UNIVERSITY OF CAPE COAST

LASER INDUCED THERMOELECTRIC PROPERTIES OF CHIRAL CARBON NANOTUBES

BY

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DECLARATION

Candidate's Declaration

I hereby declare that, except for the references to other people's work duly cited, this work is the result of my original research and that no part of it has been presented for any degree in this university or elsewhere.

.... Date: 03-08-2011

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Supervisor's Declaration

We hereby declare that the preparation and presentation of this thesis were supervised in accordance with the guidelines on supervision of thesis laid down by the University of Cape Coast.

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ABSTRACT

An investigation of laser stimulated thermopower in chiral CNT in the first Brillouin zone is presented. The electrical and thermal conductivities of a chiral CNT were calculated using a tractable analytical approach. This was done by solving the Boltzmann kinetic equation with energy dispersion relation obtained in the tight binding approximation to determine the electrical and thermal properties of chiral carbon nanotubes. The electroconductivity σ and the electron thermal conductivities χ_{cz}, χ_{zz} along the circumferential and axial directions respectively of laser induced chiral CNT are calculated. The resistivity ρ and differential thermoelectric power α_{cz} along the circumferential and axial α_{zz} are obtained. The results obtained are numerically analyzed. The parameters α, ρ and χ are found to oscillate in the presence of laser radiations. We have also noted that the presence of the laser source lowered the figure of merit. The figure of merit is enhanced mainly by increasing Δ_s or decreasing Δ_z in the presence of the laser. At room temperature (300K) the value of ZT recorded for the chiral CNT in the presence of laser was greater than one.

Based on our findings we propose the prospect of using a monochromatic laser induced chiral carbon nanotube as a good quality and highly efficient thermoelement.

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DEDICATION

I dedicate this work to my wife Mary and children Emmanuel, Eugenia and Michael.

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CHAPTER ONE

INTRODUCTION

History of Thermoelectricity

The thermoelectric effect is the direct conversion of temperature differences to electric voltage and vice versa. A thermoelectric device creates a voltage when there is a different temperature on each side. Conversely when a voltage is applied to a thermoelectric device, temperature difference is created between the two sides of the device. This effect is known as Peltier effect. At atomic scale, an applied temperature gradient causes charged carriers (i.e. electrons or holes) in the thermoelectric material to diffuse from the hot side to the cold side, similar to a classical gas that expands when heated; hence, the thermally induced current.

Traditionally, the term thermoelectric effect or thermoelectricity encompasses three separately identified effects known as the Seebeck effect, the Peltier effect, and the Thomson effect.

In 1821 Thomas Johann Seebeck found that a circuit made from two dissimilar metals, with junctions at different temperatures would deflect a compass magnet. Seebeck initially believed this was due to magnetism induced by the temperature difference. However, it was quickly realized that it was an electrical current that is induced, which by Ampere's law deflects the magnet. More specifically, the temperature difference produces an electric potential (voltage) which can drive an electric current in a closed circuit. The voltage produced is proportional to the temperature difference between the two junctions. The proportionality constant S is defined as the Seebeck coefficient or thermoelectric power and is obtained from the ratio of the voltage generated ΔV and the applied temperature difference ΔT (i.e. $S = {}^{\Delta V}/_{\Delta T}$) [1]. The Seebeck voltage does not depend on the distribution of temperature along the metals between the junctions. This effect is the physical basis for a thermocouple, which is used often for temperature measurement. Jean-Charles Peltier, a French physicist in 1834 discovered the calorific effect of an electric current at the junction of two different metals [2]. This effect which is named after her discoverer as Peltier effect occurs when a current passes through a wire. The current will carry thermal energy so that the temperature of one end of the wire decreases and the other increases. The Peltier coefficient Π_{12} is defined as the heat emitted per unit time per unit current flow from conductor 1 to conductor 2. Therefore, this heat labeled Q, is directly proportional to the current I, passing through the junction as described by the relation $dQ = \Pi_{12} dI$. An interesting consequence of this effect is that the direction of heat transfer is controlled by the polarity of the current; reversing the polarity will change the direction of transfer.

Twenty years later, William Thomson (later Lord Kelvin) issued a comprehensive explanation of the Seebeck and Peltier Effects and described their interrelationship. The Seebeck and Peltier coefficients are related through thermodynamics. The Peltier coefficient is simply the product of Seebeck coefficient and the absolute temperature. This thermodynamic derivation led Thomson to predict a third thermoelectric effect, now known as the Thomson effect. In the Thomson effect, heat is absorbed or produced when current flows in a material with a temperature gradient [3]. The heat is proportional to both the electric current and the temperature gradient. The proportionality constant, known as the Thomson coefficient is related by thermodynamics to the Seebeck coefficient. The Thomson effect was experimentally confirmed in 1856. The Thomson coefficient is positive if heat is generated when positive current flows from a higher temperature to lower temperature [4]. The Peltier–Seebeck and Thomson effects can in principle be thermodynamically reversible, whereas Joule heating is not.

Figure of Merit

In 1912, Altenkirch [5,6] introduced the concept of a figure of merit when he showed that good thermoelectric materials should possess large Seebeck coefficients, high electrical conductivity to minimize Joule heating and low thermal conductivity to retain heat at the junctions that will help maintain a large temperature gradient. Ioffe in 1957 [7] provided a theory that presented the figure of merit as $Z = S^2\sigma / k$ which he used to qualify the efficiency of thermoelectric materials. Presently thermoelectric materials are ranked by a dimensionless figure of merit, ZT, which is defined as $ZT = S^2\sigma T/k$, where S is the thermopower or Seebeck coefficient, σ is the electrical conductivity, k is the thermal conductivity, and T is the absolute temperature. To be competitive compared with conventional refrigerators and generators, one must develop materials with $ZT > 3$. Yet in five decades the room-temperature ZT of bulk semiconductors has increased only marginally, from about 0.6 to 1. Figure 1 shows progress over the years since the discovery of the thermoelectric properties of Bi_2Te_3 and its alloys with Sb and Se in the 1950s [8]. The challenge lies in the fact that the parameters S, σ, and k are interdependent so changing one alters the others, making optimization extremely difficult. The only way to reduce k without affecting S and σ in bulk materials is to use semiconductors of high atomic weight such as Bi_2Te_3 and its alloys with Sb, Sn, and Pb. High atomic weight reduces the speed of sound in the material, and thereby decreases the thermal conductivity. Although it is possible in principle [9] to develop bulk semiconductors with $ZT > 3$, there are no candidate materials on the horizon.

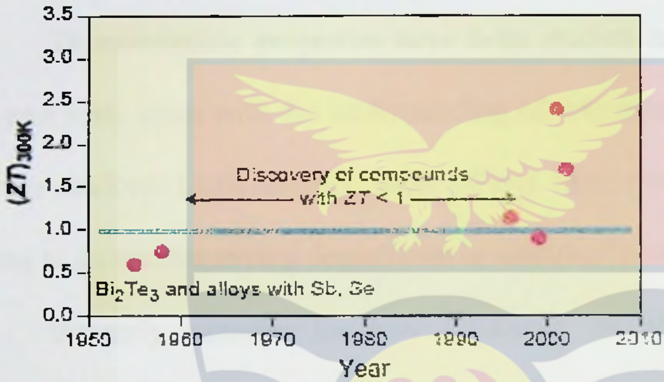


Figure 1: Thermoelectric improvements. History of thermoelectric figure of merit, *ZT*, at 300 K. Since the discovery of the thermoelectric properties of Bi2Te3 and its alloys with Sb and Se in the 1950s, no bulk material with $(ZT)_{300K} > 1$ has been discovered. Recent studies in nanostructured thermoelectric materials have led to a sudden increase in $(ZT)_{300K} > 1$.

In 2002, Hideo Iwasaki et al [10] used the Harman method to evaluate the figure of merit ZT of thermoelectric materials in the temperature region below room temperature. In this method only resistance measurement by direct current (dc) and alternating current (ac) methods are required to obtain the ZT values. The Harman method uses the formula $ZT = \left({R_{dc}}/{R_{ac}} - 1 \right) / x$, where R_{dc}, R_{ac} and x are the resistance value by the dc and ac methods and x is the rate of the heat flow to the heat bath, respectively. The heat effect is experimentally confirmed to be negligibly small and so they used $x=1$ which corresponds to a sufficient adiabatic condition.. They found Harman method for determining ZT to be simple and precise.

Thermoelectric materials

Thermoelectric properties have been studied in many materials over the past forty years with the understanding of determining good materials for thermo devices. Unfortunately, these efforts have met with limited success owing to an accompanying degradation in electrical properties [11].

Recently, attention has been refocused, owing to the appearance of new materials like the multiquantum wells and superlattices [12]. Superlattices of semiconductors and semimetals are expensive for mass production, even though, they show enhancement in the thermoelectric figure of merit Z, hence the need to search for new materials.

Thermoelectricity is a widely used method for cooling and heating, sensing, heat retention, and thermal management. In its core, it takes advantage of materials and structures with a sustainable chemical potential difference between the hot and cold ends of a given sample. Looking at the widespread use of semiconductors in microelectronics and optoelectronics, it is hard to imagine that the initial excitement was due to their promise in refrigeration, but not in electronics [13]. The discovery in the 1950s that semiconductors can act as efficient heat pumps led to premature expectations of environmentally benign solid-state home refrigerators and power generators containing no moving parts.

In semiconductors, electrons and holes carry charge, whereas lattice vibrations or phonons dominate heat transport. Electrons (or holes) and phonons have two length scales associated with their transport which are wavelength, λ, and mean free path, *l*. By nanostructuring semiconductors with sizes comparable to wavelength λ, sharp edges and peaks in their electronic density of states are produced, whose location in energy space depends on size. By matching the peak locations and shape with respect to the Fermi energy, one can tailor the thermopower *S*. Furthermore, such quantum confinement also increases electronic mobility, which could lead to high values of electrical conductivity. Hence, quantum confinement allows manipulation of $S^2\sigma$ that is otherwise difficult to achieve in bulk materials [8]. Many bulk thermoelectric materials are alloys because alloy scattering of the short-wavelength acoustic phonons suppresses thermal conductivity without substantially altering $S^2\sigma$. It is entirely possible, that the increase of *ZT* may be less dependent on quantum confinement of electrons and holes, and more on phonon dynamics and transport. For example, if the size of a semiconductor is smaller than the mean free path of phonons and larger than that of electrons or holes, one can reduce thermal conductivity by boundary scattering without affecting electrical transport.

Over the past decade, these questions about quantum effects have received increasing attention, and their answers hold promise [14, 15] in increasing *ZT*. L. D. Hicks et al. [14] in their paper proposed that it may be possible to increase *ZT* of certain materials by preparing them in quantum-well superlattice structures. They have done calculations to investigate the potential for such an approach, and also evaluated the effect of anisotropy on the figure of merit. Their calculations showed that layering has the potential to increase significantly the figure of merit of a highly anisotropic material such as Bi_2Te_3, provided that the superlattice multilayers are made in a particular orientation. This result opens the possibility of using quantum-well superlattice structures to enhance the performance of thermoelectric coolers.

Mensah et al [12] investigated the thermoelectric effect in a semiconductor superlattice in a nonquantized electric field for electrons of the lowest miniband in the linear approximation of temperature gradient ∇T. They obtained analytical expressions for the thermopower α and the heat conductivity coefficient χ as functions of the superlattice parameters such as its bandwidth Δ, period d, temperature T, concentration and electric field E. Their results confirmed the fact that depending on the relation between Δ and other characteristic energies of the carrier charge, the carrier charges can behave either as a quasi-two-dimensional or as a three-dimensional electron gas. They proposed the prospect of using a superlattice as a good-quality and highly efficient thermoelement.

In the past few years, reports have suggested that nanostructured thin-film superlattices [16] of Bi_2Te_3 and Sb_2Te_3 have $ZT = 2.4$ at room temperature, whereas PbSeTe/PbTe quantum dot superlattices [17] have ZT between 1.3 and 1.6. Currently the materials with the highest thermoelectric figure of merit ZT are Bi_2Te_3 alloys. Therefore these compounds are the best thermoelectric refrigeration elements. However, since the 1960s only slow progress has been made in enhancing ZT, either in Bi_2Te_3 alloys or in other thermoelectric materials. So far, the materials used in applications have all been in bulk form.

Over the past decade, researchers in thermoelectricity have leveraged their knowledge of band gap engineering from electronics and optoelectronics to create nanostructured thermoelectric materials and devices.

Hsu *et al.* [18] reported of the synthesis of a new class of materials that could potentially be used for power generation. It is encouraging to see that the new class of materials $AgPb_m SbTe_{2+m}$ has $ZT = 2$ at 800 K for $m = 18$. Although the temperature may be too high for refrigeration, it is appropriate for power generation. However, what is interesting is the discovery that this material contains regions 2 to 4 nm in size that is rich in Ag-Sb and is epitaxially embedded in a matrix that is depleted of Ag and Sb. Presumably, the electronic band structure and vibrational properties of these nano regions are different from those of the surrounding material, suggesting quantum confinement.

Lyeo *et al.* [19] have reported on an experimental technique called Scanning Thermoelectric Microscopy (SThEM) that can probe thermoelectric transport at nanoscales. By heating a sharp metallic tip to about 10 K above the temperature of a sample and bringing them in contact under ultrahigh vacuum, they create a temperature gradient within a localized region in the sample right under the tip. The thermoelectric effect in this sample region creates a potential difference, which can be measured between the tip and the sample. By scanning the tip laterally, one can map out the thermopower profile in a sample. Lyeo *et al.* demonstrated this by mapping out the thermopower of a *pn* homojunction. Because *p*- and *n*-doped semiconductors have positive and negative thermopowers, respectively, a *pn* homojunction produces a large swing in thermopower over a length scale that is on the order of the depletion region. What is remarkable is that they showed the spatial resolution to be on the order of 2 to 4 nm in highly doped semiconductors, which creates the possibility of probing semiconductor nanostructures for thermoelectricity. Interestingly, this resolution is on the order of the nanostructure size discovered by Hsu *et al.* [18] in $AgPb_{18}SbTe_{20}$. Lyeo *et al.* [19] showed that through SThEM thermoelectricity could be used to facilitate the next generation of electronics and optoelectronics.

Takashiri et al. [20] have investigated the structure and thermoelectric properties of boron doped nanocrystalline $Si_{0.8}Ge_{0.2}$ thin films for potential application in micro thermoelectric devices. The nanocrystalline $Si_{0.8}Ge_{0.2}$ thin films were grown by low-pressure chemical vapor deposition on a sandwich of $Si_3N_4/SiO_2/Si_3N_4$ films deposited on a Si (100) substrate. The $Si_{0.8}Ge_{0.2}$ film was doped with boron by ion implantation. They studied structure of the thin film by means of atomic force microscopy, x-ray diffraction, and transmission electron microscopy. It was found that the film has column-shaped crystal grains ~100nm in diameter oriented along the thickness of the film. The electrical conductivity and Seebeck coefficient are measured in the temperature range between 80–300°K and 130–300 K, respectively. The thermal conductivity was measured at room temperature. As compared with bulk silicon-germanium and microcrystalline film alloys of nearly the same Si/Ge ratio and doping concentrations, the $Si_{0.8}Ge_{0.2}$ nanocrystalline film exhibits a twofold reduction in the thermal conductivitity, an enhancement in the Seebeck coefficient, and a reduction in the electrical conductivity.

Enhanced heat carrier scattering due to the nanocrystalline structure of the films and a combined effect of boron segregation and carrier trapping at grain boundaries are believed to be responsible for the measured reductions in the thermal and electrical conductivities, respectively.

Carbon-based materials (diamond and in-plane graphite) display the highest measured thermal conductivity of any known material at moderate temperatures [21]. The discovery of carbon nanotubes in 1991 [22] has led to speculation that this new material could have a thermal conductivity greater than that of diamond and graphite [23]. Aside this material has found a lot of application in electronic and mechanical devices. It is, therefore, not surprising that the material has received a lot of attention over the past decade [24-31]. The thermal conductivity of materials in general is partitioned into charge carriers (i.e., electron or hole) component χ_e which depends on the electronic band structure, electron scattering and electron-phonon interaction, and lattice component χ_L which depends mainly on phonon and phonon scattering. In dielectrics, $\chi_L \gg \chi_e$ while in metals $\chi_e \gg \chi_L$. In semiconductors, the value of the thermal conductivity χ is strongly dependent on the composition of the semiconductor, and the value of χ_L is generally greater than the value of χ_e.

So far, all publications on the thermal conductivity of carbon nanotubes have paid attention to only the lattice thermal conductivity and completely neglected electron thermal conductivity. For example, Hone et al. [23] found that the conductivity of carbon nanotubes was temperature dependent, and was almost a linear relationship. They suggested that the conductivity decreases smoothly with temperature, and displays linear temperature dependence below 30 K. However, Berber et al. [32] suggested that the graph of the temperature dependence of thermal conductivity looked less linear and that it shows a positive slope from low temperatures up to 100 K where it peaks around 37000 W/mK. Then, the thermal conductivity drops dramatically down to around 3000 W/mK when the temperature approaches 400 K. Similar relationship has been found by Mensah et al. [33] for electron thermal conductivity χ_e.

Mensah et al. [34] have also studied the electron thermal conductivity of carbon nanotubes. They observed that the temperature dependence of χ_e in carbon nanotubes is similar to that obtained by Berber et al. and that χ_e peaks at unusually high values. They further observed the dependence of χ_e on the geometric chiral angle θ_h, temperature T, the real overlapping integrals for jumps along the tubular axis Δ_z and the base helix Δ_s. Interestingly, they again noted that varying these parameters could give rise to unusual high electron thermal conductivity whose peak values shift towards higher temperatures. For example, at Δ_z=0.020 eV and $\Delta_s = 0.0150eV$ the peak value of χ_e occurs at 104K and is about 41000s W/mK which compares well with that reported for a 99.9% isotropically enriched ^{12}C diamond crystal.

Thermoelectric (TE) power has been reported for a random array of carbon nanotubes (CNT) [35-37] as well as for individual tubes [38]. Similar investigations were made on quantum wires [39, 40] and artificial nanostructures, such as superlattices [41]. Past work on CNT was mostly made on randomly dispersed tubes but Shamim M. et al. [42] reported on the TE properties of cross aligned and co aligned junctions made between functionalized single-wall CNTs (SWCNTs) and multiwall CNTs (MWCNTs).

Mensah et al. have studied the differential thermopower of the chiral carbon nanotube [43]. They used the approach stated in [12] together with the model developed in [44] to determine the thermopower a, of the chiral CNT. The approach requires the creation of phenomenological models that yield analytically tractable results [44]. The justification for this approach can be established from the work of Miyamoto *et al.* [45], where they computed the current excited in carbon and BC_2N nanotubes immersed in an electrostatic field. [43] They observed that the thermopower strongly depends on the geometric chiral angle (GCA) θ_h, electric field E, temperature T, the real overlapping integrals for jumps along the tubular axis Δ_z and the base helix Δ_s. Mensah et al. in their paper highly recommended that the manipulation of the parameters E, T, Δ_z and Δ_s can give rise to high thermopower values [43].

Using the semiclassical approach Mensah et al. [46] investigated and reported on the giant electrical power factor in single-walled chiral carbon nanotubes. They observed that the resistivity ρ, thermopower α, and power factor P are all temperature dependent. Based on their findings they predicted a giant electrical power factor and hence proposed the use of carbon nanotubes as thermoelements for refrigeration.

In their studies Guo-Dong Zhan et al. [47] investigated the thermoelectric properties of single-wall carbon nanotube (SWCNT)/ceramic nanocomposites produced by spark-plasma-sintering. They found that the ZT increases with increasing temperature and has a value of 0.018 at 850 K which is two orders of magnitude higher than that of pure SWNTs. Therefore CNT/ceramic composites exhibit thermoelectric properties, suggesting potential for use as a promising thermoelectric material. As compared to other thermoelectric materials, however, the electrical conductivity of the CNT/ceramic composites is low. This can be further improved if pure metallic SWNTs can be applied, due to the much higher electrical conductivity of SWCNTs. The researchers have earlier on discovered that incorporation of single-walled carbon nanotubes into nanoceramics leads to a dramatically improved electrical conductivity of the composites combined with a significant decrease in thermal conductivity [48-51], suggesting that the carbon nanotube reinforced nanoceramic composites might make promising thermoelectric materials.

Mensah and Buah-Bassuah [52] have theoretically investigated the photostimulated thermomagnetic effect by electrons in a semiconductor superlattice (SL). In their work, they indicated the possibility of controlling the thermopower α, the electron thermal conductivity χ, and the electroconductivity σ of the SL with the help of laser radiation. They found the parameters α, χ, and σ to oscillate in the presence of laser therefore are amplitude dependent. Changing the amplitude of the laser source can result in changes of the thermopower α, the electron thermal conductivity χ, and the electroconductivity σ of the SL. Mensah and Buah-Bassuah proposed the prospect of using laser induced SL as a good-quality and highly efficient thermoelement.

Objectives

The main objectives of this work is to investigate

1. How the chiral CNT parameters Δ_s Δ_z, θ_h, the d.c. electric field E_o and the laser source E_s affects the resistivity, thermopower and the electron thermal conductivity of chiral CNT.
2. How the laser affects the resistivity, thermopower and the electron thermal conductivity of chiral CNT.
3. Whether the laser can improve the figure of merit of the chiral CNT.

Justification and Relevance

Based on the good work done by Mensah and Buah-Bassuah [52] on a Semiconductor Superlattice, this work seeks to use laser to control the resistivity, thermopower and the electron thermal conductivity of Chiral Carbon Nanotubes. Just as laser induced SL has been found to be a good-quality and highly efficient thermoelement, it is possible for laser induced Chiral CNT to behave similarly.

Statement of Problem

Researchers are working extensively to find materials which can be used as good thermoelements and are cheap to produce. This work seeks to determine whether chiral carbon nanotubes which are now cheap and easy to produce can be a good candidate.

Scope and Delimitation

In this work, we have used semiclassical approach to investigate theoretically the laser stimulated thermopower and thermal conductivity in chiral CNTs. The electrical and thermal properties of chiral carbon nanotubes will also be considered with the aim of determining whether the figure of merit can improve as a result of the presence of laser. Even though there are different forms of carbon nanotubes, our investigations were carried specifically on chiral CNT.

Structure of Thesis

The rest of the chapters are organized as follows:

Chapter two will be a review of the history and some of the physical properties of CNTs. In Chapter three, the Boltzmann kinetic equation with energy dispersion will be employed to determine the differential thermoelectric power α_{cz} along the circumferential and axial α_{zz} directions of chiral CNTs. Results obtained in the previous chapter will be discussed in Chapter four. Finally, we draw our conclusions in Chapter five.

CHAPTER TWO

A REVIEW OF CARBON NANOTUBES

The History of Discovery of Carbon Nanotubes

Carbon nanotubes are cylindrical structures of nanometric size, based on a hexagonal lattice of carbon atoms. Carbon nanotubes (CNTs) are allotropes of carbon whose structures can be thought of as rolled two-dimensional graphene sheets [53]. Their dimensions are typically a few nanometers across and up to 100 micrometers long.

In 1976, Endo from Japan collaborated with Oberlin in France to research on carbon fibers using vapor-growth technique. In studies of filamentous carbon fibers by electron microscopy, they reported on the occasional observation of carbon nanotubes consisting of a single wall of graphene [54, 55].

In 1985, while Harry Kroto of the University of Sussex in the UK and Richard Smalley from Rice University in the US were studying the nature of interstellar matter to determine the forms of carbon-containing materials found between the stars, they detected, for the first time (by mass spectroscopy) a closed cluster containing precisely 60 carbon atoms [56]. It was named buckminsterfullerene after an architect R. Buckminster Fuller who pioneered the use of geodesic domes in architecture. This cluster, which is called C_{60} or fullerene, exhibits a very unique structure and stability [57, 58]. The original observation of fullerenes in mass spectrometry was not anticipated, it was discovered by accident [56]. Studies on C_{60} were hindered because there was no known technique for producing it in appreciable quantities.

In 1990, Krätschmer and Huffman succeeded in using the arc discharge technique to produce the famed Buckminster fullerene on a large scale [59]. The discovery of fullerenes and their production in bulk in 1990 were the first steps towards the era of carbon nanotubes.

Sumio Iijima, a Japanese electron microscopist of NEC Fundamental Research Laboratory in Tsukuba, Japan was the first to give experimental evidence of the existence of carbon nanotubes in 1991. Using High Resolution Transmission Electron Microscopy (HRTEM), he examined electron microscope images of the soot deposited on the carbon cathode during the arc- evaporation synthesis of fullerenes. Iijima found that the central core of the cathodic deposit contained a variety of closed graphitic structures including nanoparticles and strange tube-like carbon structures [60] of a type which had never previously been observed. The new found strange tube-like carbon structures that consisted of several concentric tubes of carbon atoms, cylindrical in shape, exquisitely thin and impressively long were later called multiple-walled carbon nanotubes (MWCNTs). These early structures had the form of cylinders within cylinders, nested inside each other like Russian dolls. Iijima's discovery is considered to be the first citation of carbon nanotubes (CNT).

Two years after his first observation of MWCNTs, Iijima et al. [61] of NEC Fundamental Research Laboratory in Tsukuba and Bethune et al. [62] of Almaden Research Centre in California simultaneously and independently observed single walled carbon nanotubes (SWCNTs). Although carbon nanotubes were observed four decades ago, it was not until the discovery of C_{60} and theoretical studies of possible other fullerene structures that the scientific community realized their importance. Theoretical predictions about structure and electronic properties of CNTs followed quickly [63-66].

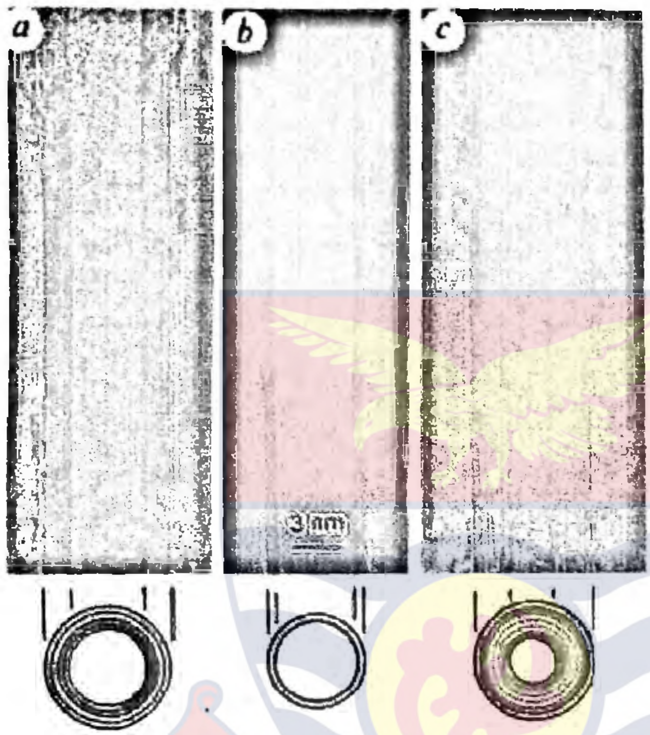


Figure 2: The Observation of transmission electron microscopy of multi-walled coaxial CNT [18]. The cross section of each nanotube is illustrated. The CNTs consist of (a) five graphene sheets and an outer diameter of 6.7 nm, (b) two graphene sheets and an outer diameter of 5.5 nm, and (c) seven sheets and an outer diameter of 6.5 nm.

Soon methods were developed to produce single-walled carbon nanotubes (SWCNT) [67,68]. Since this pioneering work, carbon nanotube research has developed into a leading area in nanotechnology expanding at an extremely fast pace. Although lijima is credited with their official discovery, carbon nanotubes were probably already observed thirty years earlier by Roger Bacon at Union Carbide in Parma, OH. Bacon began carbon arc research in 1956 to investigate the properties of carbon fibers. He was studying the melting of graphite under high temperatures and pressures and probably found carbon nanotubes in his samples. In his paper, published in 1960, he presented the observation of carbon nanowhiskers under SEM investigation of his material [69] and he proposed a scroll like-structure. Nanotubes were also produced and imaged directly by Endo in the 1970's via high resolution transmission electron microscopy (HRTEM) when he explored the production of carbon fibers by pyrolysis of benzene and ferrocene at 1000°C [55]. He observed carbon fibers with a hollow core and a catalytic particle at the end. He later discovered that the particle was iron oxide from sand paper. Iron oxide is now well-known as a catalyst in the modern production of carbon nanotubes.

Allotropes of Carbon

Carbon is the most versatile element in the periodic table, owing to the type, strength, and number of bonds it can form with many different elements. The diversity of bonds and their corresponding geometries enable the existence of structural isomers, geometric isomers, and enantiomers. These are found in large, complex, and diverse structures and allow for an endless variety of organic molecules.

Carbon can bind in a sigma (σ) bond and a pi (π) bond while forming a molecule; the final molecular structure depends on the level of hybridization of the carbon orbitals. An sp^1 hybridized carbon atom can make two σ bonds and two π bonds, sp^2 hybridized carbon forms three σ bonds and one π bond, and an sp^3 hybridized carbon atom forms four σ bonds. The number and nature of the bonds determine the geometry and properties of carbon allotropes.

Due to the many possible configurations of the electronic states of a carbon atom (which is known as hybridization of atomic orbitals), the carbon atom can bond with itself and with other atoms in endlessly varied combinations of chains and rings. Graphite and diamond are well known naturally occurring allotropes of carbon.

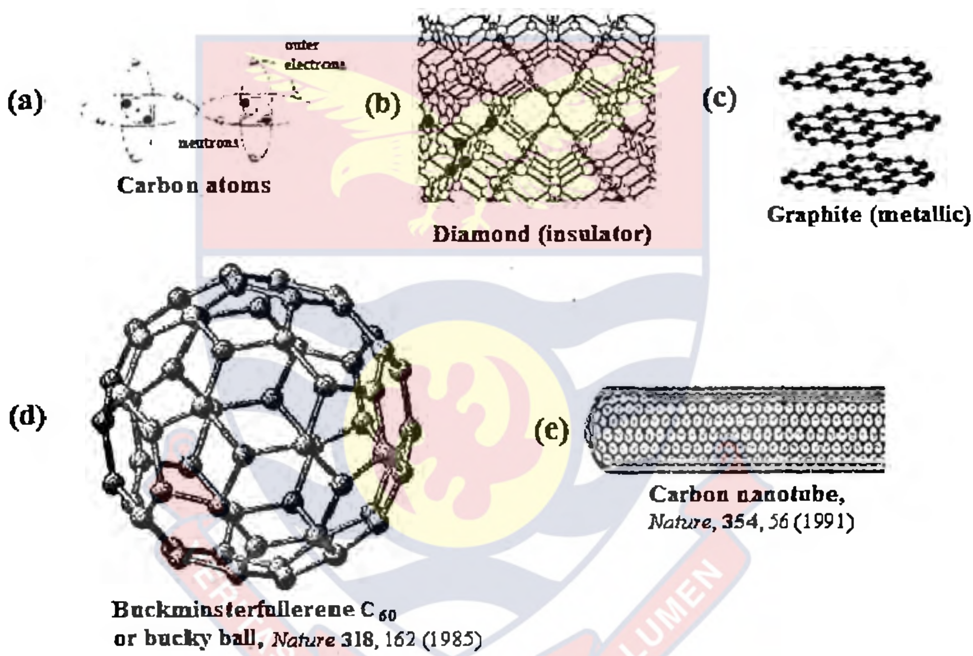


Figure 3: (a) Electronic configuration of isolated carbon atoms; (b) Diamond (c) Graphite (d) Buckminsterfullerene C_{60}; (e) Carbon nanotube.

The electronic configuration of isolated carbon atoms and the allotropes of carbon are illustrated in Figure 3. The carbon atoms in diamond, each of which is sp^3 hybridized, are arranged in a rigid three-dimensional (3D) structure and are bonded to each other by strong σ-bonds (as indicated in

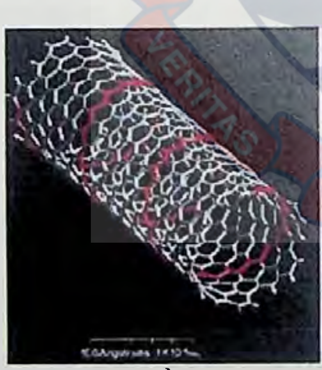
Figure 3 (b)). The carbon atoms in graphite, each of which is sp^2 hybridized, are arranged in sheets of atoms called graphenes, and are bonded to each other by strong σ-bonds and weak π-bonds. The sheets in graphite are held together by weak Van der Waal's force, so these sheets can move over each other fairly, but in diamond the atoms are held rigidly. Diamond is therefore hard while graphite is soft. The free π-electrons in the π-bonds of graphite explain why graphite is a conductor. The valence electrons of carbon atoms in diamond are held tightly in strong σ-bonds and are therefore not available for conduction. This explains why diamond is an insulator.

A third form of carbon, now known as buckminsterfullerene or simply fullerene (C_{60}) was discovered in 1980 by Kroto et al. C_{60}, also referred to as bucky ball, is a tiny molecular cage of 60 carbon atoms that make up the mathematical shape called a truncated icosahedron (Figure 3 (d)). The shape of this structure happens to be the same as the shape of a football (12 pentagons and 20 hexagons).

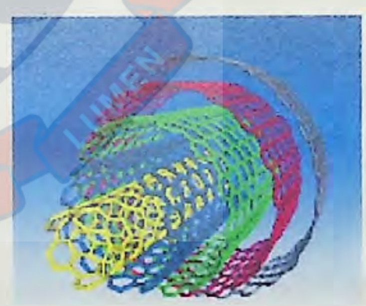
The fourth allotrope of carbon is the tubular form of the fullerenes, which are called carbon nanotubes (Figure 3 (e)). CNTs consist of graphene sheets rolled into perfect cylinders with mind-bending aspect ratios; often bring only a nanometer in diameter but many micrometers in length. These tiny cylinders of grapheme are closed at each end with caps containing six pentagonal rings. These cylindrical structures of carbon atoms take two forms: single-walled nanotubes (SWCNTs) or multi-walled nanotubes (MWCNTs). A SWCNT is basically a single layer of pure-carbon atoms rolled into a seamless tube capped at each end by half-spherical fullerene structures. The diameter of a SWCNT is of the order of 1 nm or 10^{-9} m [61]. All of its atoms form a single covalently bound network. MWCNTs on the other hand, consist of a collection of concentric graphene cylinders and are larger structures than SWCNTs. A MWCNT can be considered as a mesoscale graphite system, whereas a SWCNT is a single large molecule.

Classification Of Carbon Nanotubes

Considering the cylindrical wall(s) of CNTs, they can be classified into single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs). A single-wall carbon nanotube (SWCNT) can be described as a graphene sheet rolled into a cylindrical shape so that the structure is one dimensional with axial symmetry, and in general exhibiting a spiral conformation, called chirality [70]. On the other hand, a tube comprising several, concentrically arranged graphene sheet cylinders is referred to as a multi-walled carbon nanotube (MWCNT). In plates 1and 2, examples of a SWCNT and a MCWNT are shown.



a)



b)

Plate 1 : Single-Walled Carbon Nanotubes

Plate 2 : Multi-Walled Carbon Nanotubes with five walls. www.azonano.com

There are different types of CNTs each having their own different properties. When CNTs are synthesized a bunch of different types of CNTs are produced. These CNTs can be well aligned or nestled depending on the synthesis method, the catalysts used and other reaction conditions such as temperature [71-75].

In general the multi-walled carbon nanotubes (MWCNTs) have a larger diameter than the single-walled carbon nanotubes (SWCNTs). Single-wall nanotubes with only one single layer generally have a diameter of 1 to 5 nm. The properties of SWCNT are more stable than MWCNT so it is more favourable. MWCNT is a little bigger than SWCNT because MWCNT has about 50 layers. MWCNT's inner diameter is from 1.5 to 15 nm and the outer diameter is from 2.5 nm to 30 nm. Distances between the walls are mostly found to be between 0.1 and 0.4 nm [61]. Depending on the number of walls, CNTs may have different conductive properties. For example, MCWNTs have metallic conducting properties, whereas SWCNTs can have semi conducting properties as well as metallic conducting properties. This depends on the so-called chirality of the SWCNTs [76,77].

Both SWCNT and MWCNT are usually many microns long and hence they can fit well as components in submicrometer-scale devices [53] and nanocomposite structures that are very important in emerging technologies. SWCNTs have better defined shapes of cylinder than MWCNTs, thus a MWCNT has more possibilities of structure defects and its nanostructure is less stable. Most researchers focus on SWCNT and develop applications based on SWCNT due to the physical stability of SWCNT [78-85].

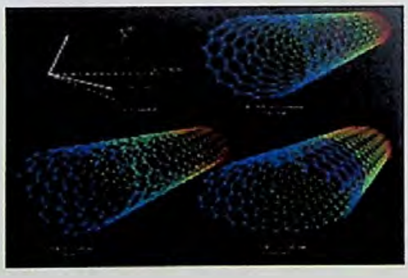
The second form of classification is common among both MWCNTs and SWCNTs and depends on the arrangement of carbon atoms in a given tube or how the two-dimensional graphene sheet is "rolled up". The primary symmetry classification of a carbon nanotube is that it can either be an achiral (symmorphic) or chiral (non-symmorphic). An achiral carbon nanotube is defined by a carbon nanotube whose mirror image has an identical structure to the original one.

There are only two cases of achiral nanotubes:

a) armchair and

b) zigzag nanotubes

The names of armchair and zigzag arise from the shape of the cross-sectional ring, as shown at the edge of the nanotubes in Figure 4 and 5. An armchair nanotube corresponds to the case of $n = m$, that is $C_h = (n,n)$; and a zigzag nanotube corresponds to the case of $m = 0$ or $C_h = (n,0)$. Chiral nanotubes exhibit a spiral symmetry whose mirror image cannot be superposed on to the original one. All (n,m) chiral vectors other than (n,n) and $(n,0)$ correspond to chiral nanotubes. Looking at the hexagonal symmetry of the lattice, we need to consider only $0 < |m| < n$ in $C_h = (n,m)$ for chiral nanotubes. Plate 3 shows a 3D model of the three types of single-walled CNT.



www.dolcera.com

Plate 3. 3-D models of the three types of single-walled carbon nanotubes.

Armchair nanotubes are formed when $n = m$, hence it is an (n, n) tube structure and the chiral angle ,θ, is 30°. Zigzag nanotubes are formed when either n or m is zero, hence it is referred to $(n, 0)$ or $(m, 0)$ tube structure and chiral angle ,θ, is 0°, also referred to as the zigzag axis . Chiral nanotubes are formed when neither n nor m is zero and also $n \neq m$., hence it is general chiral (n, m) nanotube which corresponds to a chiral angle lying between 0°<θ<30°.

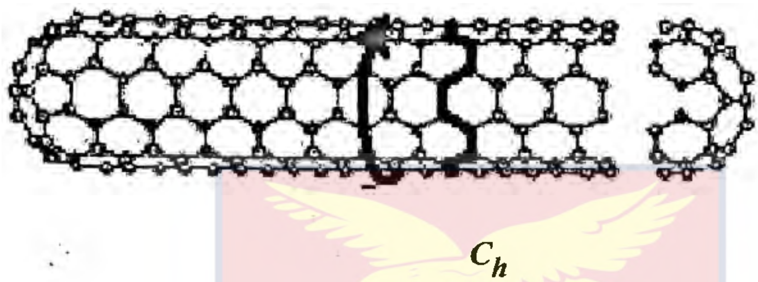


Figure 4 : Structure of Armchair Carbon Nanotube: n = m, θ=30°.

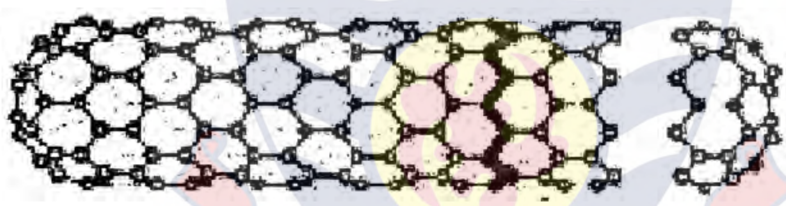


Figure 5: Structure of Zigzag Carbon Nanotube: n or m = 0, θ=0°.

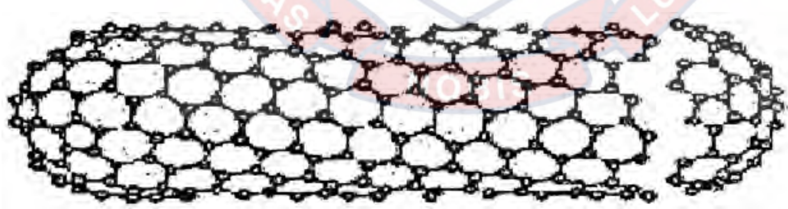


Figure 6: Structure of Chiral Carbon Nanotube: n or m ≠ 0 and also n ≠ m, 0°<θ<30°. www.cnx.org

There are two possible high symmetry structures for carbon nanotubes, known as “zigzag “and “armchair” and these are illustrated in figures 4 and 5. In practice it is believed that most carbon nanotubes do not have these highly symmetric forms but have structures in which the hexagons are arranged helically around the tube axis as in figure 6.

Of course, a carbon nanotube is not visible by bare eye, and a bundle of 100 of them is necessary to be spotted with the best optical microscope. Using Scanning Tunnelling Microscopy (STM) [86-88], the crystalline structure of the tubes was verified. Despite their small diameter, their length can be micrometers [89], which make nanotubes the (geometrically) most anisotropic molecules in the world. The chiral angles of zigzag as well as armchair carbon nanotube are shown in figure 7. Figure 8 shows a graphitic sheet with (n,m) indices.

Figure 7: Zigzag and Armchair Carbon Nanotubes Showing Chiral Angles

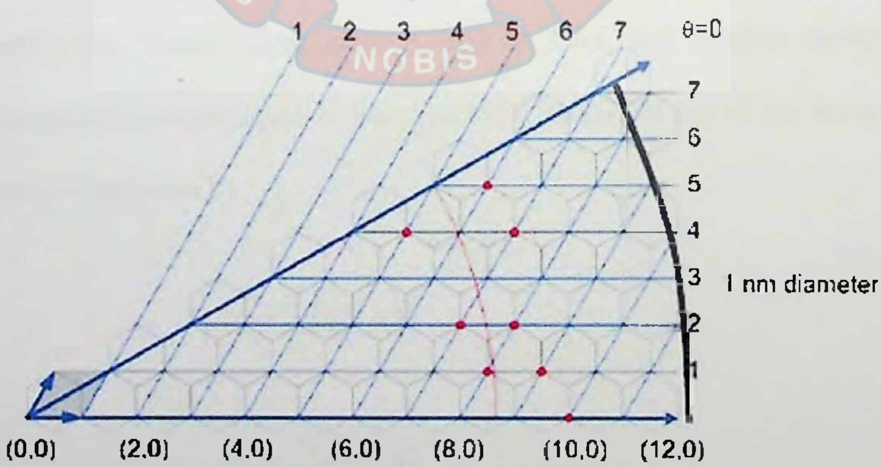


Figure 8: Graphene Sheet with (n,m) indices

Chiral vector

The structure of a SWCNT is specified uniquely by the chiral vector. The chiral vector of a CNT is the vector that, when graphene is rolled to form the CNT, lies along the circumference of the circular cross-section of the CNT. Thus the magnitude of the chiral vector is equal to the circumference of the cross-section of the CNT. The honeycomb lattice of graphene can be considered as a hexagonal lattice with a basis of two inequivalent carbon atoms, say A and B illustrated in Figure 9.

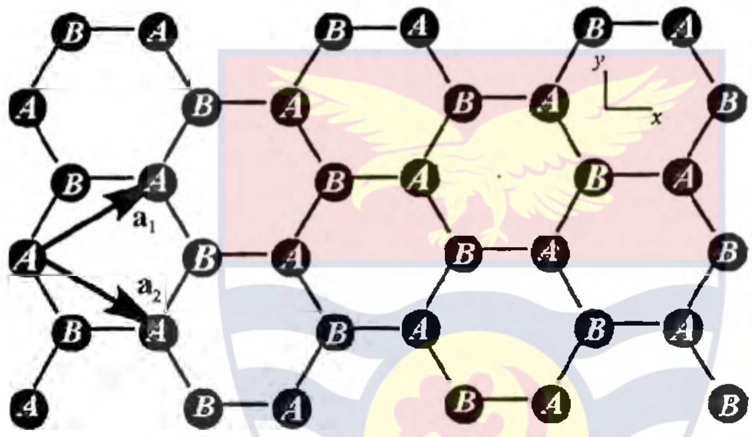


Figure 9: The honeycomb lattice of graphene showing the two hexagonal sublattices. a_1 and a_2 are the basis vectors of any of the hexagonal sublattices.

Therefore the carbon atom sites A and B form two distinct hexagonal sublattices of the honeycomb lattice. The basis vectors of any of the hexagonal sublattices are given by

$$a_1 = \frac{a}{2}\left(\sqrt{3}\mathbf{i} + \mathbf{j}\right) \quad (1)$$

$$a_2 = \frac{a}{2}\left(\sqrt{3}\mathbf{i} - \mathbf{j}\right) \quad (2)$$

where i and j are the unit vectors along the x and y axes, and

$a = |a_1| = |a_2| = a_{c-c}\sqrt{3} = 1.42\sqrt{3}\text{Å}$ is the lattice constant of graphene. The vectors a_1 and a_2 defined above are not orthogonal and the scalar product between them gives

$$a_1 \cdot a_1 = a_2 \cdot a_2 = a^2, \quad \text{and } a_1 \cdot a_2 = \frac{a^2}{2} \tag{3}$$

If we cut open the carbon nanotube along the tube axis and through the reference atom, we can imagine spreading out the nanotube into a graphene sheet that could exactly match a portion of an infinitely large graphene sheet. Figure 11 shows the hexagonal carbon network that can be thought of as the infinitely large graphene sheet [65,90]. The dotted lines at the left and right represent the cut made along the CNT. Location (0,0) represents the reference atom and is the location that the chiral vector C_h starts from. The angles θ and Φ always combine to form 30° [91].

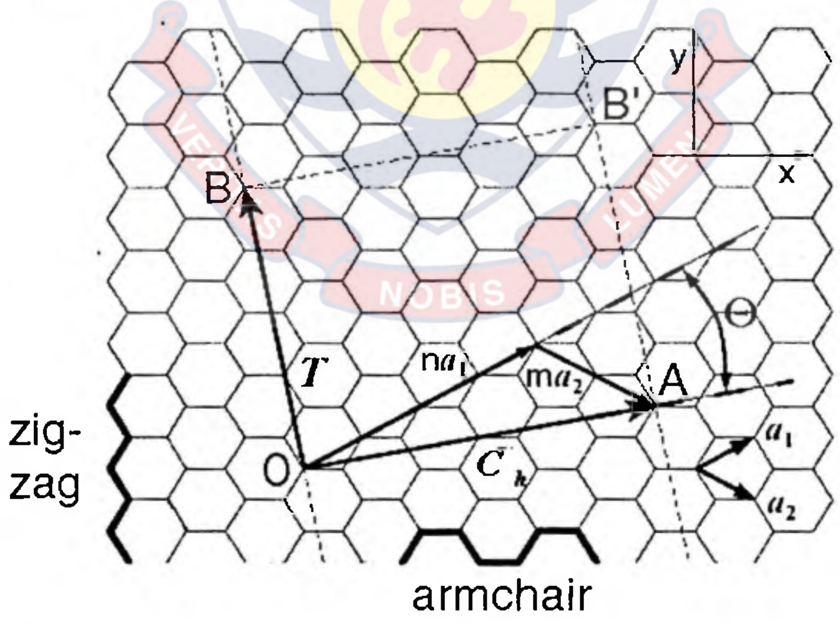


Figure 10: Hexagonal network of a graphene sheet with some essential lattice parameters

In Figure 10, a model of a SWCNT with index $(n.m) = (4,2)$ is constructed when the dotted strip is rolled up in such a way that point O coincides with point A, and point B coincides with point B'. θ denotes the chiral angle of a specific tube and varies between $0 \leq \theta \leq 30°$ The chiral vector, C_h is perpendicular to the translational vector, **Tr.** Therefore the translational vector **Tr** is parallel to the nanotube axis, while the chiral vector C_h lies along the circumference of the cross section of the nanotube.

An armchair CNT corresponds to the case when n = m. In this case, the chiral vector (n, n) bisects the angle between a_1 and a_2 thereby making the chiral angle to become 30°. A zigzag CNT corresponds to the case when m = 0, and in this case the chiral vector (n, 0) lies along the vector a_1 so the chiral angle become 0°. All other chiral vectors (n,m), where $n \neq m$, n or $m \neq 0$ with chiral angles intermediate between 0° and 30°, correspond to chiral CNTs.

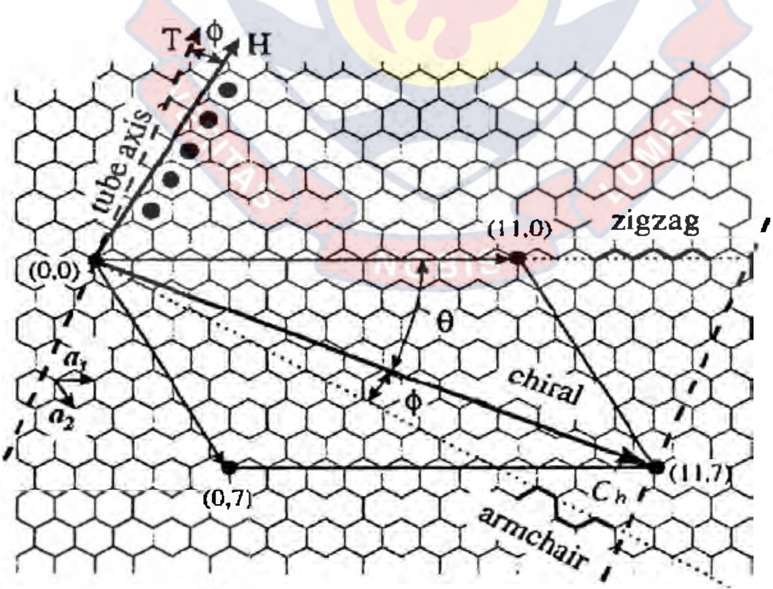


Figure 11: Unrolled sheet of Graphite that can be rolled into the three types of Carbon nanotubes.

The chiral vector C_h can be expressed in terms of the real space basis vectors a_1 and a_2 of the hexagonal lattice of graphene as follows,

$$C_h = na_1 + ma_2 \equiv (n, m) \tag{4}$$

where n and m are integers. Due to the hexagonal symmetry of the honeycomb lattice of graphene, n and m are such that $0 \leq |m| \leq n$.

The magnitude $|C_h|$ of the chiral vector is

$$|C_h| = \sqrt{C_h \cdot C_h} = a\sqrt{n^2 + m^2 + nm} \tag{5}$$

Therefore the diameter d_t of a CNT in terms of the chiral vector (n,m), is

$$d_t = \frac{|C_h|}{\pi} = \frac{a\sqrt{n^2 + m^2 + nm}}{\pi} \tag{6}$$

The chiral angle θ shown in Figure 10 is the angle between the chiral vector C_h and the vector a_1. Therefore, in terms of n and m, θ is given by

$$C_h \cdot a_1 = |C_h||a_1|\cos\theta \tag{7}$$

or

$$\cos\theta = \frac{C_h \cdot a_1}{|C_h||a_1|} = \frac{2n + m}{2\sqrt{n^2 + m^2 + nm}} \tag{8}$$

Because of the hexagonal symmetry of the honeycomb lattice of graphene, θ is restricted to values in the range $0 \leq \theta \leq 30°$. The chiral angle θ specifies the orientation of the hexagons with respect to the nanotube axis as well as the spiral symmetry of the nanotube. It can be seen from Eq (7) that an armchair (n, n) CNT corresponds to a chiral angle of 30°, and a zigzag (n, 0) CNT corresponds to $\theta = 0^{\circ}$.

Translational vector

The translational vector Tr is parallel to the nanotube axis and perpendicular to the chiral vector C_h in the unrolled honeycomb lattice of a nanotube in Figure 10. The translational vector Tr can be expressed in terms of the hexagonal basis vectors a_1 and a_2 as

$$Tr = t_1 a_1 + t_2 a_2 \equiv (t_1, t_2) \tag{9}$$

where t_1 and t_2 are integers. From Figure 10, the translational vector Tr is the position vector (with respect to O) of the first equivalent lattice point B of the hexagonal lattice of graphene. Therefore t_1 and t_2 do not have a common divisor except 1. Using Eqs (4), (6), (9) and the fact that C_h T = 0, t_1 and t_2 can be obtained in terms of n and m as

$$t_1 = \frac{2m+n}{d_R}, \text{ and } t_2 = \frac{2n+m}{d_R} \tag{10}$$

where d_R is the greatest common divisor of (2m+n) and (2n+m). If d is the greatest common divisor of n and m, then it can be shown that d_R is given in terms of d [90,92] as

$$d_R = \begin{cases} d \text{ if n - m is not a multiple of } 3d \\ 3d \text{ if n - m is a multiple of } 3d \end{cases} \tag{11}$$

Using Eqs (4), (9) and (10), the length T of the translational vector T is obtained as

$$T = \sqrt{T \cdot T} = \frac{\sqrt{3}|C_h|}{d_R} \tag{12}$$

From Eqs (11) and (12), T is greatly reduced when n and m have a common divisor or when (n − m) is a multiple of 3d.

Unit cells

The vectors C_h and Tr (Figure 10) define the rectangle OAB′B, which is the unit cell of the CNT. The unit cell of all SWCNTs has the shape of a cylinder and forms a translational unit cell along the nanotube axis. The unit cell of a SWCNT can be constructed by first drawing the chiral vector C_h relative to an origin O in the graphene. Then a straight line that is normal to C_h is drawn from O and extended until it passes exactly through a lattice point B that is equivalent to O. The rectangle generated by C_h and $\overrightarrow{OB}$ gives the unrolled unit cell of the SWCNT. The length of the unit cell in the direction of the nanotube axis is the magnitude of the translational vector Tr given by Eq (12). The unrolled unit cells for (4,4) armchair, (7,0) zigzag and (5,2) chiral CNTs are shown in Figures 12, 13 and 14. For the (5,5) armchair CNT, the width of the unit cell is Tr = a, while for the zigzag CNT the width of the unit cell is Tr = √3a.

The area of a hexagon is equal to the area of a unit cell of the hexagonal lattice of graphene defined by a_1 and a_2, i.e., the area of a hexagon is $|a_1 \times a_2|$. The nanotube unit cell has an area equal to $|C_h \times Tr|$. Therefore the number of hexagons N per unit nanotube cell is

$$N = \frac{\text{area of nanotube unit cell}}{\text{area of a hexagon}}$$

$$= \frac{|C_h \times Tr|}{|a_1 \times a_2|} = \frac{2\left(n^2 + m^2 + nm\right)}{d_R}$$

$$= \frac{2|C_h|^2}{a^2 d_R} \qquad (13)$$

where $|C_h|$ and d_R are given by Eqs (5) and (11) respectively. Each hexagon contains two carbon atoms, so there are 2N carbon atoms in each nanotube unit cell.

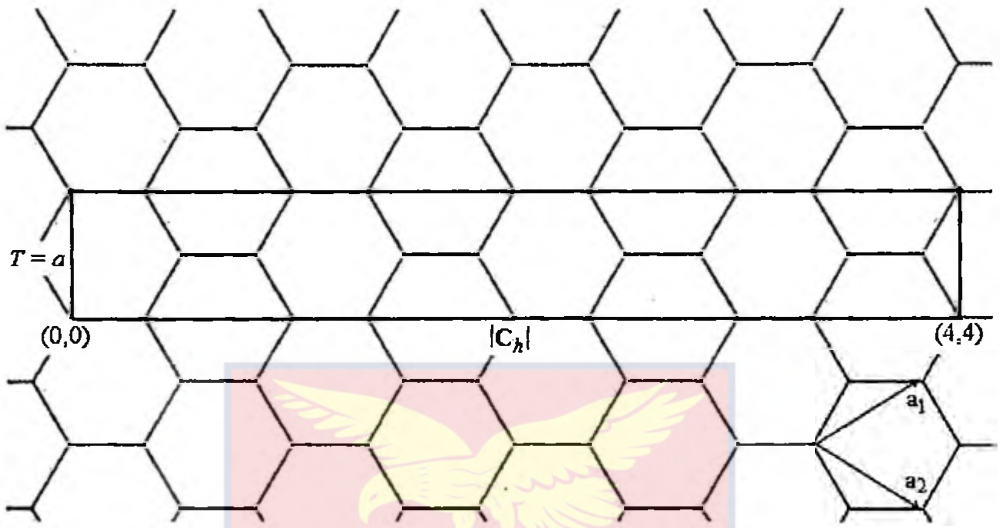


Figure 12: Unit cell of (4,4) armchair nanotube. The width of the unit cell for all armchair nanotube is T = |T| = a.

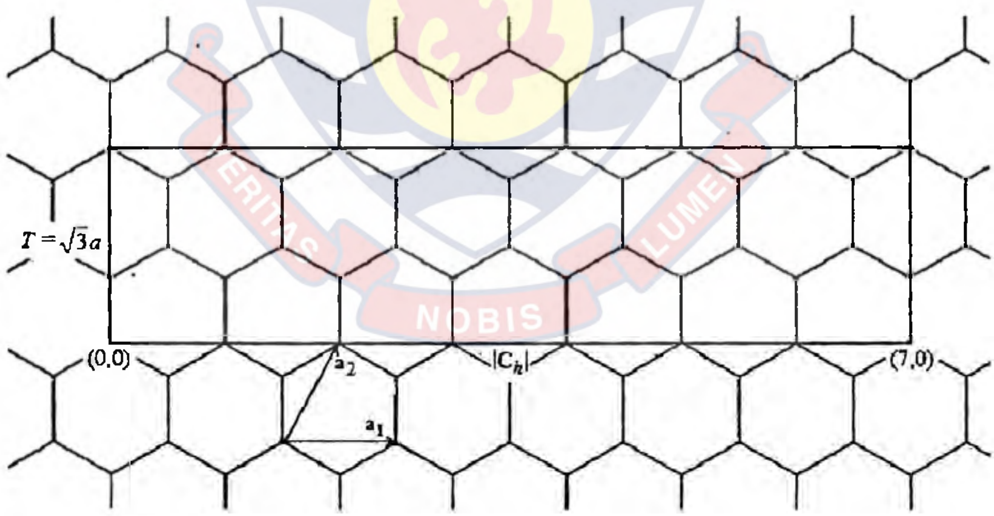


Figure 13: Unit cell of (7,0) zigzag nanotube. The width of the unit cell of all zigzag nanotubes is √3a. The length is $|C_h|$.

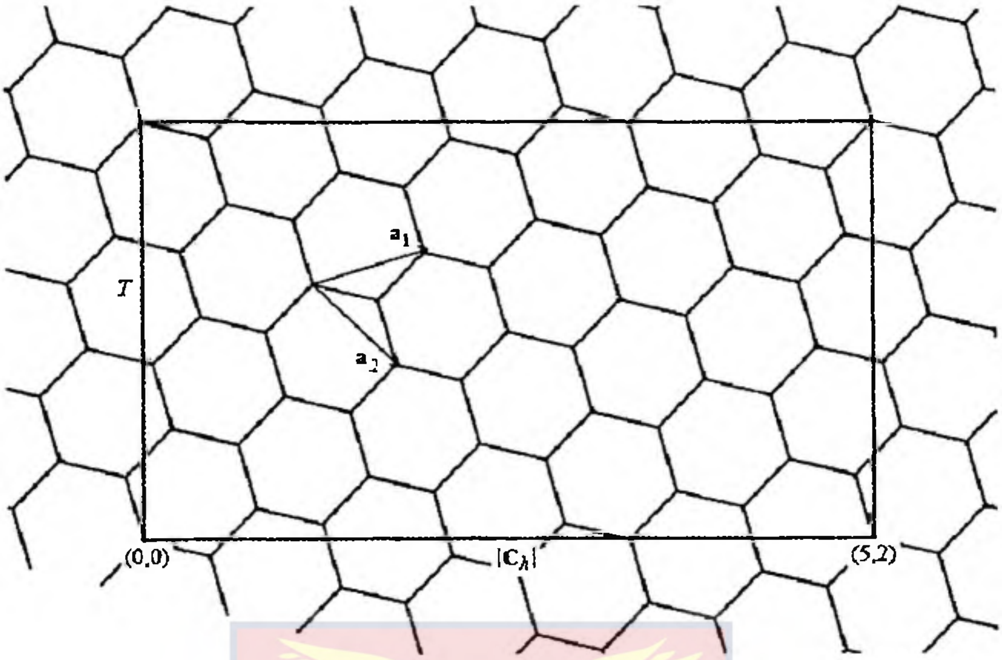


Figure 14: The unit cell of (5,2) chiral nanotube. The width and length of the unit cell is T and |C$_h$| respectively.

Symmetry vector

The symmetry vector R is the site vector (as indicated $\overrightarrow{OA}$ in Figure 10) that has the smallest component in the direction of the chiral vector C_h. The coordinates of carbon atoms in a nanotube unit cell are represented by iR, where i = 1 . . . N is an integer. When a carbon site vector iR goes out of the nanotube unit cell, it is shifted to lie within the unit cell through translation by an integral number of Ch or Tr, using periodic boundary conditions. R can be expressed in terms of a_1 and a_2 as [93]

$$R = pa_1 + qa_2 \equiv (p,q) \quad \textbf{(14)}$$

where p and q are integers and have no common divisor except 1, and are such that

$$0 \le t_1 q - t_2 p \le N \text{ and } 0 \le mp - nq \le N \quad \textbf{(15)}$$

N is the number of hexagons per unit cell of the CNT. The symmetry vector R can be considered as a rotation about the nanotube axis by ψ followed by a translation τ along the nanotube axis. This reflects the basic space group symmetry operations of a chiral CNT denoted by R = (ψ|τ) and illustrated in Figure 15. In this case, the component of R in the direction of the chiral vector C_h gives the angle ψ of rotation scaled by $|C_h|$ /dt, while the component in the direction of the translational vector Tr gives the translation τ of the basic symmetry operation of the one-dimensional space group of the CNT. The integers (p, q) then represents the lattice vector obtained when the symmetry operator acts on (0, 0),

i.e. (ψ|τ)(0, 0) = (p, q),

and $(\psi|\tau)^2$, $(\psi|\tau)^3$, . . . , $(\psi|\tau)^N$ are all distinct symmetry operations of an Abelian group denoted by C_N, where $(\psi|\tau)^N = E$ is the identity operation.

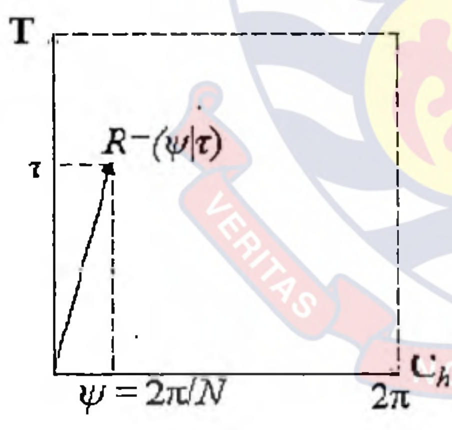


Figure 15: Space group symmetry operation R = (ψ|τ) [93]. ψ is the angle of rotation around the nanotube axis and τ is the translation in the direction of Tr; Nψ = 2π and Nτ = MT.

It can be shown that τ and the rotational angle ψ are given as [93]

$$\tau = \frac{|R \times C_h|}{|C_h|} = \frac{(mp - nq)Tr}{N} \quad (16)$$

$$\psi = \frac{|Tr \times R|}{Tr} \frac{2\pi}{|C_h|} = \frac{2\pi}{N} \tag{17}$$

The symmetry operator $(\psi|\tau)^N$ brings a lattice point to an equivalent lattice point, where

$$NR = C_h + MTr \tag{18}$$

and

$$M \equiv mp - nq \tag{19}$$

is an integer. M is the number of Tr vectors that is necessary for bringing a lattice point to its equivalent lattice point.

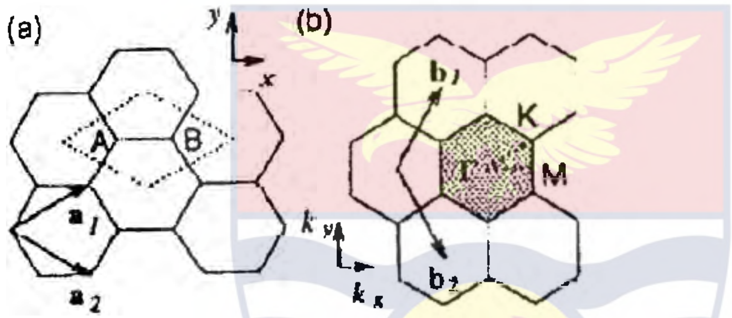


Figure 16: (a) The unit cell and (b) Brillouin zone of graphene are shown as the dotted rhombus and shaded hexagon respectively. A and B are inequivalent carbon atoms. The points Γ, K, and M are high symmetry points in the Brillouin zone.

One of the most remarkable properties of a given (*n*,*m*) carbon nanotubes is that depending on their structure and diameter, conducting or semiconducting nanotubes are possible. The condition for metallic or conducting nanotubes is that $(2n+m)$ or equivalently $(n-m)$ is a multiple of 3. That is for a given (*n*,*m*) nanotube, if $2n+m=3i$ or $n-m=3i$ (where *i* is an integer), then the nanotube is metallic, otherwise the nanotube is a semiconductor [93]. This leads to the cases that all armchair nanotubes are metallic or conducting, and zigzag nanotubes are only metallic or conducting if n is a multiple of 3. Figure 17 shows which carbon nanotubes (n,m) are predicted to be metallic and which are semiconducting, denoted by the yellow and blue circles respectively. It can be seen from this diagram that approximately one third of carbon nanotubes are metallic or conducting while the other two thirds are semiconducting. These basic predictions from the theory have been verified using Scanning Tunnelling Microscope studies [94,95]

Figure 17: Graphene showing atoms of metallic and semiconducting CNTs (n,m) which are denoted by the yellow and blue circles respectively [96].

Synthesis of carbon nanotubes

In this section we describe some of the synthesis methods for producing and purifying carbon nanotubes, with primary emphasis on single-wall nanotubes (SWCNT's). After Iijima's discovery [22], various methods where exploited to produce CNT's in sufficient quantities to be further studied. Some of these included arc-discharge, laser vaporisation of graphite and chemical vapour deposition (CVD). The general principle of nanotube growth involves producing reactive carbon at a very high temperature; these atoms then accumulate in regular patterns on the surface of metal particles that stabilize the formation of fullerenes resulting in a long chain of assembled carbon atoms. The CNT synthesis methods to be discussed are the arc-discharge of graphite, laser vaporisation of graphite and thermal synthesis.

Arc-Discharge Method of Synthesizing Carbon Nanotubes

The arc-discharge methodology originally used by Iijima [60] produced large quantities of multiwalled carbon nanotubes MWCNTs, typically greater than 5 nm in diameter, which have multiple carbon shells in a structure resembling that of Russian doll. In recent years, single-walled nanotubes (SWCNT's) using this method also have been grown and have become available in large quantities. The original arc-discharge apparatus, shown in Figure 18, consists of two graphite electrodes closely placed to each other (about 1 mm apart) in an atmosphere of helium at a 400 mbar and enclosed in a chamber. When a dc voltage is applied across the graphite electrodes, an arc is struck between the electrodes, resulting in the evaporation of the carbon from the anode to form plasma. Some of the plasma re-condenses as a hard cylindrical rod on the cathodic graphite. The central part of this deposit contains both MWCNTs and nanoparticles. This method produced very little amount of MWCNTs, making further progress in research in CNTs rather slow.

The arc-discharge tube provides a simple and traditional tool for generating the high temperatures of about 3000^0 C needed for the vaporization of carbon atoms into plasma [67-68].

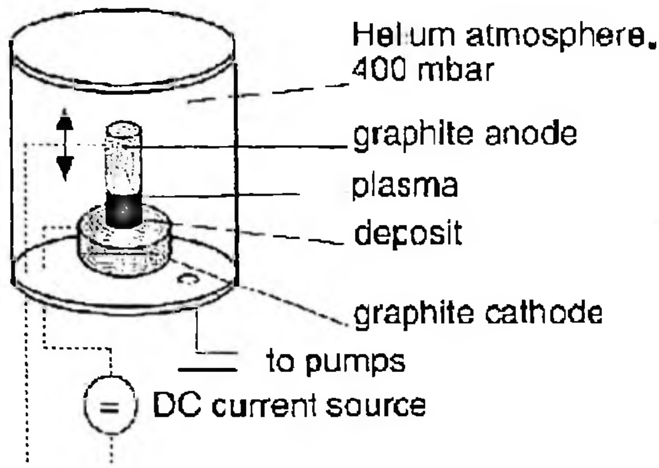


Figure 18: Schematic diagram of the arc discharge apparatus.

Modifications to the arc-discharge method by Ebbeson and Ajayan [67] greatly improved the quantity of CNTs obtained by the arc-discharge method. The arc-discharge is done in a vessel through which an inert gas flows at a controlled pressure (Figure 19). This technique has been used for the synthesis of single-wall and multi-wall carbon nanotubes, and ropes of single-wall nanotubes [97]. Typical conditions for operating the arc-discharge tube for the synthesis of carbon nanotubes include the use of carbon rod electrodes of 5-20 mm diameter separated by -1 mm with a voltage of 20-25V across the electrodes and a dc electric current of 50-120A flowing between the electrodes. The arc is typically operated in -500 torr He with a flow rate of 5-15ml/s for cooling purposes. When the arc is in operation, carbon deposits form on the negative electrode. As the carbon nanotubes form, the length of the positive electrode (anode) decreases (see Fig.19). As the anode is being consumed the electrodes are adjusted to keep them at approximately 1 mm or less apart.

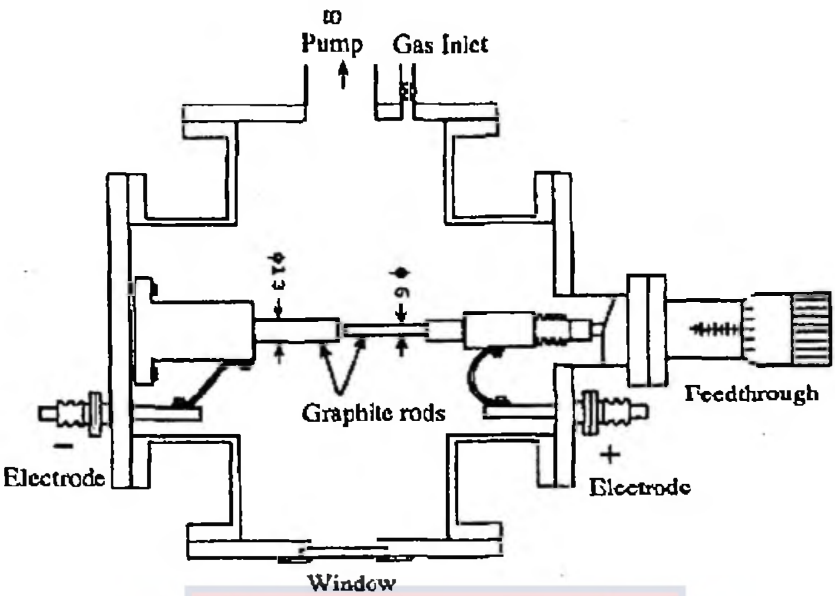


Figure 19: Cross-sectional view of a carbon arc generator that can be used to synthesize carbon nanotubes.

If multi-wall carbon nanotube is to be produced, then the synthesis requires no catalyst and the nanotubes formed are found in bundles in the inner region of the cathode deposit where the temperature is a maximum (3000°C). The nanotube bundles are roughly aligned in the direction of the electric current flow [68, 98]. Surrounding the nanotubes is a hard grey shell consisting of nanoparticles, fullerenes and amorphous carbon [99-101]. Adequate cooling of the growth chamber is necessary to maximize the nanotube yield in the arc growth process.

The current that produces the arc, which is usually about 100A, depends on the size of the rods, their separation and the gas pressure. Though the purity and yield depend sensitively on the gas pressure in the vessel, very high pressure does not improve the sample quality but results in a fall in total yield. The current is another important factor which affects the yield [68,102]. Very high current will produce a hard sintered material with few free nanotubes. Therefore the current should be kept low, but high enough to maintain a stable plasma. Also to produce good quality nanotube samples, it is essential that the electrodes and the chamber are effectively cooled.

Catalysts used to prepare isolated single-wall carbon nanotubes include transition metals such as Co, Ni, Fe and rare earths such as Y and Gd, while mixed catalysts such as Fe/Ni, Co/Ni and Co/Pt have been used to synthesize ropes of single-wall nanotubes.

Laser Vaporization Synthesis Method

The first large-scale production of SWCNTs was achieved in 1996 by the Smalley group at Rice University. This method of carbon nanotube growth produced SWCNTs of excellent quality but requires high powered lasers while producing small quantities of material. The Laser Vaporization Synthesis also called Laser ablation has been found to be the most efficient method for synthesizing bundles of single-wall carbon nanotubes with a narrow diameter distribution. Early reports of the laser synthesis technique [103,104] revealed high yields with about 70%-90% conversion of graphite to single-wall nanotubes in the condensing vapor of the heated flow tube operating at 1200^0C.

The laser ablation technique uses a 1.2 atom % of cobalt/nickel with 98.8 atom% of graphite composite target that is placed in a 1200°C quartz tube furnace with an inert atmosphere of 500 Torr of Ar or He and vaporized with a laser pulse. Two sequenced laser pulses are used to evaporate a target containing carbon mixed with a small amount of transition metal from the target. Figure 20 shows the quartz tube furnace used for producing CNTs.

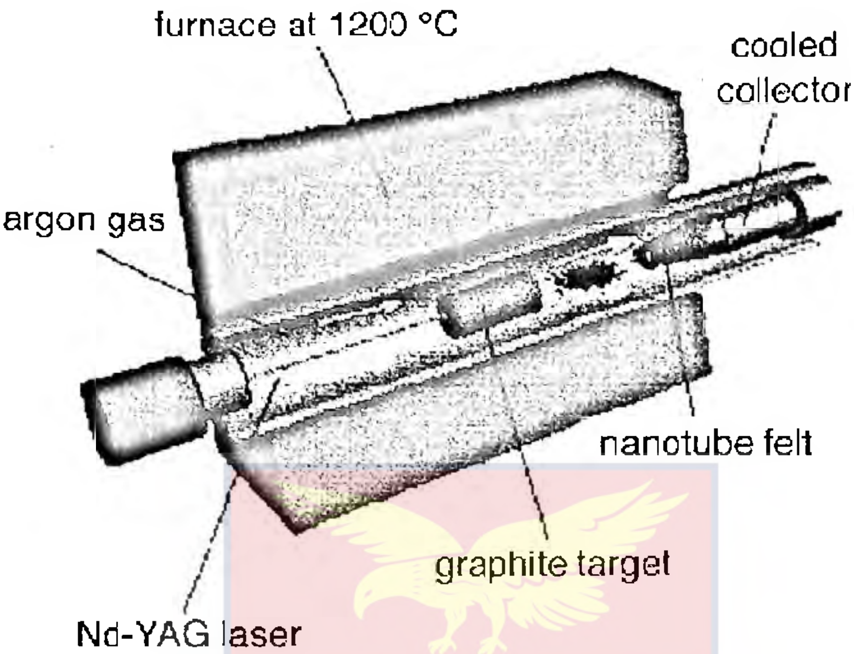


Figure 20: Single-walled nanotubes produced in a quartz tube heated to 1200°C by the laser vaporization method, using a graphite target and a cooled collector for nanotubes [105]

Flowing argon gas sweeps the entrained nanotubes from the high temperature zone to the water-cooled Cu collector downstream, just outside the furnace [104,106]. The material thus produced appears in a scanning electron microscope (SEM) image as a mat of "ropes" 10-20 nm in diameter and up to 100 µm or more in length. Under transmission electron microscope (TEM) examination, each rope is found to consist primarily of a bundle of single-wall carbon nanotubes aligned along a common axis. A detailed transmission electron microscopy study of carbon nanotubes prepared by the laser vaporization method [104] has shown that the carbon nanotube chiral indices *(n,m)* are mainly 44% of (10,10), 20% of (9,9) and some (12,8). The single-wall nanotubes are held together by weak van der Waals inter-nanotube bonds to form a two-dimensional triangular lattice with a lattice constant of 1.7 nm, and an inter-tube separation of 0.315 nm at closest approach within a rope [104]

Thermal synthesis

Thermal synthesis is considered a "medium temperature" method, since the hot zone of the reaction never exceeds a temperature of 1200°C. Thermal synthesis relies on only thermal energy and, in almost all cases, on active catalytic species such as Fe, Ni, and Co to break down carbon feedstock and produce CNTs. Depending on the carbon feedstock, Mo and Ru are sometimes added as promoters to render the feedstock more active for the formation of CNTs. CVD, HiPco, and flame synthesis are considered thermal CNT synthesis methods.

Chemical vapor deposition (CVD)

Endo et al [107] were the first to report on the use of CVD method to produce defective MWCNTs in 1993. Dai et al [108] successfully adapted CO-based CVD to produce SWCNT at Rice University in 1996. The CVD process encompasses a wide range of synthesis techniques, from the gram-quantity bulk formation of nanotube material to the formation of individual aligned SWCNTs on SiO_2 substrates for use in electronics. CVD can also produce aligned vertical MWCNTs for use as high-performance field emitters [109]. Additionally, CVD in its various forms produces SWCNT material of higher atomic quality and higher percent yield than the other methods currently available and, as such, represents a significant advance in SWCNT production. The majority of SWCNT production methods developed lately have direct principle related to CVD.

In a CVD furnance, gaseous carbon feedstock (CO) is flowed over transition metal nanoparticles at temperatures between 550 and 1200°C. Carbon reacts with the nanoparticles to produce SWCNTs as shown in Figure 21. The CVD method can be used to produce SWCNTs of diameters between 0.4 and 5 nm, and depending on the conditions, feedstock, and catalyst, the yield can exceed 99% (weight percent of final material) and the final product can be completely free of amorphous carbon.

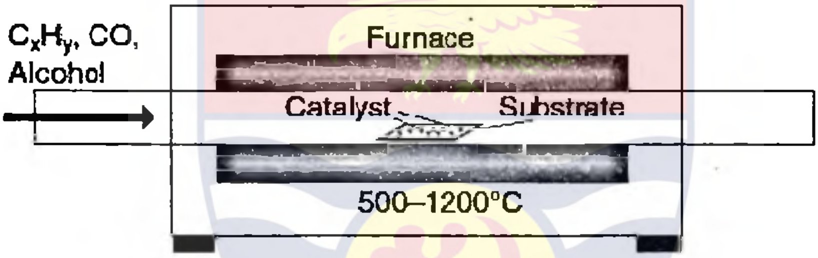


Figure 21: Schematic of a CVD furnace.

High-pressure carbon monoxide synthesis (HiPco)

One of the recent methods for producing SWCNTs in gram to kilogram quantities is the HiPco process shown in Figure 22 [110,111]. Though related to CVD synthesis, HiPco deserves a separate mention, since in recent years it has become a source of high-quality, narrow-diameter distribution SWCNTs around the world. The metal catalyst is formed *in situ* when $Fe(CO)_5$ or $Ni(CO)_4$ is injected into the reactor along with a stream of carbon monoxide (CO) gas at 900 to 1100°C and at a pressure of 30 to 50 atm. The reaction to make SWCNTs is the disproportionation of CO by nanometer-size metal catalyst particles. Yields of SWCNT material from HiPco process are claimed to be up to 97% atomic purity. The SWCNTs made by this process have diameters between 0.7 and 1.1nm. Tuning the pressure in the reactor and the catalyst composition, it is possible to tune the diameter range of the nanotubes produced [112].

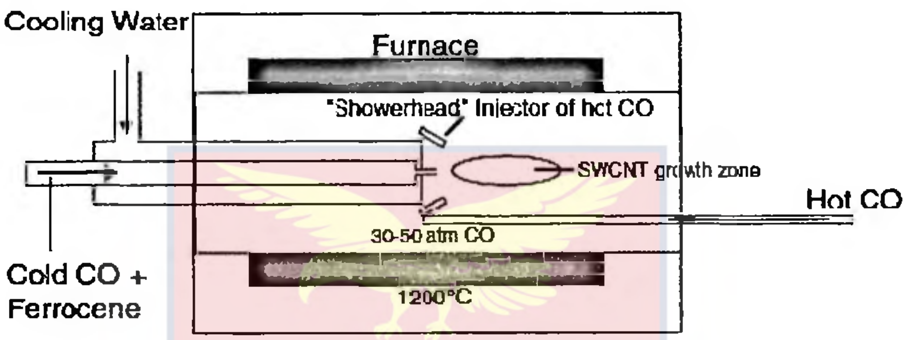


Figure 22: Schematic of a HiPco furnace. The CO gas + catalyst precursor is injected cold into the hot zone of the furnace, while excess CO gas is "showered" on it from all sides. Empirically this leads to the highest yield and longest individual nanotubes formed by this process.

Flame synthesis

Though still not a viable method for the production of high-quality SWCNTs, the so-called flame synthesis has the potential to become an extremely cheap and simple way to produce nanotubes. Flame synthesis has been shown to produce MWCNTs since the early 1990s [113]. Vander Wal et al.[114] were the first to exhibit the production of SWCNTs by using flame synthesis method. In this method, a hydrocarbon flame composed of 10% ethylene or acetylene with Fe or Co (cobaltacene, ferrocene, cobalt acetylacetonate) particles interspersed and diluted in H_2 and either He or Ar was ignited.

Since then, many other groups have been able to produce SWCNTs using similar methods, [114-119] and there has been a brief review written by Height et al [120] on the specifics of various methods for both MWCNT and SWCNT production. The current yields are low, but it is extremely attractive and potentially very cheap to be able to produce nanotubes with technology which is no more complicated than fire.

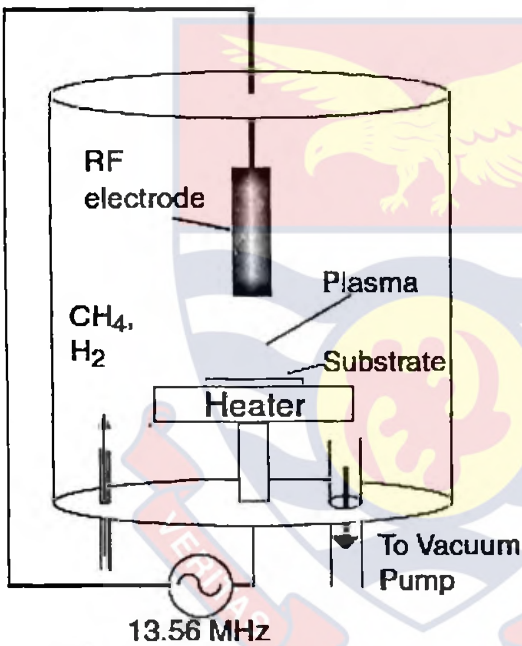


Figure 23: Schematic of a direct radiofrequency PECVD system.

Purification

In many of the synthesis methods that have been reported, carbon nanotubes are found along with other materials, such as amorphous carbon and carbon nanoparticles. Purification generally refers to the isolation of carbon nanotubes from other entities.

Three basic methods have been used with limited success for the purification of the nanotubes: gas phase, liquid phase, and intercalation methods [121]. The classical chemical techniques for purification (such as filtering, chromatography, and centrifugation) have been tried, but not found to be effective in removing the carbon nanoparticles, amorphous carbon and other unwanted species. Heating preferentially decreases the amount of disordered carbon relative to carbon nanotubes. Heating could thus be useful for purification, except that it results in an increase in nanotube diameter due to the accretion of epitaxial carbon layers from the carbon in the vapor phase resulting from heating.

The gas phase method removes nanoparticles and amorphous carbon in the presence of nanotubes by an oxidation or oxygen-burning process [98,122]. Much slower layer-by-layer removal of the cylindrical layers of multi-wall nanotubes occurs because of the greater stability of a perfect graphene layer to oxygen than disordered or amorphous carbon or material with pentagonal defects [122,123]. This method was in fact first used to synthesize a single-wall carbon nanotube. The oxidation reaction for carbon nanotubes is thermally activated with an energy barrier of 225 kJ/mol in air [123]. The gas phase purification process also tends to burn off many of the nanotubes. The carbon nanotubes obtained by gas phase purification are generally multi-wall nanotubes with diameters in the range 20-200Å and 10 nm-lμm in length [98] since the smaller diameter tubes tend to be oxidized with the nanoparticles.

Using a potassium permanganate $KMn0_4$ treatment method, the removal of nanoparticles and other unwanted carbons has been carried out in the liquid phase with some success. This method tends to give higher yields than the gas phase method, but results in nanotubes of shorter length [121,124].

Finally, the intercalation of unpurified nanotube samples with $CuCl_2$ - KCl results in intercalation of the nanoparticles and other carbon species, but not the nanotubes which have closed cage structures. Thus subsequent chemical removal of the intercalated species can be carried out [125].

A method for the purification of samples containing single-wall nanotube ropes in the presence of carbon nanoparticles, fullerenes and other contaminants has also been reported in [126].

In chapter three, the Boltzmann kinetic equation with energy dispersion will be employed to determine the electrical resistivity ρ, the differential thermoelectric power α and the electron thermal conductivity χ along the circumferential and axial directions of chiral CNTs.

CHAPTER THREE

LASER INDUCED THERMOELECTRIC PROPERTIES OF CHIRAL CARBON NANOTUBES

The carrier (electron or hole) current density j, electrical conductivity σ, thermopower α, electrical power factor P, the thermal current density q, the electron thermal conductivity χ_e of a chiral SWCNT are calculated as functions of the geometric chiral angle θ_h, temperature T, the real overlapping integrals for jumps along the nanotube axis Δ_z and along the base helix Δ_s. The calculation is done using the approach in reference [12] together with the phenomenological model of a SWNT developed in references [127] and [44]. This model yields physically interpretable results and gives correct qualitative descriptions of various electronic processes, which are corroborated by the first-principle numerical simulations of Miyamoto et al [45].

The dependence of these thermoelectric functions on T, θ_h, Δ_z and Δ_s are analysed numerically in chapter four, using MATLAB (Student Edition). The MATLAB is a simulation tool which can handle mathematical expressions with complex variables better and give detail results. Analysing the results obtained numerically help to give physical interpretation to the parameters of chiral CNT.

Carrier current density

Consider a SWCNT under a temperature gradient ∇T placed in an electric field applied along the nanotube axis. The carrier current density in the

SWCNT is calculated in the semiclassical approximation [12] by starting with the Boltzmann kinetic equation

$$\frac{\partial f(r,p,t)}{\partial t}+v(p)\frac{\partial f(r,p,t)}{\partial r}+eE\frac{\partial f(r,p,t)}{\partial p}=\frac{\partial(r,p,t)-f_0(p)}{\tau} \quad (20)$$

where $f(r, p, t)$ is the distribution function, $f_0(p)$ is the equilibrium distribution function, $v(p)$ is the electron velocity, E is the magnitude of the constant electric field, r is the electron position, p is the electron dynamical momentum, t is time elapsed, τ is the electron relaxation time and e is the electron charge. The collision integral is taken in the τ approximation and further assumed constant. The exact solution of Equation (20) presents some difficulties; therefore it is solved using perturbation approach where the second term is treated as the perturbation. In the linear approximation of ∇T and ∇μ, the solution to the Boltzmann kinetic equation is

$$f(p)=\tau^{-1}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)f_0\left(p-e\int_{t-t}^{t}\left[E_0+E_s\cos wt^{'}\right]dt^{'}\right)dt$$
$$+\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\left\{\left[\varepsilon\left(p-e\int_{t-t}^{t}\left[E_0+E_s\cos wt^{'}\right]dt^{'}\right)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$
$$\times v\left(p-e\int_{t-t}^{t}\left[E_0+E_s\cos wt^{''}\right]dt^{''}\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t}^{t}\left[E_0+E_s\cos wt^{''}\right]dt^{''}\right) \quad (21)$$

$\varepsilon(p)$ is the tight-binding energy of the electron, and μ is the chemical potential. The carrier current density j is defined as

$$j=e\sum_p v(p)f(p) \quad (22)$$

Substituting Eqn. (21) into Eqn. (22) we have

$$j=e\tau^{-1}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\sum_p v(p)f_0\left(p-e\int_{t-t}^{t}\left[E_0+E_s\cos wt^{'}\right]dt^{'}\right)$$

$$+e\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\sum_p v(p)\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \qquad (23)$$

Making the transformation

$$p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\rightarrow p\,,$$

we obtain for the current density

$$j=e\tau^{-1}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\sum_p v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)f_0(p)$$

$$+e\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\sum_p\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times\left\{v(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \qquad (24)$$

Using the phenomenological model [44,127,128], a SWCNT is considered as an infinitely long periodic chain of carbon atoms wrapped along a base helix as shown in Figure 24, and the real honeycomb crystalline structure of graphite is ignored.

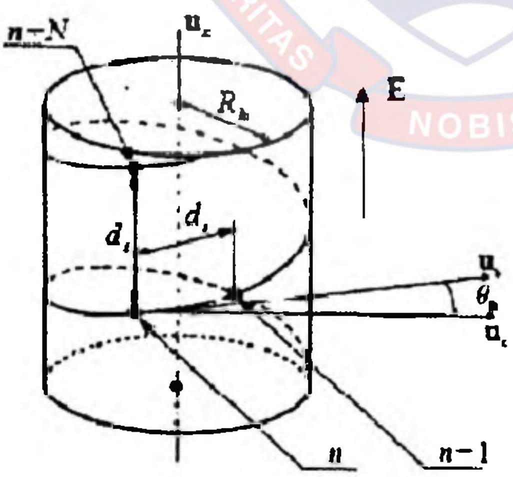


Figure 24: The schematic of the carbon nanotube geometry. All carbon atoms are numbered consecutively. Adapted from [44, 127].

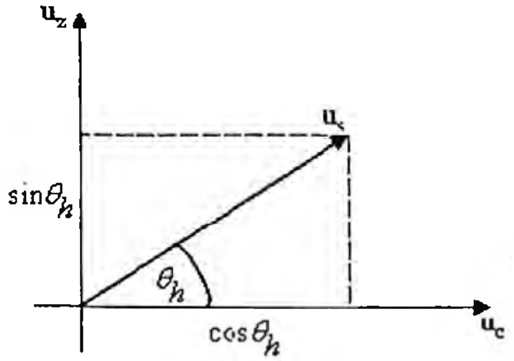


Figure 25: u_z and u_c are orthogonal unit vectors and u_s makes an angle θ_h with u_c.

The motion of electrons in the SWCNT is resolved along the nanotube axis in the direction of the unit vector u_z and unit vector u_s tangential to the base helix. The unit tangential vector u_s in turn makes an angle of θ_h with the circumferential unit vector u_c. u_c is defined to be the unit vector tangential to the circumference of the nanotube. θ_h is the geometric chiral angle (GCA).

The current density in the phenomenological model is in the form

$$j = S' u_s + Z' u_z \tag{25}$$

where S′ and Z′ are respectively components of the current density along the base helix and along the nanotube axis.

As defined in Figure 24 and illustrated in Figure 25, u_c is always perpendicular to u_z, therefore u_s can be resolved along u_c and u_z as follows

$$u_s = u_c \cos \theta_h + u_z \sin \theta_h \tag{26}$$

According to Eq (26), j can be expressed in terms of u_c and u_z as

$$j = u_c (S' \cos \theta_h) + u_z (Z' + S' \sin \theta_h) \equiv j_c u_c + j_z u_z \tag{27}$$

It implies that,

$$j_c = S' \cos \theta_h \tag{28}$$

$$j_z = Z' + S' \sin \theta_h \tag{29}$$

The interference between the axial and helical paths connecting a pair of atoms is neglected so that transverse motion quantization is ignored [44, 127]. This approximation best describes doped chiral carbon nanotubes, and is experimentally confirmed in [129].

Thus if in Equation (24) the transformation

$$\sum_p \rightarrow \frac{2}{(2\pi\hbar)^2} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

is made, Z′ and S′ respectively become,

$$Z' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z v_z\left(p - e\int_{t-t'}^{t} \left[E_0 + E_z \cos wt''\right] dt''\right) f_0(p)$$

$$+ \frac{2e}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{[\varepsilon(p) - \mu]\frac{\nabla_z T}{T} + \nabla_z \mu\right\}$$

$$\times \left\{v_z(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\} v_z\left(p - e\int_{t-t'}^{t} \left[E_0 + E_z \cos wt''\right] dt''\right) \qquad \textbf{(30)}$$

and

$$S' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z v_s\left(p - e\int_{t-t'}^{t} \left[E_0 + E_s \cos wt''\right] dt''\right) f_0(p)$$

$$+ \frac{2e}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{[\varepsilon(p) - \mu]\frac{\nabla_s T}{T} + \nabla_s \mu\right\}$$

$$\times \left\{v_s(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\} v_s\left(p - e\int_{t-t'}^{t} \left[E_0 + E_s \cos wt''\right] dt''\right) \qquad \textbf{(31)}$$

(Refer Appendices A7 and A8)

where the integrations are carried out over the first Brillouin zone, $\hbar$ is Planck's constant, v_s, p_s, E_s, $\nabla_s T$, and $\nabla_s \mu$ are the respective components of v, p, E, ∇T and $\nabla \mu$ along the base helix, and v_z, p_z, E_z, $\nabla_z T$, and $\nabla_z \mu$ are the respective components of v, p, E, ∇T and $\nabla \mu$ along the nanotube axis.

The energy dispersion relation for a chiral nanotube obtained in the tight binding approximation [127] is

$$\varepsilon(p) = \varepsilon_0 - \Delta_s \cos\frac{P_s d_s}{\hbar} - \Delta_z \cos\frac{P_z d_z}{\hbar} \tag{32}$$

where ε_0 is the energy of an outer-shell electron in an isolated carbon atom, Δ_z and Δ_s are the real overlapping integrals for jumps along the respective coordinates, p_s and p_z are the components of momentum tangential to the base helix and along the the nanotube axis, respectively.

The components v_s and v_z of the electron velocity v are respectively calculated from the energy dispersion relation Equation (32) as

$$v_s(p) = \frac{\partial \varepsilon(p)}{\partial P_s} = \frac{\Delta_s d_s}{\hbar} \sin\frac{P_s d_s}{\hbar} \tag{33}$$

$$v_s\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt^{"}\right]dt^{"}\right) = \frac{\partial \varepsilon}{\partial P_s}\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt^{"}\right]dt^{"}\right)$$

$$= \frac{\Delta_s d_s}{\hbar} \sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt^{"}\right]dt^{"}\right)$$

$$= \frac{\Delta_s d_s}{\hbar}\left\{\sin\frac{P_s d_s}{\hbar} \cos\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt^{"}\right]dt^{"}\right)\right.$$

$$\left. - \cos\frac{P_s d_s}{\hbar} \sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt^{"}\right]dt^{"}\right)\right\} \tag{34}$$

$$v_z(p) = \frac{\partial \varepsilon(p)}{\partial P_z} = \frac{\Delta_z d_z}{\hbar} \sin\frac{P_z d_z}{\hbar} \tag{35}$$

and

$$v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)=\frac{\partial\varepsilon}{\partial P_z}\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)$$

$$=\frac{\Delta_z d_z}{\hbar}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_z d_z}{\hbar}\sin\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\} \quad (36)$$

To calculate the carrier current density for a non-degenerate electron gas, the Boltzmann equilibrium distribution function $f_0(p)$ is expressed as

$$f_0(p)=C\exp\left(\frac{\Delta_s\cos\frac{P_s d_s}{\hbar}+\Delta_z\cos\frac{P_z d_z}{\hbar}+\mu-\varepsilon_0}{kT}\right) \quad (37)$$

where

$$C=\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\exp\left(-\frac{\mu-\varepsilon_0}{kT}\right) \qquad \text{(Refer Appendix A20)}$$

n_0 is the surface charge density, $I_n(x)$ is the modified Bessel function of order n defined by

$$I_n(x)=\frac{1}{\pi}\int_0^{\pi}d\theta\cos n\theta\exp(x\cos\theta) \quad (38)$$

$\Delta_s^*=\frac{\Delta_s}{kT}$ and $\Delta_z^*=\frac{\Delta_z}{kT}$ and k is Boltzmann's constant.

Now, substituting Equations (32) - (37) into Equations (30) and (31), and carrying out the integrals, the following expressions are obtained for S′ and Z′.

$$S'=-\sigma_s(E)E_{sn}^*-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T \quad (39)$$

$$Z' = -\sigma_z(E)E^*_{zn} - \sigma_z(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta^*_z \frac{I_0(\Delta^*_z)}{I_1(\Delta^*_z)} + 2 - \Delta^*_s \frac{I_1(\Delta^*_s)}{I_0(\Delta^*_s)}\right\}\nabla_z T \qquad (40)$$

Where we have defined E^*_{sn} as

$$E^*_{sn} = E_n + \nabla_s \frac{\mu}{e}$$

(Refer Appendices A47 and A48)

The electric field is applied along the nanotube axis (see Figure A1 in Appendix A), so we used the fact that $E_s = E_z \sin\theta_h = E \sin\theta_h$

Also $\sigma_i(E)$ is defined by

$$\sigma_i(E) = \frac{e^2\tau\Delta_i d_i^2 n_0}{\hbar^2}\frac{I_1(\Delta^*_i)}{I_0(\Delta^*_i)}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{1}{1+\left(\frac{ed_iE_0}{\hbar} + nw\right)^2\tau^2}\right], \; i = s,z \qquad (41)$$

(Refer Appendix A25)

Substituting Equation (39) into Equation (28), the following is obtained for the circumferential carrier current density j_c,

$$j_c = -\sigma_s(E)\sin\theta_h\cos\theta_h E^*_{zn}$$

$$-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta^*_s \frac{I_0(\Delta^*_s)}{I_1(\Delta^*_s)} + 2 - \Delta^*_z \frac{I_1(\Delta^*_z)}{I_0(\Delta^*_z)}\right\}\nabla_z T \qquad (42)$$

The following is obtained for the axial carrier current density j_z after substituting Equation (40) into Equation (29),

$$j_z = -\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\}E^*_{zn} - \left\{\sigma_z(E)\frac{k}{e}\left[\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta^*_z \frac{I_0(\Delta^*_z)}{I_1(\Delta^*_z)} + 2 - \Delta^*_s \frac{I_1(\Delta^*_s)}{I_0(\Delta^*_s)}\right]\right.$$

$$\left. + \sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta^*_s \frac{I_0(\Delta^*_s)}{I_1(\Delta^*_s)} + 2 - \Delta^*_z \frac{I_1(\Delta^*_z)}{I_0(\Delta^*_z)}\right]\right\}\nabla_z T \qquad (43)$$

Let us define

$$\xi = \frac{\varepsilon_0 - \mu}{kT}, \quad A_i = \frac{I_1(\Delta_i^*)}{I_0(\Delta_i^*)}, \quad B_i = \frac{I_0(\Delta_i^*)}{I_1(\Delta_i^*)} - \frac{2}{\Delta_i^*}, \quad i = s, z \tag{44}$$

Then Eqs (42) and (43) respectively become

$$j_c = -\sigma_s(E)\sin\theta_h \cos\theta_h E_{zn}^* - \sigma_s(E)\frac{k}{e}\sin\theta_h \cos\theta_h \{\xi - \Delta_s^* B_s - \Delta_z^* A_z\}\nabla_z T \tag{45}$$

and

$$j_z = -\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\}E_{zn}^*$$

$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta_z^* B_z - \Delta_s^* A_s\right] + \sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta_s^* B_s - \Delta_z^* A_z\right]\right\}\nabla_z T \tag{46}$$

Equations (45) and (46) define the carrier current density. The circumferential σ_{cz} and axial σ_{zz} components of the electrical conductivity in the CNT are obtained from Equations (45) and (46) respectively. In fact the coefficients of the electric field $-E_{zn}^*$ in these equations define σ_{cz} and σ_{zz} as follows,

$$\sigma_{cz} = \sigma_s(E)\sin\theta_h \cos\theta_h \tag{47}$$

$$\sigma_{zz} = \sigma_z(E) + \sigma_s(E)\sin^2\theta_h \tag{48}$$

Resistivity, thermopower and power factor

The resistivities ρ_{cz} and ρ_{zz} along the circumferential and axial directions are defined respectively by

$$\rho_c = \frac{1}{\sigma_{cz}} = \frac{1}{\sigma_s(E)\sin\theta_h \cos\theta_h} \tag{49}$$

(Refer Appendix A63)

and

$$\rho_z = \frac{1}{\sigma_{zz}} = \frac{1}{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h} \tag{50}$$

(Refer Appendix A64)

The differential thermoelectric power is defined as the ratio $\frac{|E_{zn}^*|}{|\nabla T|}$ in an open circuit (i.e. when j = 0). Thus setting j_c to zero in Equation (42), the thermoelectric power α_{cz} along the circumferential direction is obtained as follows

$$0 = -\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^* - \sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^* B_s - \Delta_z^* A_z\}\nabla_z T$$

$$\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^* = -\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^* B_s - \Delta_z^* A_z\}\nabla_z T$$

$$\frac{E_{zn}^*}{\nabla_z T} = -\frac{\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^* B_s - \Delta_z^* A_z\}}{\sigma_s(E)\sin\theta_h\cos\theta_h}$$

$$\alpha_{cz} = \left|\frac{E_{zn}^*}{\nabla_z T}\right| = \frac{k}{e}\{\xi - \Delta_s^* B_s - \Delta_z^* A_z\} \tag{51}$$

(Refer Appendix A65)

Similarly, the thermoelectric power α_{zz} along the axial direction is obtained from Equation (43) as follows (i.e. when $j_z = 0$)

$$0 = -\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\}E_{zn}^*$$
$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta_z^* B_z - \Delta_s^* A_s\right] + \sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta_s^* B_s - \Delta_z^* A_z\right]\right\}\nabla_z T$$

$$\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\}E_{zn}^* =$$
$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta_z^* B_z - \Delta_s^* A_s\right] + \sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta_s^* B_s - \Delta_z^* A_z\right]\right\}\nabla_z T$$

$$\frac{E^{*}_{zn}}{\nabla_z T} = -\frac{\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta^{*}_z B_z - \Delta^{*}_s A_s\right]\right.}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h} + \frac{\left.\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta^{*}_s B_s - \Delta^{*}_z A_z\right]\right\}}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}$$

$$\alpha_{zz} = \left|\frac{E^{*}_{zn}}{\nabla_z T}\right| = \frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta^{*}_z B_z - \Delta^{*}_s A_s\right]$$

$$+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta^{*}_s B_s - \Delta^{*}_z A_z\right] \qquad (52)$$

(Refer Appendix A66)

Finally the electrical power factor P is defined as

$$P = \sigma\alpha^2 = \frac{\alpha^2}{\rho}$$

Therefore the power factor along the circumferential and axial directions are given respectively by

$$P_c = \frac{\alpha^2_{cz}}{\rho_c} \qquad (53)$$

$$P_z = \frac{\alpha^2_{zz}}{\rho_z} \qquad (54)$$

In summary, we have obtained analytical expressions for the carrier current density *j*, the electrical resistivity ρ, thermopower α and electrical power factor *P* in a chiral SWCNT. It can be seen from these expressions that ρ, α and *P* depend on the geometric chiral angle θ_h, temperature T, the real overlapping integrals for jumps along the tubular axis Δ_z and the base helix Δ_s. The dependence of ρ, α and *P* on T, θ_h, Δ_s and Δ_z will be discussed in chapter four.

Thermal current density and electron thermal conductivity in Chiral Carbon Nanotubes

In this section, an expression for the thermal current density in a laser induced carbon nanotube under a temperature gradient and placed in an electric field is calculated. From this expression, the electron thermal conductivity is obtained as a function of the GCA θ_h, temperature T, the real overlapping integrals for jumps along the tubular axis Δ_z and the base helix Δ_s. In addition, the thermoelectric figure of merit is also estimated as a function of θ_h, T, Δs and Δz.

Consider a SWNT under a temperature gradient ∇T, and placed in a weak electric field E along the nanotube axis. The thermal current density q is given by

$$q = \sum_{p} [\varepsilon(p) - \mu] v(p) f(p) \tag{55}$$

where f(p) and ε(p) are given by Equations (21) and (32). *v(p)*, the electron velocity has components $v_s(p)$ and $v_z(p)$ given by Eqs (33), (34), (35) and (36). Substituting Equation (21) into Equation (55) we have

$$q = \tau^{-1} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \sum_p [\varepsilon(p) - \mu] v(p) f_0\left(p - e \int_{t-t'}^{t} [E_0 + E \cos wt''] dt'' \right)$$

$$+ \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \sum [\varepsilon(p) - \mu] v(p) \left\{ \left[\varepsilon\left(p - e \int_{t-t'}^{t} [E_0 + E \cos wt''] dt'' - \mu \right) \right] \frac{\nabla T}{T} + \nabla \mu \right\}$$

$$\times v\left(p - e \int_{t-t'}^{t} [E_0 + E \cos wt''] dt'' \right) \frac{\partial f_0}{\partial \varepsilon} \left(p - e \int_{t-t'}^{t} [E_0 + E \cos wt''] dt'' \right) \tag{56}$$

Making the transformation

$$p - e\int [E_0 + E\cos wt'']dt'' \rightarrow p,$$

we obtain for the thermal current density

$$q = \tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \sum_p \left[\varepsilon\left(p - e\int_{t-t'}^{t}[E_0 + E\ \cos wt'']dt''\right) - \mu\right]$$

$$\times v\left(p - e\int_{t-t'}^{t}[E_0 + E\cos wt'']dt''\right)f_0(p)$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \sum_p \left[\varepsilon\left(p - e\int_{t-t'}^{t}[E_0 + E\ \cos wt'']dt''\right) - \mu\right]\left\{[\varepsilon(p) - \mu]\frac{\nabla T}{T} + \nabla\mu\right\}$$

$$\times\left\{v(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\} v\left(p - e\int_{t-t'}^{t}[E_0 + E\ \cos wt'']dt''\right) \qquad (57)$$

We resolve the thermal current density along the tubular axis (z axis) and the base helix respectively, neglecting the interference between the axial and the helical paths connecting a pair of atoms, so that transverse motion quantization is ignored.

Then using the following transformation:

$$\sum_p \rightarrow \frac{2}{(2\pi\hbar)^2}\int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

we obtain the thermal current density along the tubular axis Z′ and along the base helix S′ respectively as follows,

$$Z' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t}[E_0 + E_z\cos wt'']dt''\right) - \mu\right]$$

$$\times\ v_z\left(p - e\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt''\right)f_0(p)$$

$$+\frac{2}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt''\right) - \mu\right]$$

$$\times\left\{[\varepsilon(p)-\mu]\frac{\nabla_z T}{T} + \nabla_z\mu\right\}\left\{v_z(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v_z\left(p - e\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt''\right) \quad (58)$$

and

$$S' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right) - \mu\right]$$

$$\times v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right)f_0(p)$$

$$+\frac{2}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right) - \mu\right]$$

$$\times\left\{[\varepsilon(p)-\mu]\frac{\nabla_s T}{T} + \nabla_s\mu\right\}\left\{v_s(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v_s\left(p - e\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right) \quad (59)$$

(Refer Appendices B6 and B7)

where the integrations are carried out over the first Brillouin zone.

The thermal current density in the phenomenological model is in the form

$$q = S'u_s + Z'u_z$$

Using Equation (26), q can be expressed in terms of u_c and u_z as follows,

$$q = u_c S' \cos\theta_h + u_z (Z' + S' \sin\theta_h) \equiv q_c u_c + q_z u_z$$

where the circumferential q_c and axial q_z thermal current densities are respectively

$$q_c = S' \cos\theta_h \ \ and \ \ q_z = Z' + S' \sin\theta_h \quad (60)$$

For a non-degenerate electron gas, we use the Boltzmann equilibrium distribution function $f_0(p)$ given by Eq (37), i.e.,

$$f_0(p) = C\exp\left(\frac{\Delta_s \cos\frac{P_s d_s}{\hbar} + \Delta_z \cos\frac{P_z d_z}{\hbar} + \mu - \varepsilon_0}{kT}\right) \tag{61}$$

where C is determined by the condition

$$C = \frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\exp\left(-\frac{\mu - \varepsilon_0}{kT}\right)$$

and n_0 is the surface charge density, $I_n(x)$ is the modified Bessel function of order n and k is Boltzmann's constant.

The components v_s and v_z of the electron velocity v are given by

$$v_s(p) = \frac{\partial\varepsilon(p)}{\partial P_s} = \frac{\Delta_s d_s}{\hbar}\sin\frac{P_s d_s}{\hbar} \tag{62}$$

$$v_s\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right) = \frac{\partial\varepsilon}{\partial P_s}\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)$$

$$= \frac{\Delta_s d_s}{\hbar}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right.$$
$$\left. - \cos\frac{P_s d_s}{\hbar}\sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right\} \tag{63}$$

$$v_z(p) = \frac{\partial\varepsilon(p)}{\partial P_z} = \frac{\Delta_z d_z}{\hbar}\sin\frac{P_z d_z}{\hbar} \tag{64}$$

and

$$v_z\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right) = \frac{\partial\varepsilon}{\partial P_z}\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)$$

$$= \frac{\Delta_z d_z}{\hbar}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right.$$
$$\left. - \cos\frac{P_z d_z}{\hbar}\sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right\} \tag{65}$$

Using Eqs (60) – (65) and the fact that $E_s = E_z \sin\theta_h$, $\nabla_s T = \nabla_z T \sin\theta_h$, and

$E^{*}_{sn} = E_n + \nabla_s \frac{\mu}{e}$, we obtain the circumferential q_c and axial q_z thermal current

densities after a cumbersome calculation as follows,

$$q_c = -\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_s^*}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta_z^* A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}E^*_{zn}$$

$$-\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\left\{\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a) + \frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + \frac{\Delta_s^*\Delta_z^*}{2}B_s A_z$$

$$\left.\mathrm{x}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + (\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}\nabla_z T \tag{66}$$

$$q_z = -\frac{kT}{e}\left\{\sigma_z(E)\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_z^*}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta_s^* A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_s^*}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta_z^* A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}E^*_{zn}$$

$$-\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_z^*}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - 2\Delta_s^*\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right.\right.$$

$$+\frac{(\Delta_z^*)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + \frac{\Delta_z^*\Delta_s^*}{2}A_s B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right] + \sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - 2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + \frac{\Delta_s^*\Delta_z^*}{2}A_z B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\left(\Delta_z^*\right)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg]\Bigg\}\nabla_z T \tag{67}$$

(Refer Appendices B99 and B102)

Here we have used the definitions given in Equation (44) and the definitions

$$C_i = 1-\frac{3I_0\left(\Delta_i^*\right)}{\Delta_i^* I_1\left(\Delta_i^*\right)}+\frac{6}{\Delta_i^{*2}},\quad i = s, z \tag{68}$$

$$\sigma_s(E)=\frac{e^2\tau\Delta_s d_s^{\,2}\, n_0}{(\hbar)^2}\frac{I_1\left(\Delta_s^*\right)}{I_0\left(\Delta_s^*\right)},\quad \Delta_i^* = \frac{\Delta_i}{kT},\quad i = s, z \tag{69}$$

From Equation (66) and (67), the electron thermal conductivity χ_e is given by

$$\chi_{ec} = \sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\Bigg\{\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{\left(\Delta_s^*\right)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z^*}{2}B_sA_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+\left(\Delta_z^*\right)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\} \tag{70}$$

(Refer Appendix B103)

$$\chi_{ez} = \frac{k^2T}{e^2}\Bigg\{\sigma_z(E)\Bigg[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^*}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-2\Delta_s^*\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\left(\Delta_z^*\right)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+\frac{\Delta_z^*\Delta_s^*}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\left(\Delta_s^*\right)^2\left(1-\frac{A_s}{\Delta_s^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg]+\sigma_s(E)\sin^2\theta_h\Bigg[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Big]\Big\} \quad \textbf{(71)}$$

(Refer Appendix B104)

where χ_{ec} and χ_{ez} are respectively the circumferential and axial components of the electron thermal conductivity. It can be observed from Equations (70) and (71) that χ_{ec} and χ_{ez} depend on the geometric chiral angle θ_h, temperature T, the real overlapping integrals for jumps along the tubular axis Δ_z and the base helix Δ_s. The results for χ_{ec} and χ_{ez} will be analysed numerically in chapter four. In order to check our results, the Onsagar relations are determined in the next section.

Onsagar Relations

In this section, we consider the ground state level (i.e. n = 0) for both the electrical current densities and the electron thermal conductivities of the chiral CNT.

When n = 0, the circumferential and axial electrical current densities found in Equations (45) and (46) now become

$$j_c=-\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^*-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\}\nabla_z T \quad \textbf{(72)}$$

and

$$j_z=-\{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\}E_{zn}^*$$

$$-\left\{\sigma_z(E)\frac{k}{e}[\xi-\Delta_z^*B_z-\Delta_s^*A_s]+\sigma_s(E)\frac{k}{e}\sin^2\theta_h[\xi-\Delta_s^*B_s-\Delta_z^*A_z]\right\}\nabla_z T \quad \textbf{(73)}$$

where

$$\sigma_i(E) = \frac{e^2\tau\Delta_i d_i^2 n_0}{\hbar^2}\frac{I_1(\Delta_i^*)}{I_0(\Delta_i^*)}J_0^2(a)\left[\frac{1}{1+\left(\frac{ed_iE_0}{\hbar}\right)^2\tau^2}\right],\ i = s,z \tag{74}$$

Using Equations (47) and (51), Equation (72) can be written in the form

$$j_c = \sigma_{cz}E_{zn}^* - \sigma_{cz}\alpha_{cz}\nabla_z T \tag{75}$$

Similarly, using Equations (48) and (52), Equation (73) can be written as

$$j_z = \sigma_{zz}E_{zn}^* - \sigma_{zz}\alpha_{zz}\nabla_z T \tag{76}$$

When n = 0, we also obtained the circumferential and axial thermal current densities as

$$q_c = -\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\xi J_0^2(a) - \frac{\Delta_s^*}{2}B_s(1+3J_0^2(a)) - \Delta_z^* A_z J_0^2(a)\right\}E_{zn}^*$$

$$-\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\left\{\xi^2 J_0^2(a) - \frac{\Delta_s^*}{2}\xi B_s\left(1+3J_0^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z J_0^2(a) + \frac{(\Delta_s^*)^2}{2}C_s\left(1+J_0^2(a)\right) + \frac{\Delta_s^*\Delta_z^*}{2}B_s A_z$$

$$\left. \times\ \left(1+3J_0^2(a)\right) + (\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)\right\}\nabla_z T \tag{77}$$

$$q_z = -\frac{kT}{e}\left\{\sigma_z(E)\left[\xi J_0^2(a) - \frac{\Delta_z^*}{2}B_z\left(1+3J_0^2(a)\right) - \Delta_s^* A_s J_0^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi J_0^2(a) - \frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right) - \Delta_z^* A_z J_0^2(a)\right]\right\}E_{zn}^*$$

$$-\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2 J_0^2(a) - \frac{\Delta_z^*}{2}\xi B_z\left(1+3J_0^2(a)\right) - 2\Delta_s^*\xi A_s J_0^2(a)\right.\right.$$

$$\left. + \frac{(\Delta_z^*)^2}{2}C_z\left(1+J_0^2(a)\right) + \frac{\Delta_z^*\Delta_s^*}{2}A_s B_z\left(1+3J_0^2(a)\right) + (\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)J_0^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2 J_0^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3J_0^2(a)\right)-2\Delta_z^*\xi A_z J_0^2(a)\right.$$

$$+\frac{\left(\Delta_s^*\right)^2}{2}C_s\left(1+J_0^2(a)\right)+\frac{\Delta_s^*\Delta_z^*}{2}A_z B_s\left(1+3J_0^2(a)\right)$$

$$\left.\left.+\left(\Delta_z^*\right)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)\right]\right\}\nabla_z T \tag{78}$$

Now we eliminate E_{zn}^* between Equations (72) and (77), and between Equations (73) and (78) and then compare our results with the Onsagar relations. From Equation (72), we have

$$E_{zn}^*=-\frac{j_c}{\sigma_s(E)\sin\theta_h\cos\theta_h}-\frac{k}{e}\left\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\right\}\nabla_z T \tag{79}$$

Eqn. (79) is substituted into Eqn. (77)

$$q_c=\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right)\right.$$

$$\left.-\Delta_z^*A_z J_0^2(a)\right\}\frac{j_c}{\sigma_s(E)\sin\theta_h\cos\theta_h}$$

$$+\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right)\right.$$

$$\left.-\Delta_z^*A_z J_0^2(a)\right\}\frac{k}{e}\left\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\right\}\nabla_z T$$

$$-\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\left\{\xi^2 J_0^2(a)\right.$$

$$-\frac{\Delta_s^*}{2}\xi B_s\left(1+3J_0^2(a)\right)-2\Delta_z^*\xi A_z J_0^2(a)$$

$$+\frac{\left(\Delta_s^*\right)^2}{2}C_s\left(1+J_0^2(a)\right)+\frac{\Delta_s^*\Delta_z^*}{2}B_s A_z\left(1+3J_0^2(a)\right)$$

$$\left.+\left(\Delta_z^*\right)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)\right\}\nabla_z T$$

$$q_c = \frac{kT}{e}\left\{\xi J_0^2(a) - \frac{\Delta_s^*}{2} B_s\left(1+3J_0^2(a)\right) - \Delta_z^* A_z J_0^2(a)\right\} j_c$$

$$-\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\left[\left\{\xi^2 J_0^2(a) - \frac{\Delta_s^*}{2}\xi B_s\left(1+3J_0^2(a)\right) - 2\Delta_z^*\xi A_z J_0^2(a)\right.\right.$$

$$+\frac{(\Delta_s^*)^2}{2} C_s\left(1+J_0^2(a)\right) + \frac{\Delta_s^*\Delta_z^*}{2} B_s A_z\left(1+3J_0^2(a)\right) + (\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right) J_0^2(a)\Big\}$$

$$-\left\{\xi J_0^2(a) - \frac{\Delta_s^*}{2} B_s\left(1+3J_0^2(a)\right) - \Delta_z^* A_z J_0^2(a)\right\}\left\{\xi - \Delta_s^* B_s - \Delta_z^* A_z\right\}\Big]\nabla_z T \quad \textbf{(80)}$$

Also making E_{zn}^* the subject in Equation (73), we get

$$E_{zn}^* = \frac{j_z}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h} - \left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta_z^* B_z - \Delta_s^* A_s\right]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta_s^* B_s - \Delta_z^* A_z\right]\right\}\nabla_z T \quad \textbf{(81)}$$

Substituting Eq (81) into (78) we obtain

$$q_z = \frac{kT}{e}\left\{\sigma_z(E)\left[\xi J_0^2(a) - \frac{\Delta_z^*}{2} B_z\left(1+3J_0^2(a)\right) - \Delta_s^* A_s J_0^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi J_0^2(a) - \frac{\Delta_s^*}{2} B_s\left(1+3J_0^2(a)\right) - \Delta_z^* A_z J_0^2(a)\right]\right\}$$

$$\text{x}\ \frac{j_z}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}$$

$$+\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi J_0^2(a) - \frac{\Delta_z^*}{2} B_z\left(1+3J_0^2(a)\right) - \Delta_s^* A_s J_0^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi J_0^2(a) - \frac{\Delta_s^*}{2} B_s\left(1+3J_0^2(a)\right) - \Delta_z^* A_z J_0^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi - \Delta_z^* B_z - \Delta_s^* A_s\right]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi - \Delta_s^* B_s - \Delta_z^* A_z\right]\right\}\nabla_z T$$

$$-\frac{k^2T}{e^2}\{\sigma_z(E)[\xi^2 J_0^2(a)-\frac{\Delta_z^*}{2}\xi B_z(1+3J_0^2(a))$$

$$-2\Delta_s^*\xi A_s J_0^2(a)+\frac{(\Delta_z^*)^2}{2}C_z(1+J_0^2(a))$$

$$+\frac{\Delta_z^*\Delta_s^*}{2}A_s B_z(1+3J_0^2(a))+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)J_0^2(a)]$$

$$+\sigma_s(E)\sin^2\theta_h[\xi^2 J_0^2(a)-\frac{\Delta_s^*}{2}\xi B_s(1+3J_0^2(a))$$

$$-2\Delta_z^*\xi A_z J_0^2(a)+\frac{(\Delta_s^*)^2}{2}C_s(1+J_0^2(a))+\frac{\Delta_s^*\Delta_z^*}{2}A_z B_s(1+3J_0^2(a))$$

$$+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)]\}\nabla_z T$$

Simplifying we get

$$q_z=\frac{kT}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}[\xi J_0^2(a)-\frac{\Delta_z^*}{2}B_z(1+3J_0^2(a))-\Delta_s^*A_sJ_0^2(a)]\right.$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s(1+3J_0^2(a))-\Delta_z^*A_zJ_0^2(a)\right]\right\}j_z$$

$$-\frac{k^2T}{e^2}\left(\left\{\sigma_z(E)[\xi^2 J_0^2(a)-\frac{\Delta_z^*}{2}\xi B_z(1+3J_0^2(a))-2\Delta_s^*\xi A_s J_0^2(a)\right.\right.$$

$$+\frac{(\Delta_z^*)^2}{2}C_z(1+J_0^2(a))+\frac{\Delta_z^*\Delta_s^*}{2}A_sB_z(1+3J_0^2(a))+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)J_0^2(a)]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2 J_0^2(a)-\frac{\Delta_s^*}{2}\xi B_s(1+3J_0^2(a))-2\Delta_z^*\xi A_z J_0^2(a)\right.$$

$$\left.\left.+\frac{(\Delta_s^*)^2}{2}C_s(1+J_0^2(a))+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s(1+3J_0^2(a))+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)\right]\right\}$$

$$-\{\sigma_z(E)[\xi J_0^2(a)-\frac{\Delta_z^*}{2}B_z(1+3J_0^2(a))-\Delta_s^* A_s J_0^2(a)]$$

$$+\sigma_s(E)\sin^2\theta_h\,[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s(1+3J_0^2(a))-\Delta_z^* A_z J_0^2(a)]\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}[\xi-\Delta_z^* B_z-\Delta_s^* A_s]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h[\xi-\Delta_s^* B_s-\Delta_z^* A_z]\right\}\Bigg)\nabla_z T$$

$$q_z=\frac{kT}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}[\xi J_0^2(a)-\frac{\Delta_z^*}{2}B_z(1+3J_0^2(a))-\Delta_s^* A_s J_0^2(a)]\right.$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s(1+3J_0^2(a))-\Delta_z^* A_z J_0^2(a)\right]\right\}j_z$$

$$-\left(\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2 J_0^2(a)-\frac{\Delta_z^*}{2}\xi B_z(1+3J_0^2(a))-2\Delta_s^*\xi A_s J_0^2(a)\right.\right.\right.$$

$$\left.+\frac{(\Delta_z^*)^2}{2}C_z(1+J_0^2(a))+\frac{\Delta_z^*\Delta_s^*}{2}A_s B_z(1+3J_0^2(a))+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)J_0^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2 J_0^2(a)-\frac{\Delta_s^*}{2}\xi B_s(1+3J_0^2(a))-2\Delta_z^*\xi A_z J_0^2(a)\right.$$

$$\left.\left.+\frac{(\Delta_s^*)^2}{2}C_s(1+J_0^2(a))+\frac{\Delta_s^*\Delta_z^*}{2}A_z B_s(1+3J_0^2(a))+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)\right]\right\}$$

$$-\frac{k^2T}{e^2}(\sigma_z(E)+\sigma_s(E)\sin^2\theta_h)\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}[\xi J_0^2(a)\right.$$

$$-\frac{\Delta_z^*}{2}B_z(1+3J_0^2(a))-\Delta_s^* A_s J_0^2(a)]$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s(1+3J_0^2(a))-\Delta_z^* A_z J_0^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi-\Delta_z^{\bullet}B_z-\Delta_s^{\bullet}A_s\right]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi-\Delta_s^{\bullet}B_s-\Delta_z^{\bullet}A_z\right]\right\}\nabla_z T \quad \textbf{(82)}$$

Equation (80) and (82) are in the form of the Onsagar relations given by

$$q_c=\Pi_{cz}j_c-X_{cz}\nabla_z T \quad \textbf{(83)}$$

and

$$q_z=\Pi_{zz}j_c-X_{zz}\nabla_z T \quad \textbf{(84)}$$

Where X is the electron thermal conductivity when the carrier current density j is zero and Π, the Peltier coefficient, is given by $\Pi=\alpha T$. As usual α is the thermopower.

Comparing Equation (80) and Equation (83), we obtain the circumferential component of the Peltier coefficient Π as follows

$$\Pi_{cz}=\frac{k}{e}\left\{\xi J_0^2(a)-\frac{\Delta_s^{\bullet}}{2}B_s\left(1+3J_0^2(a)\right)-\Delta_z^{\bullet}A_zJ_0^2(a)\right\}T$$

$$=\alpha_{cz}T \quad \textbf{(85)}$$

This implies that,

$$\alpha_{cz}=\frac{k}{e}\left\{\xi J_0^2(a)-\frac{\Delta_s^{\bullet}}{2}B_s\left(1+3J_0^2(a)\right)-\Delta_z^{\bullet}A_zJ_0^2(a)\right\} \quad \textbf{(86)}$$

Again comparing Equation (82) and Equation (84), we obtain the axial component of Π as follows

$$\Pi_{zz}=\frac{k}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_z^{\bullet}}{2}B_z\left(1+3J_0^2(a)\right)-\Delta_s^{\bullet}A_sJ_0^2(a)\right]\right.$$

$$+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right)-\Delta_z^*A_zJ_0^2(a)\right]\Bigg\}T$$

$$=\alpha_{zz}T \tag{87}$$

This implies that,

$$\alpha_{zz}=\frac{k}{e}\Bigg\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_z^*}{2}B_z\left(1+3J_0^2(a)\right)-\Delta_s^*A_sJ_0^2(a)\right]$$

$$+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right)-\Delta_z^*A_zJ_0^2(a)\right]\Bigg\}T \tag{88}$$

Now, comparing Equations (80) and (83), the circumferential component of the electron thermal conductivity X_{cz} (when j = 0) is as follows

$$X_{cz}=\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\Bigg[\Bigg\{\xi^2J_0^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3J_0^2(a)\right)-2\Delta_z^*\xi A_zJ_0^2(a)$$

$$+\frac{(\Delta_s^*)^2}{2}C_s\left(1+J_0^2(a)\right)+\frac{\Delta_s^*\Delta_z^*}{2}B_sA_z\left(1+3J_0^2(a)\right)+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^{''}}\right)J_0^2(a)\Bigg\}$$

$$-\left\{\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right)-\Delta_z^*A_zJ_0^2(a)\right\}\left\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\right\}\Bigg] \tag{89}$$

Now, comparing Eqns. (82) and (84), the circumferential component of the electron thermal conductivity X_{zz} (when j = 0) is as follows

$$X_{zz}=\Bigg(\frac{k^2T}{e^2}\Bigg\{\sigma_z(E)\Big[\xi^2J_0^2(a)-\frac{\Delta_z^*}{2}\xi B_z\left(1+3J_0^2(a)\right)-2\Delta_s^*\xi A_sJ_0^2(a)$$

$$+\frac{(\Delta_z^*)^2}{2}C_z\left(1+J_0^2(a)\right)+\frac{\Delta_z^*\Delta_s^*}{2}A_sB_z\left(1+3J_0^2(a)\right)+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)J_0^2(a)\Big]$$

$$+\sigma_s(E)\sin^2\theta_h\Big[\xi^2J_0^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3J_0^2(a)\right)-2\Delta_z^*\xi A_zJ_0^2(a)$$

$$+\frac{(\Delta_s^*)^2}{2}C_s\left(1+J_0^2(a)\right)+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3J_0^2(a)\right)+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)J_0^2(a)\Bigg]\Bigg\}$$

$$-\frac{k^2T}{e^2}\left(\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\right)\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)\right.\right.$$

$$\left.-\frac{\Delta_z^*}{2}B_z\left(1+3J_0^2(a)\right)-\Delta_s^*A_sJ_0^2(a)\right]$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi J_0^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3J_0^2(a)\right)-\Delta_z^*A_zJ_0^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi-\Delta_z^*B_z-\Delta_s^*A_s\right]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi-\Delta_s^*B_s-\Delta_z^*A_z\right]\right\}\Bigg) \qquad \textbf{(90)}$$

Laser Switched Off ($E_s = 0$).

When the Laser source is switched off, $E_s = 0$, $a = 0$, $w = 0$ and $J_n^2(a)$ becomes unity, therefore the expressions for the resistivity from Equations (49) and (50) ρ_{cz} and ρ_{zz} along the circumferential and axial directions are reduced to

$$\rho_c = \frac{1}{\sigma_s(E)\sin\theta_h\cos\theta_h} \qquad \textbf{(91)}$$

and

$$\rho_z = \frac{1}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h} \qquad \textbf{(92)}$$

where $\sigma_i(E) = \frac{e^2\tau\Delta_i d_i^2 n_0}{\hbar^2}\frac{I_1(\Delta_i^*)}{I_0(\Delta_i^*)}\left[\frac{1}{1+\left(ed_iE_0/\hbar\right)^2\tau^2}\right]$, $i = s, z$.

Also, the thermopower expression in Equation (52) is reduced to

$$\alpha_{zz} = \frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta_z^{*}B_z - \Delta_s^{*}A_s\right]$$

$$+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta_s^{*}B_s - \Delta_z^{*}A_z\right] \qquad (93)$$

The removal of the Laser source also causes the electron thermal conductivity χ_e to become

$$\chi_{ec} = \sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\Big\{\xi^2 - 2\Delta_s^{*}\xi B_s - 2\Delta_z^{*}\xi A_z + \left(\Delta_s^{*}\right)^2 C_s$$

$$+2\Delta_s^{*}\Delta_z^{*}B_sA_z + \left(\Delta_z^{*}\right)^2\left(1-\frac{A_z}{\Delta_z^{*}}\right) \qquad (94)$$

$$\chi_{ez} = \frac{k^2T}{e^2}\Big\{\sigma_z(E)\Big[\xi^2 - 2\Delta_z^{*}\xi B_z - 2\Delta_s^{*}\xi A_s + 2\left(\Delta_z^{*}\right)^2 C_z + 2\Delta_z^{*}\Delta_s^{*}A_sB_z$$

$$+\left(\Delta_s^{*}\right)^2\left(1-\frac{A_s}{\Delta_s^{*}}\right)\Big] + \sigma_s(E)\sin^2\theta_h\Big[\xi^2 - 2\Delta_s^{*}\xi B_s - 2\Delta_z^{*}\xi A_z$$

$$+2\left(\Delta_s^{*}\right)^2 C_s + 2\Delta_s^{*}\Delta_z^{*}A_zB_s + \left(\Delta_z^{*}\right)^2\left(1-\frac{A_z}{\Delta_z^{*}}\right)\Big]\Big\} \qquad (95)$$

where χ_{ec} and χ_{ez} are respectively the circumferential and axial components of the electron thermal conductivity.

CHAPTER FOUR

RESULTS AND DISCUSSION

In Chapter Three, a tractable analytic approach was used to calculate the electrical resistivity ρ, thermopower α and the electron thermal conductivity χ. Calculations were done for both the circumferential and axial components of the electrical resistivity, thermopower and the electron thermal conductivity. These calculations were based on solving the Boltzmann kinetic equation with energy dispersion relation obtained in the tight binding approximation.

In this chapter, the equations obtained for ρ_c, ρ_z, α_z, χ_c and χ_z shall be analyzed numerically. With appropriate choice of values for d_s, d_z, τ, θ_h and n_o, we determine how the results obtained in chapter three depend on temperature T, the overlapping integrals (Δ_s and Δ_z), the applied d. c. electric field E_o and a Laser source with a. c. electric field E_s. Typically, θ_h for a chiral SWCNT is a few degrees. For the analysis of the electrical resistivity and thermopower of a chiral SWCNT, parameters with values d_s = 1A, d_z = 2A, $\tau = 0.3 \times 10^{-12}$ s and $\theta_h = 4^o$ is considered. The Laser beam present has a frequency $w = 10^{12} s^{-1}$ and an a. c. electric field $E_s = 5 \times 10^7$ V/m. In the case of the electron thermal conductivity of a chiral SWCNT, values considered are d_s = 1 nm, d_z = 2 nm, $\tau = 0.3 \times 10^{-11}$ s and $\theta_h = 4^o$. All numerical analysis and plots were done using Mathlab 7.5 (Professional edition).

Electrical Resistivity

The electrical resistivity of a chiral SWNT for which d_s, d_z, τ, w, E_s and θ_h are given above is studied using Equations (49) and (50). In Figure 26, relationship between the circumferential electrical resistivity ρ_c and temperature T is sketched for various fixed values of the electric field E_o. The value of the d. c. electric field, E_o is chosen such that $\Omega\tau = 1$. Where $\Omega = ed_z E_o/\hbar$. Thus using the values of d_s, d_z, and τ given above, E_o is found to be 6.9063×10^7V/m. In the presence of Laser, it was observed in Figure 26 that ρ_c changed slowly at low temperatures up to about 200 K and then increased almost linearly with temperature. Explanation to this trend is that increasing the temperature causes carbon atoms in the walls of the CNT to vibrate faster thereby increasing electron – atom collisions. As a result of increasing electron – atom collisions, electrical resistivity also increases correspondingly. Also, the low value of resistivity observed is a clear indication that chiral CNT's can exhibit metallic properties. There was also a remarkable increase in resistivity as the electric field E_o was increased. As E_o is increased, the electrons in the CNT become more energetic, and so they collide with carbon atoms within the walls of the CNT, setting these carbon atoms into large amplitude oscillations which scatter the electrons.

Therefore increasing E_o causes the resistivity of the chiral CNT to increase as observed in Figure (26). Thus at high electric fields, Ohm's law is violated. However, the resistivity, ρ_c, was found to decrease markedly with increasing Δ_s as shown in Figure (27).

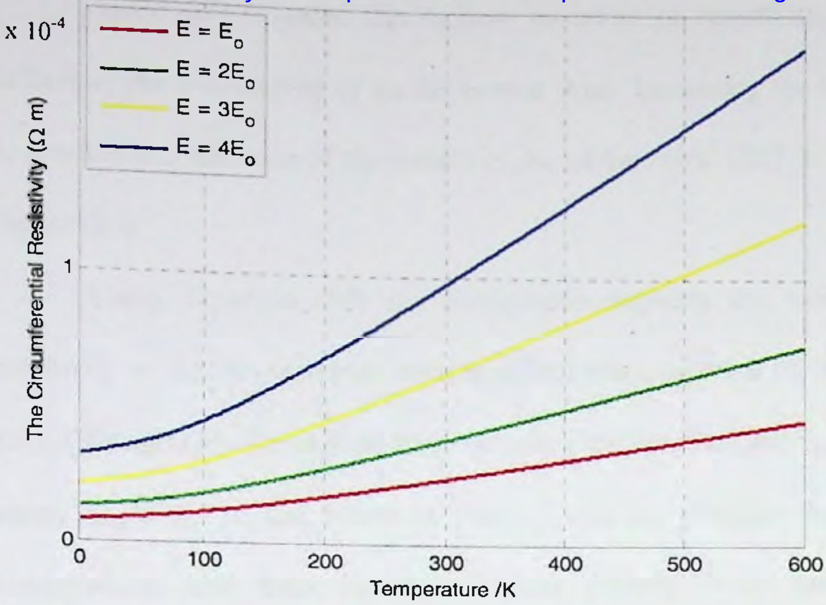


Figure 26. The dependence of ρ_c on temperature for various fixed values of the electric field $E=E_o$, $2E_o$, $3E_o$ and $4E_o$, where $E_o=6.9063 \times 10^7$V/m. $E_s = 5.0 \times 10^7$V/m, $\Delta_s = 0.018$eV and $\Delta_z = 0.024$eV.

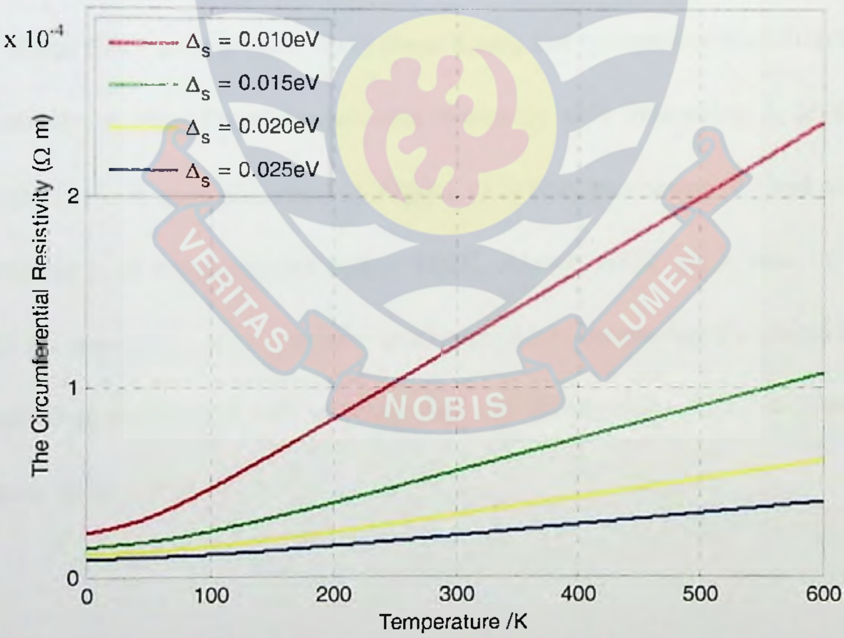


Figure 27. The dependence of ρ_c on temperature for various fixed values of Δ_s, $\Delta_z = 0.024$eV, $E_s = 5.0 \times 10^7$V/m, $E = 2E_o$, where $E_o=6.9063 \times 10^7$V/m.

Figure (28) revealed that Δ_z have no effect on resistivity, ρ_c. This is evident in the overlapping of all the curves. Also, increasing the chiral angle, θ_h resulted in a decrease of the resistivity, ρ_c, of the chiral CNT as observed in Figure (29).

Using Equation (50) the relationship between the axial electrical resistivity ρ_z and temperature were sketched and presented as Figures (30), (31), (32) and (33) for various fixed values of the electric field E_o, Δ_s, Δ_z and chiral angle θ_h. It was observed that ρ_z, like ρ_c, changes slowly at low temperatures and then increases almost linearly with temperature at temperatures above 200 K. There was also a remarkable increase in resistivity as the electric field E_o was increased (Figure 30). Even though the behavior of ρ_z with temperature is similar to that of ρ_c, the values recorded for ρ_z is greater than that of ρ_c. This means that the number of electron – atom collisions along the chiral CNT axis is more than those along the circumferential direction.The resistivity, ρ_z, was found to decrease markedly with increasing Δ_s as shown in Figure (31). It was observed in Figure (32) that increasing Δ_z had very little effect on ρ_z at temperatures below 100K. Above 100K, ρ_z is seen to increase with increasing Δ_z but in smaller amounts. Also, increasing the chiral angle, θ_h resulted in a decrease of the resistivity, ρ_z, of the chiral CNT as observed in Figure (33).

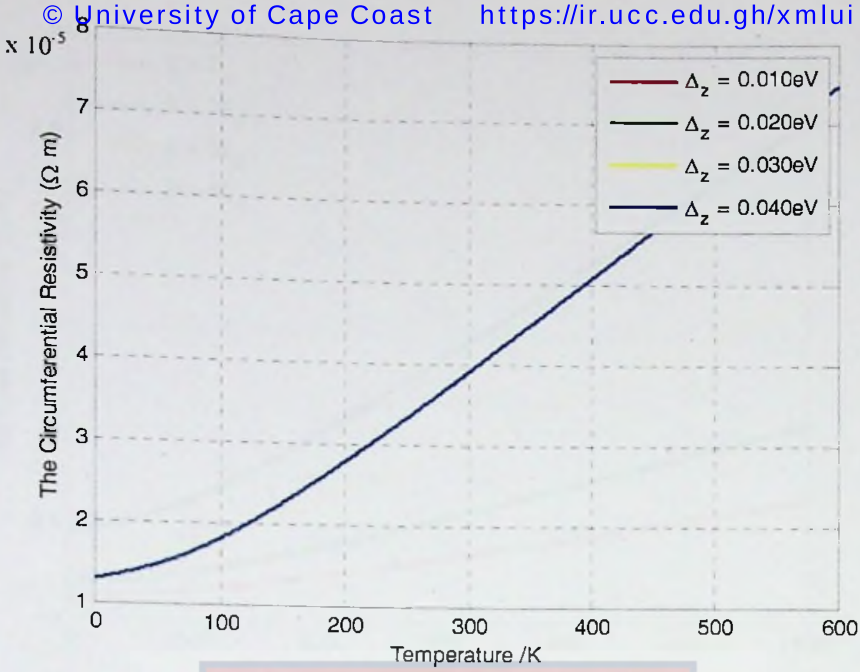


Figure 28: The dependence of ρ_c on temperature for various fixed values of Δ_z. Δ_s= 0.018eV, E_s =5.0 × 10^7V/m, E = $2E_o$, where E_o =6.9063 × 10^7V/m.

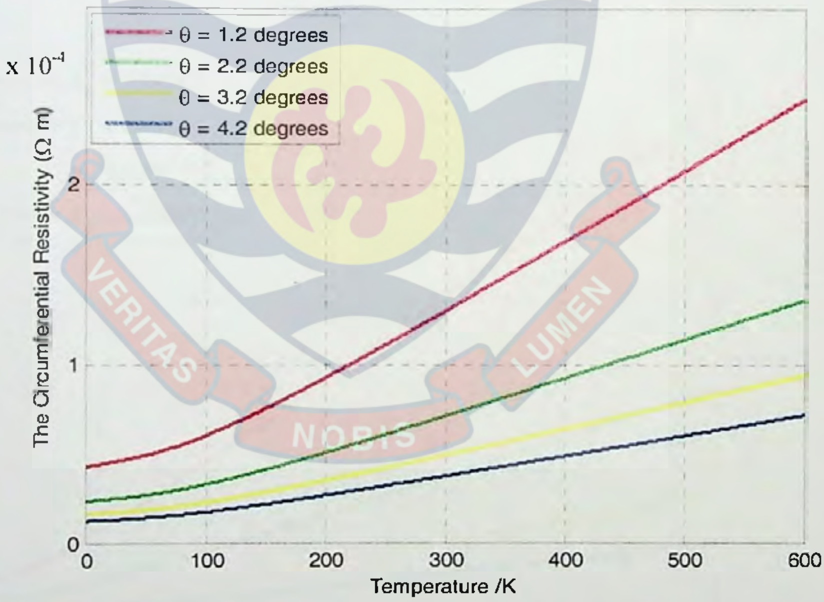


Figure 29: The dependence of ρ_c on temperature for various fixed values of chiral angle, θ_h. Δ_z =0.024eV, Δ_s = 0.018eV, E_s =5.0 × 10^7V/m, E = $2E_o$, where E_o =6.9063 × 10^7V/m.

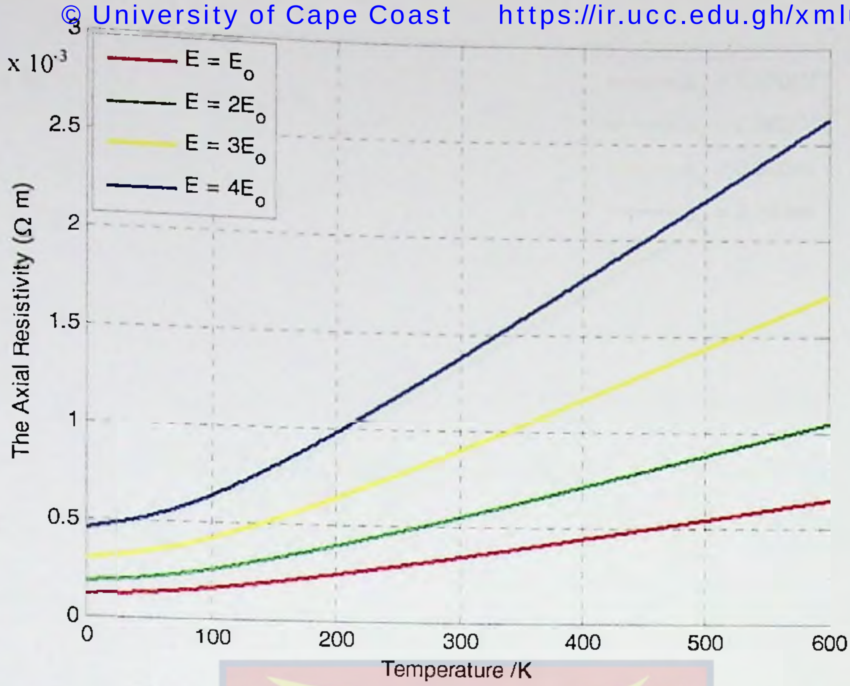


Figure 30: The dependence of ρ_z on temperature for various fixed values of the electric field $E = E_o$, $2E_o$, $3E_o$ and $4E_o$, where $E_o = 6.9063 \times 107V/m$. $E_s = 5.0 \times 107V/m$, $\Delta_s = 0.018eV$ and $\Delta_z = 0.024eV$.

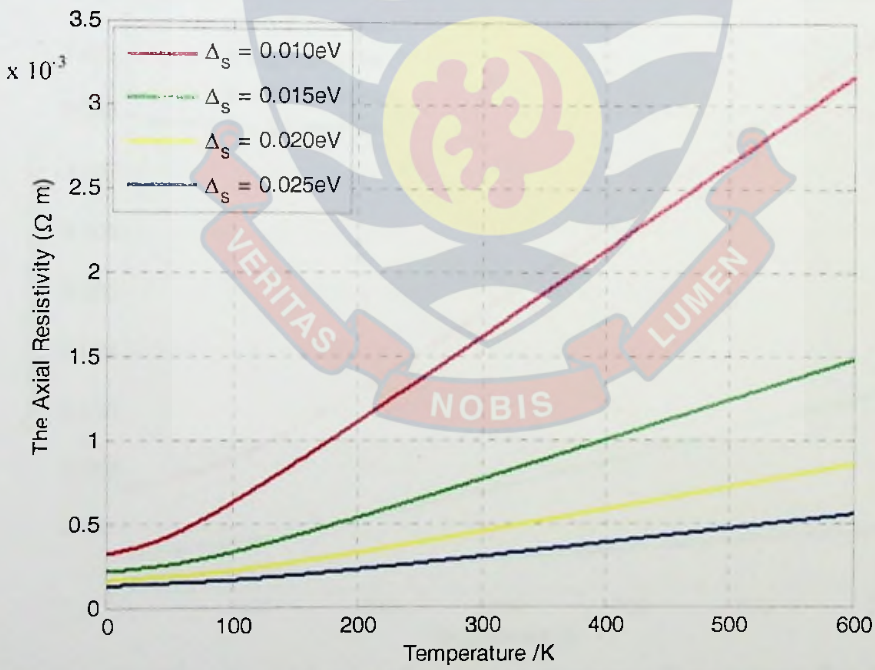


Figure 31: The dependence of ρ_z on temperature for various fixed values of Δ_s. $\Delta_z = 0.024eV$, $E_s = 5.0 \times 10^7 V/m$, $E = 2E_o$, where $E_o = 6.9063 \times 10^7 V/m$.

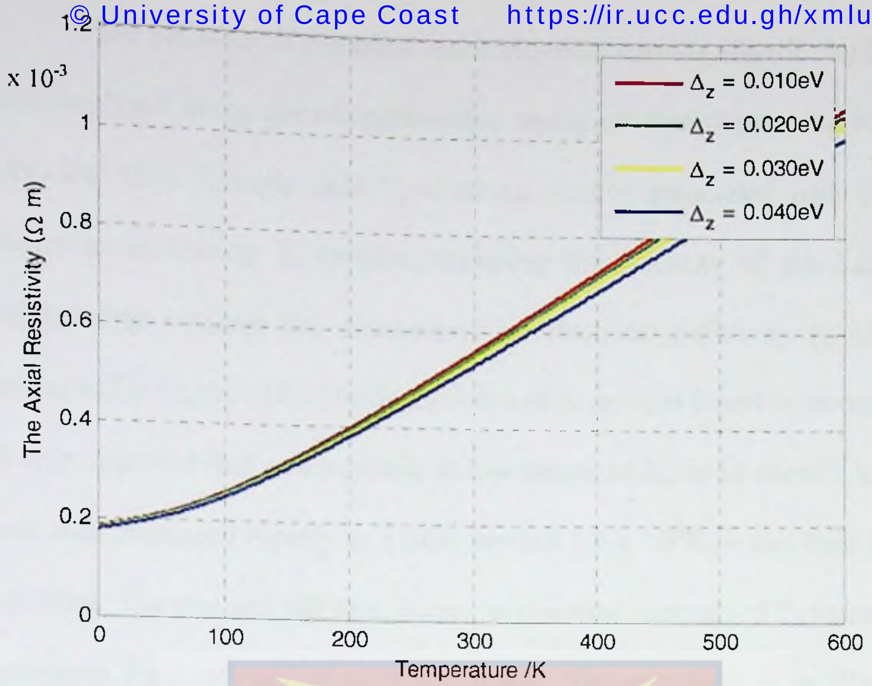


Figure 32: The dependence of ρ_z on temperature for various fixed values of Δ_z. Δ_s =0.018eV, E_s =5.0 × 10^7V/m, E =2E_o, where E_o =6.9063 × 10^7V/m.

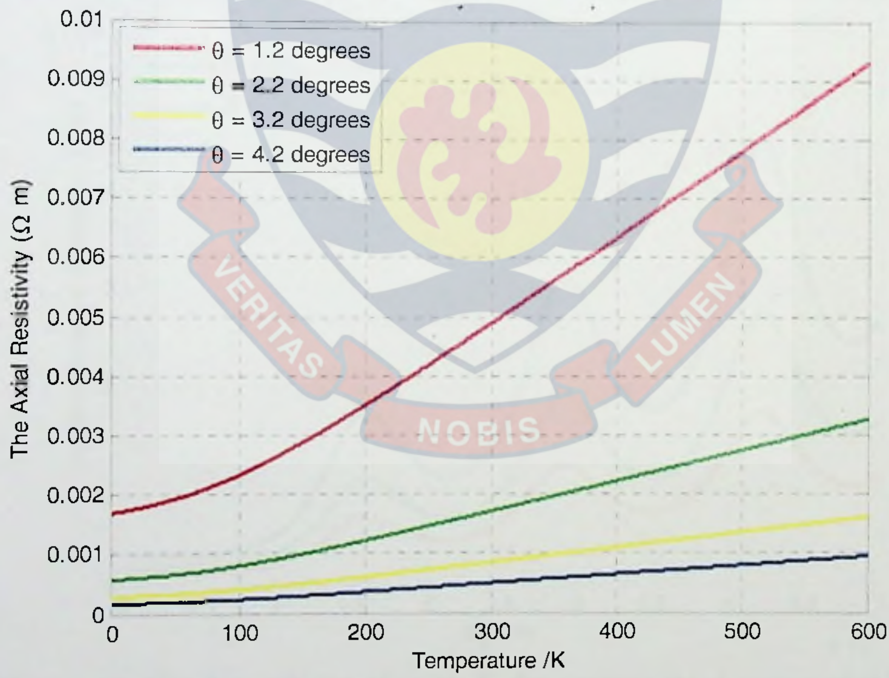


Figure 33:. The dependence of ρ_z on temperature for various fixed values of chiral angle, θ_h. Δ_z =0.024eV, Δ_s = 0.018eV, E_s =5.0 × 10^7V/m, E = 2E_o, where E_o =6.9063 × 10^7V/m.

The behavior of electrical resistivity with varying electric field E_s were also analysed along the circumferential and axial directions using Equations (49) and (50). Electric field E_s is an a.c. source associated with the Laser therefore increasing E_s implies increasing the intensity of the Laser. The relationship between the circumferential electrical resistivity ρ_c and E_s is presented in Figure (34). The dependence of ρ_c on E_s is found to be oscillatory. It was observed that ρ_c was linear at low values of E_s up to about 1 x 10^8V/m and then increased rapidly to a peak around 1.6 x 10^8V/m and then began to oscillate. The rise and fall of ρ_c occurs at constant intervals of E_s values. As E_s increases the amplitude of ρ_c also increases. The amplitude of oscillation was also found to increase with E_o but the frequency remain unchanged.

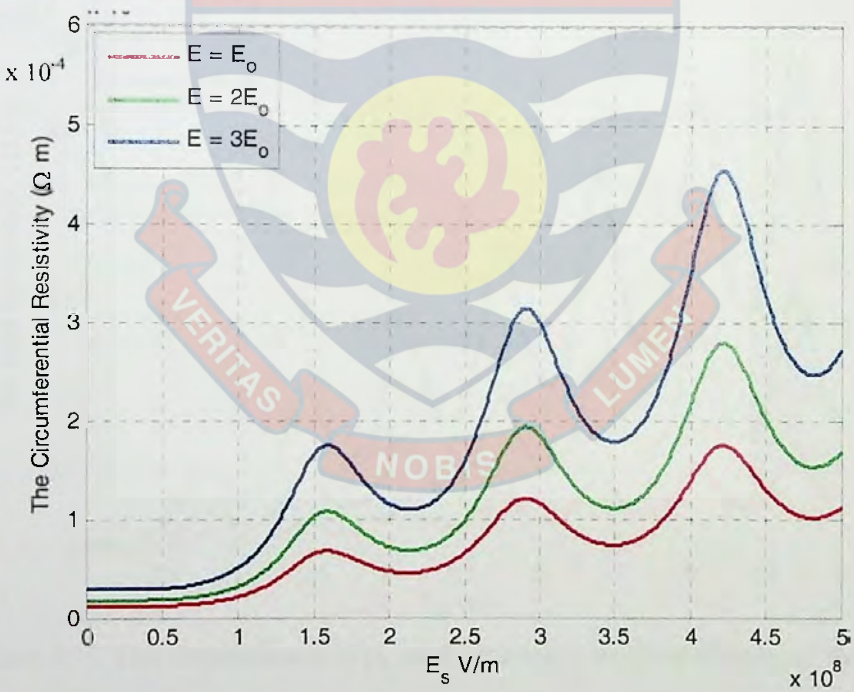


Figure 34: The dependence of ρc on E_s for various fixed values of the electric field $E = E_o$, $2E_o$ and $3E_o$, where E_o =6.9063 × 107V/m, Δs = 0.018eV and Δ_z = 0.024eV.

A sketch of the relationship between the axial electrical resistivity ρ_z and E_s is presented in Figure (35). The dependence of ρ_z on E_s is also found to be oscillatory. It was observed that ρ_z changed slowly at low values of E_s up to about 0.5×10^8V/m and then increased rapidly to a peak around 0.75×10^8V/m. The rise and fall of ρ_c occurs at constant intervals of E_s values. As E_s increases the amplitude of ρ_z also increases. The amplitude of oscillation was also found to increase with E_o but the frequency remain unchanged.

It is quite interesting to note that the ratio $\rho_c/\rho_z \approx 17$ for the same values of E_s and E_o. On the other hand for the same E_s and E_o values the number of oscillations for ρ_z is much more greater than that of ρ_c.

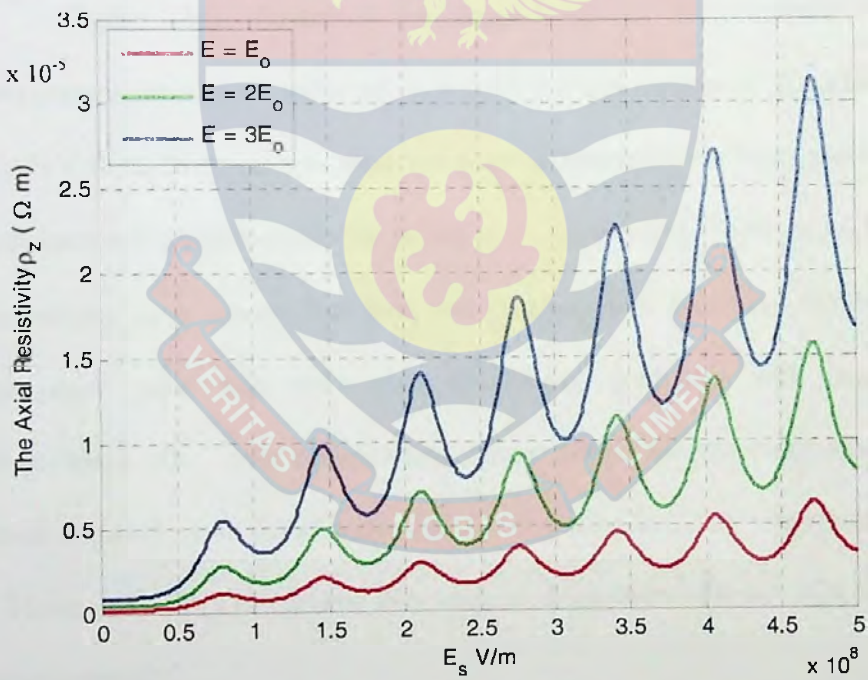


Figure 35:. The dependence of ρ_z on E_s for various fixed values of the electric field $E = E_o$, $2E_o$ and $3E_o$, where $E_o = 6.9063 \times 10^7$V/m. $\Delta_s = 0.018$eV and $\Delta_z = 0.024$eV.

Thermopower

It can be seen from Equations (51) and (52) that the thermoelectric power of a chiral CNT is dependent on the electric fields E_s and E_o, temperature T, GCA θ_h, and the overlapping integrals Δ_s and Δ_z for jumps along the circumferential and axial directions. Generally, a typical GCA θ_h for a chiral SWCNT is small, so $\sin^2\theta_h \cong 0$ (in Equation (52)). Therefore Equation (52) which defines the axial thermopower α_{zz} becomes approximately equal to Equation (51) which defines the circumferential thermopower α_{cz}. This makes the dependence of α_{zz} and α_{cz} on E_s, E_o , T, Δ_s and Δ_z for a chiral SWCNT to be similar. Based on this reason, only Equation (52) for axial thermopower α_{zz} will be sketched and analysed.

Figure (36) illustrates the dependence of thermopower α_{zz} on temperature for a fixed value of Δ_z = 0.015eV and values of Δ_s varied from 0.015eV to 0.025eV. It was observed that the thermopower decreases rapidly with increasing temperature for values of Δ_s between 0.015eV and 0.018eV. For values of Δ_s above 0.018eV, the thermopower increases rapidly to a maximum value and then start decreasing gradually with increasing temperature. At high temperatures above 500K, thermopower assumes a lower constant value for all values of Δ_s. A similar behavior was observed by J. Hone et al. in [130], where they measured the thermopower of a SWCNT experimentally.

The hyperbolic curves obtained in Figure (36) are similar to the characteristic thermopower behaviour expected for semiconducting CNTs [131]. Therefore under these conditions, the chiral CNT behaves as a semimetal. The fact that thermopower values in Figure (36) are positive over the entire range of temperature indicates that the contribution from positive (hole) carriers dominates the response.

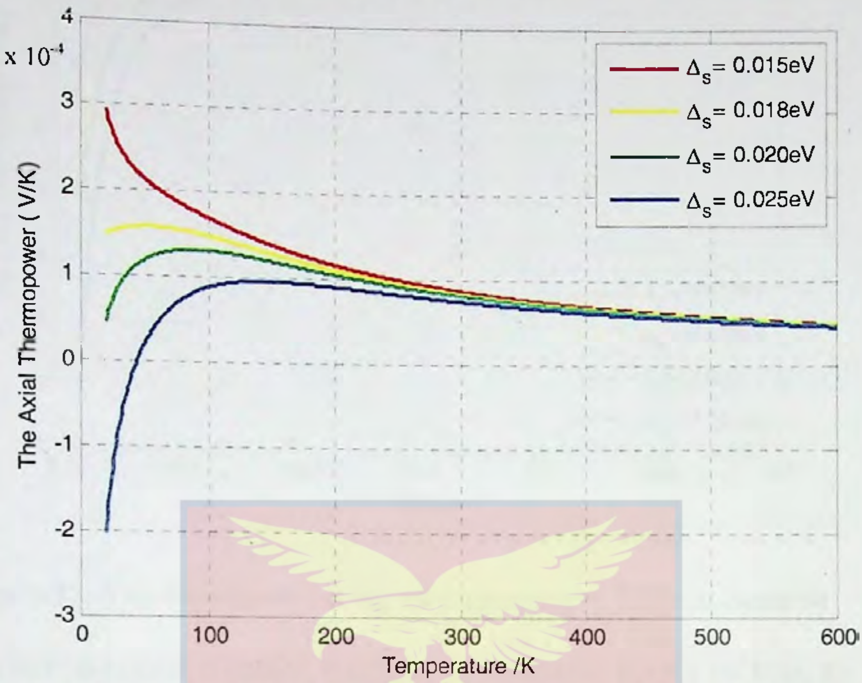


Figure 36: The dependence of α_{zz} on temperature T for Δ_s equal to 0.015eV, 0.018eV, 0.020eV, 0.025eV, Δ_z =0.015eV, E_s =5 x 10^7V/m, E= $2E_0$.

The dependence of thermopower on temperature is sketched for fixed values of Δ_z = 0.024eV, 0.027eV and 0.041eV as Figures (37), (38) and (39) respectively. In all cases, Δ_s is varied from 0.015eV to 0.025eV.

In Figures (37) and (38), the thermopower was found to increase rapidly to a maximum value, then decreases slowly to a constant value as temperature rises. All the curves were observed to have turning points at different temperatures.

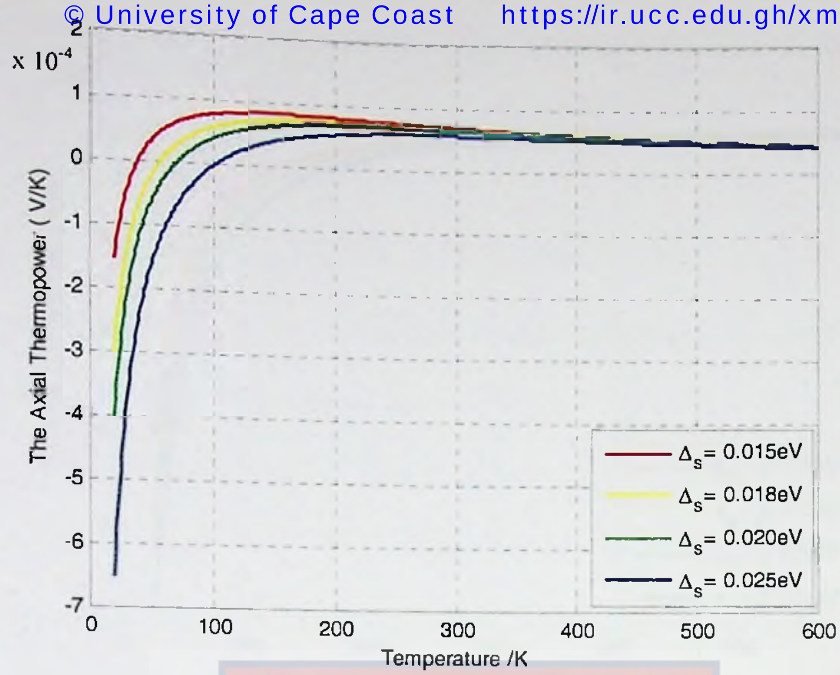


Figure 37: The dependence of α_{zz} on temperature T for Δ_s equal to 0.015eV, 0.018eV, 0.020eV, 0.025eV, Δ_z =0.024eV, E_s=5 x 10^7V/m, E= $2E_o$.

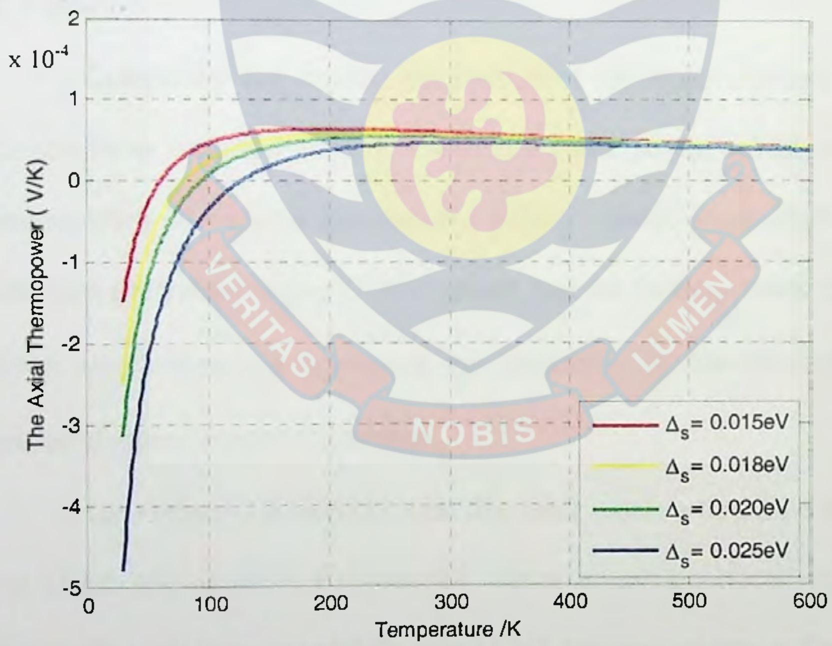


Figure 38: The dependence of α_{zz} on temperature T for Δ_s equal to 0.015eV, 0.018eV, 0.020eV, 0.025eV, Δ_z =0.027eV, E_s=5 x 10^7V/m, E= 2Eo.

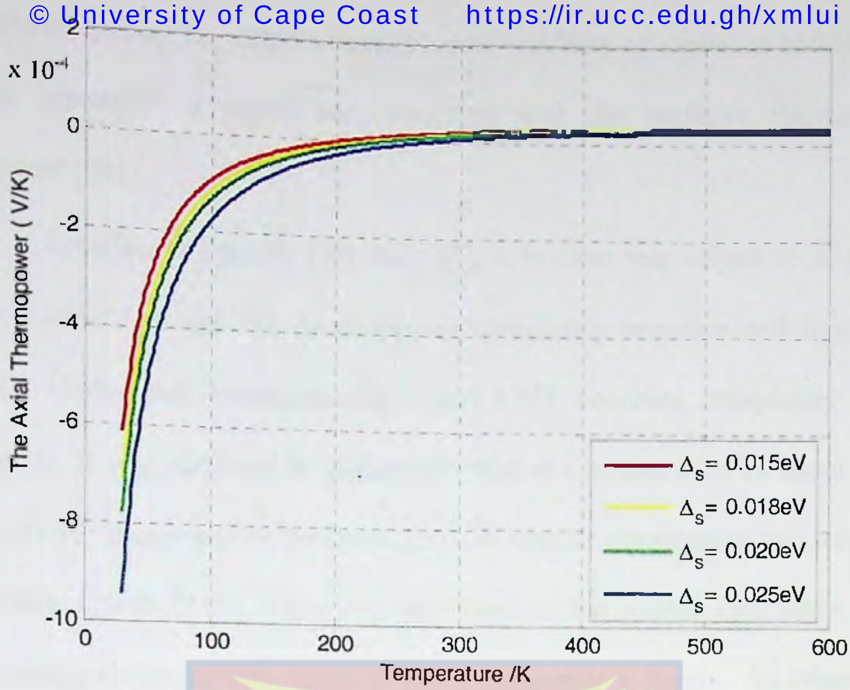


Figure 39: The dependence of α_{zz} on temperature T for Δ_s equal to 0.015eV, 0.018eV, 0.020eV, 0.025eV, Δ_z = 0.041eV, $E_s = 5 \times 10^7$V/m, $E = 2E_0$.

Comparing our results obtained with the experimentally measured thermopower in reference [36], it was noted that the theoretical curves agree reasonably well with the experimental values. Careful study of all the curves obtained (including Figure (39)) revealed that the turning points shift toward lower temperatures for a given Δ_z and increasing Δ_s, but they shift towards greater temperatures as Δ_z increases.

Interestingly, it came to light that there exists a threshold temperature for which hole conductivity switches over to electron conductivity. It means that positive thermopower of the chiral CNT becomes negative. The threshold value for the temperature shifts towards lower temperature as Δ_z is increased. This can be explained by the fact that graphite has a pair of weakly overlapping electron and hole sp^2 or π bands with near mirror symmetry about the Fermi energy E_F. Approximately equal numbers of electrons and holes in these symmetric π bands are consistent with the negative thermopower observed [36].

Looking at Figures (40) and (41), it is clear that values of Δ_z greater than 0.085eV render the thermopower completely negative and hyperbolic [131]. Under this condition, the chiral CNT becomes completely n-type material. It was observed in Figure (40) that at a temperature of about 600 K and above, thermopower becomes zero. A similar observation was made for armchair CNTs [130]. This was attributed to the mirror symmetry of the coexisting electrons and holes in the overlapping π bands. An observation made from Figure (41) shows that when Δ_z is greater than 0.25eV, increasing Δ_s does not affect the thermopower.

Analysis of the behavior of thermopower with varying E_s field was also considered at a fixed temperature of 300K in Figure (42). It is interesting to note that as E_s increases, the thermopower shows distinctive peaks. The dependence of thermopower on E_s was found to be oscillatory. It was observed that thermopower changed slowly at low values of E_s up to about 0.3 x 10^8V/m and then drops off rapidly to a minimum value around 0.75 x 10^8V/m. From this point, the thermopower increases rapidly then oscillate and drops off again. We noted that, this behavior of the thermopower repeats itself at regular intervals except that the drop off points rises as the E_s increases. Furthermore, thermopower was found to decrease as E_o increases.

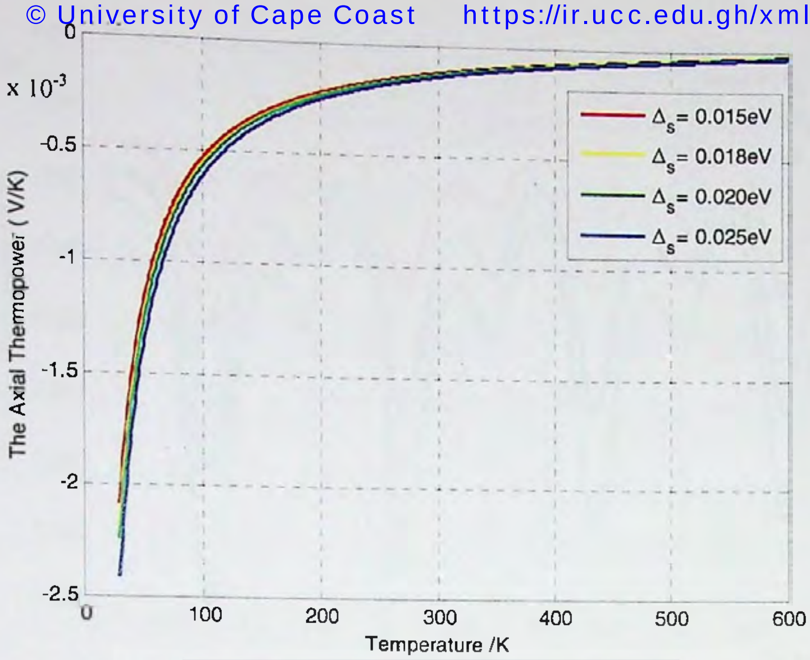


Figure 40: The dependence of α_{zz} on temperature T for Δ_s equal to 0.015eV, 0.018eV, 0.020eV, 0.025eV, Δ_z =0.085eV, E_s =5 x 10^7V/m, E= $2E_o$.

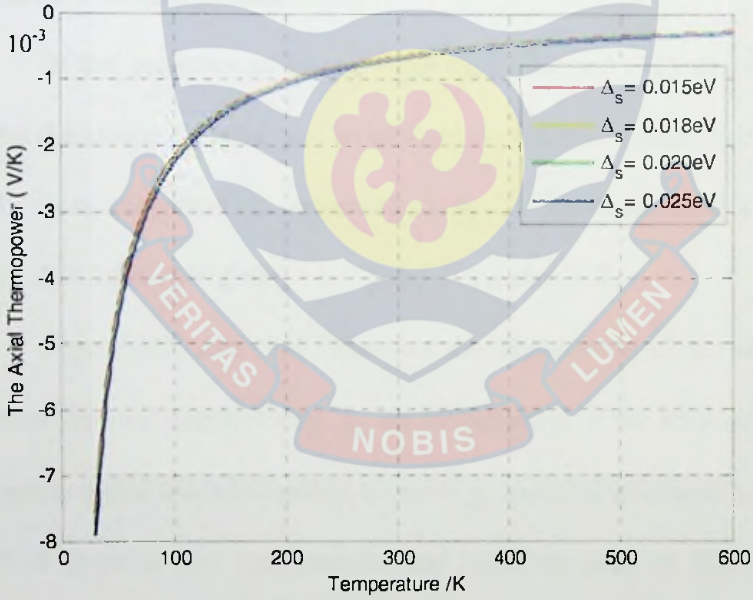


Figure 41: The dependence of α_{zz} on temperature T for Δ_s equal to 0.015eV, 0.018eV, 0.020eV, 0.025eV, Δ_z = 0.25eV, E_s =5 x 10^7V/m, E = $2E_o$.

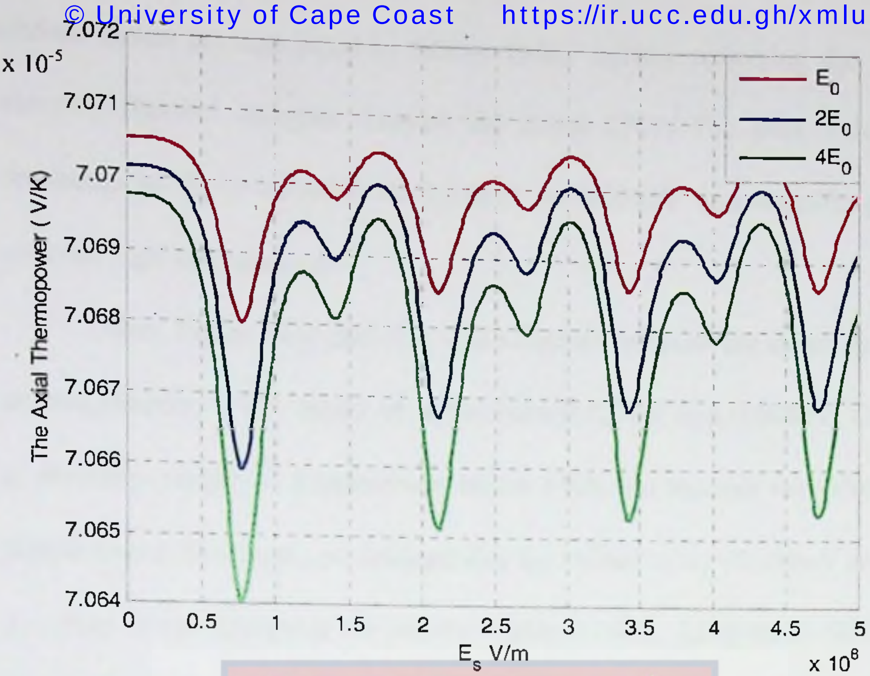


Figure 42: The dependence of α_{zz} on E_s for temperature T = 300K for E = E_0, $2E_0$ and $4E_0$, where $E_0 = 6.9063 \times 10^7$V/m $\Delta_s = 0.018$eV, $\Delta_z = 0.024$eV,

Electron Thermal Conductivity

In the presence of Laser, Equations (70) and (71) which respectively define the circumferential and axial electron thermal conductivities of a chiral CNT, were subjected to numerical analysis. We considered a SWCNT for which d_s = 1nm, d_z = 2 nm, $\tau = 0.3\times10^{-11}$ s and $\theta_h = 4°$.

Figure (43) and (44) illustrates the dependence of the circumferential electron thermal conductivity, χ_c, on temperature, T for various values of Δ_z. We noticed that the relationship between χ_c and T is nonlinear and indicates a positive slope at low temperatures and negative slope at high temperatures. The physical interpretation to the part of the graph showing positive slope is that more electrons are thermally generated to transport heat through the chiral CNT. The peak of the graph indicates the threshold temperature at which electron and heat transport through the chiral CNT is maximum. The negative slope of the graph shows that as temperature exceeds the threshold value, carbon atoms are energized to vibrate faster thereby scattering the electrons carrying thermal energies through the chiral CNT. The peak values of χ_c decreases as Δ_z is varied from 0.010eV to 0.026eV and it shifts gradually towards high temperatures.

Also, Figure (45) and (46) was sketched to show the dependence of χ_c on temperature, T for values of Δ_z between 0.027eV and 0.048eV. Generally, χ_c decreases rapidly at temperatures below 150K but become very slow at high temperatures. However, we realized that for values of Δ_z =0.036eV and above, χ_c values do not change at temperatures above 200K. Analysis to find out how GCA θ_h affects χ_c was also considered. In Figures (47) to (50), χ_c against temperature T was studied for GCA θ_h varied between 0.2° and 4.0°. It was noted that χ_c increases with increasing GCA θ_h at low temperatures and peaks at 75K.

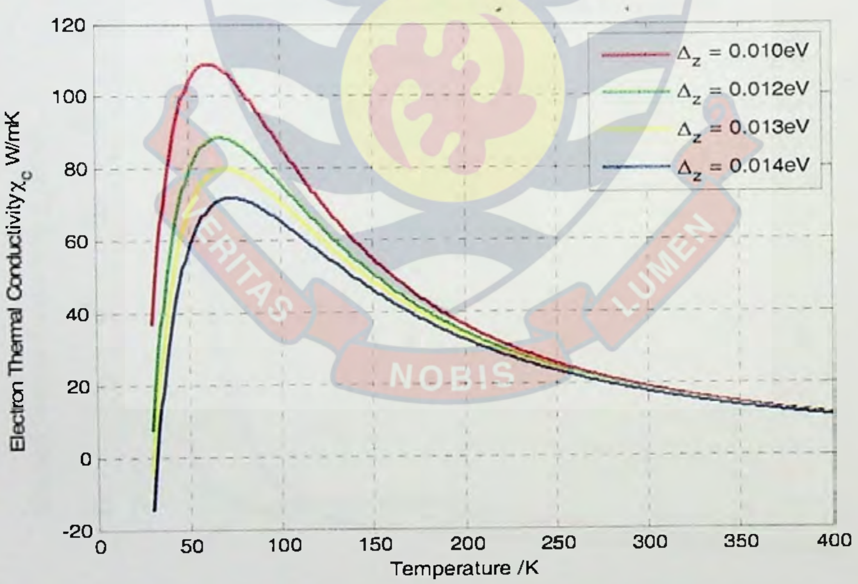


Figure 43: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $E_s = 1.5 \times 10^7$V/m and Δ_z varied from 0.010 to 0.014eV.

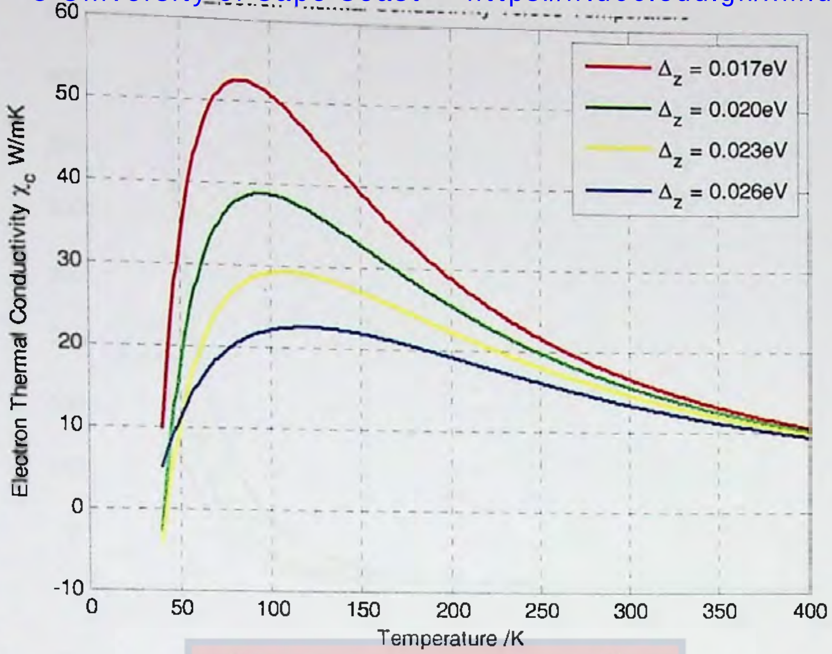


Figure 44: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $E_s = 1.5 \times 10^7$V/m and Δ_z varied from 0.017 to 0.026eV.

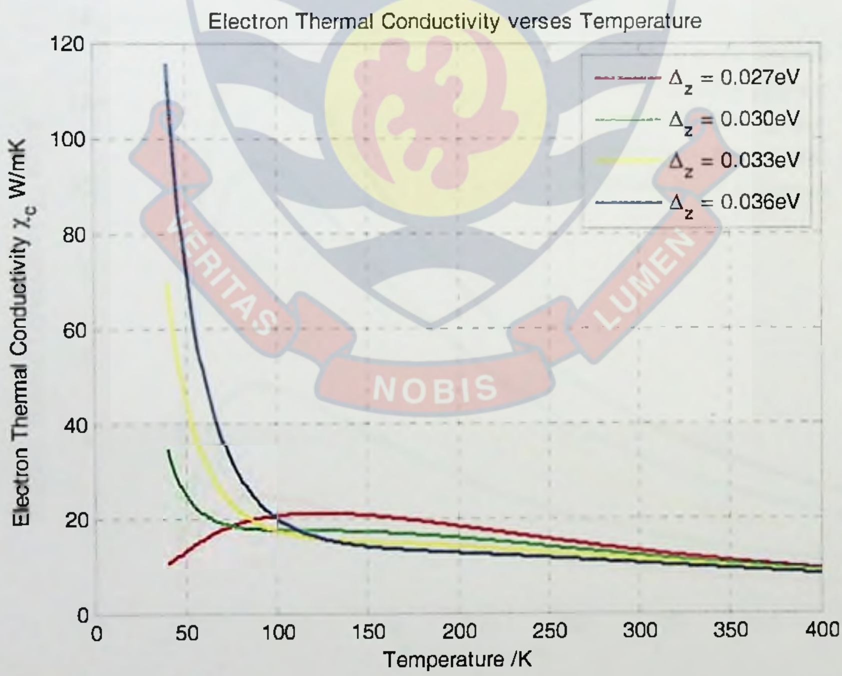


Figure 45: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $E_s = 1.5 \times 10^7$V/m and Δ_z varied from 0.027 to 0.036eV.

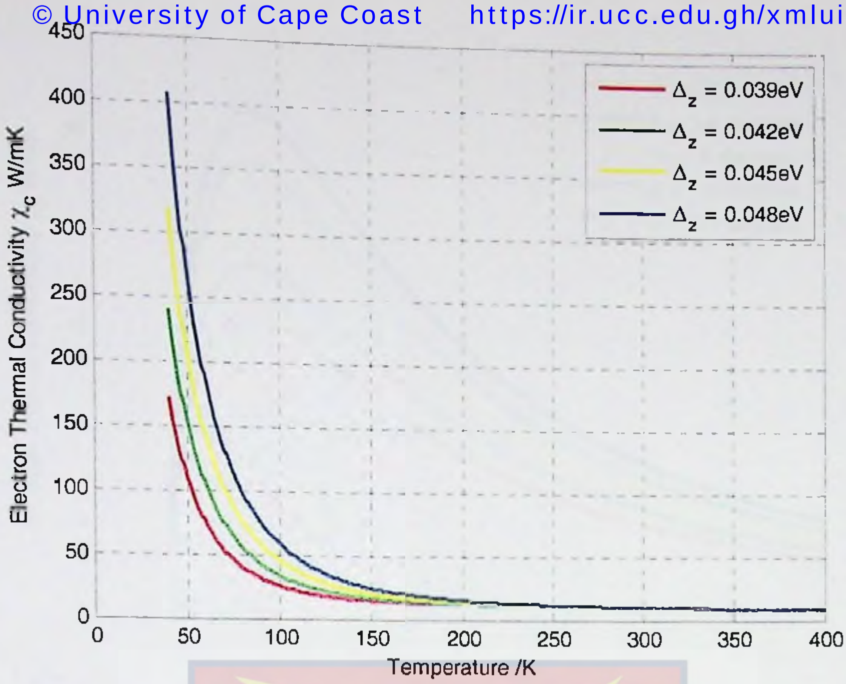


Figure 46: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $E_s = 1.5 \times 10^7$V/m and Δ_z varied from 0.039 to 0.048eV.

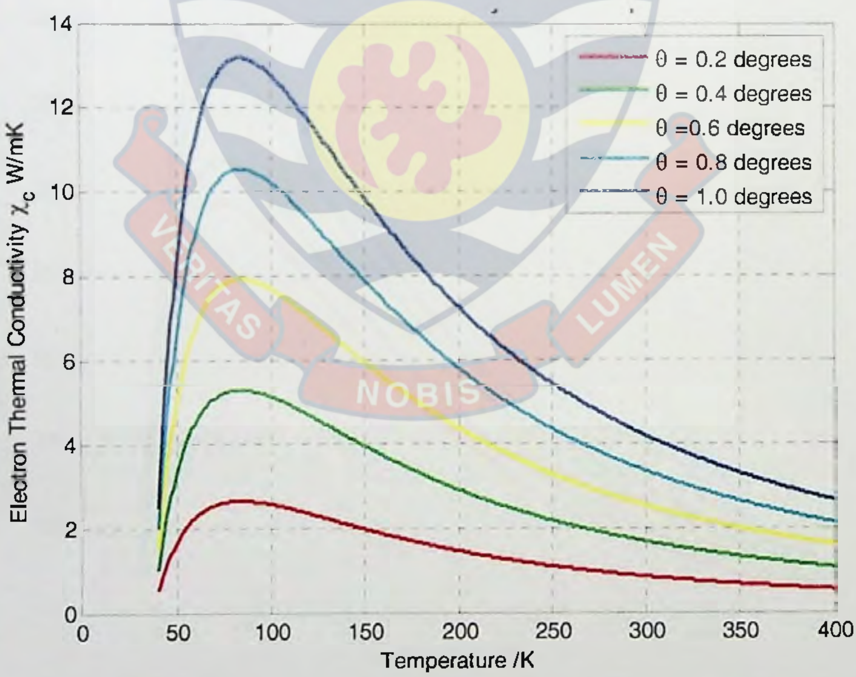


Figure 47: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $\Delta_z = 0.017$eV,. $E_s = 1.5 \times 10^7$V/m and GCA θ_h varied from 0.2^o to 1.0^o.

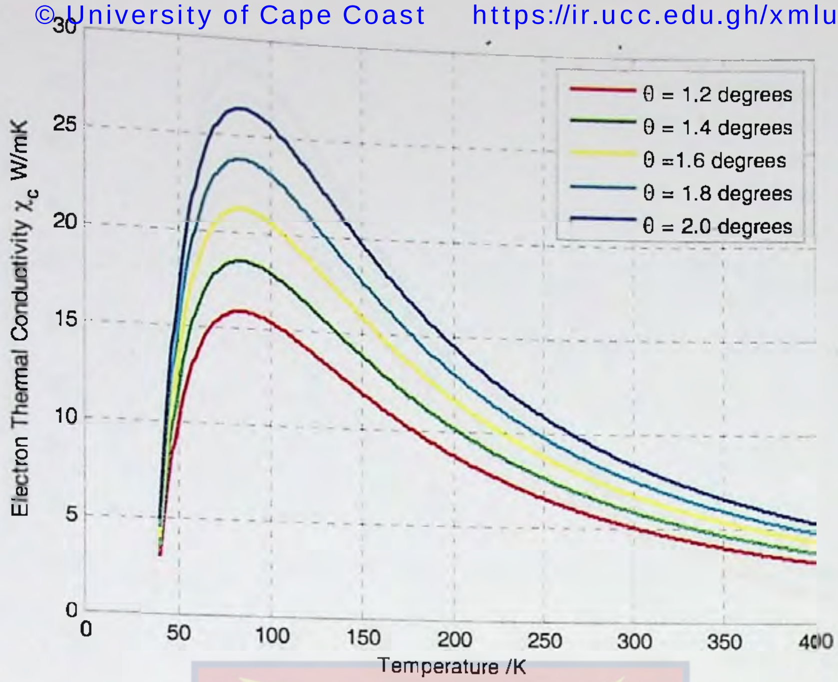


Figure 48: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $\Delta_z = 0.017$eV,. $E_s = 1.5 \times 10^7$V/m and GCA θ_h varied from 1.2^o to 2.0^o.

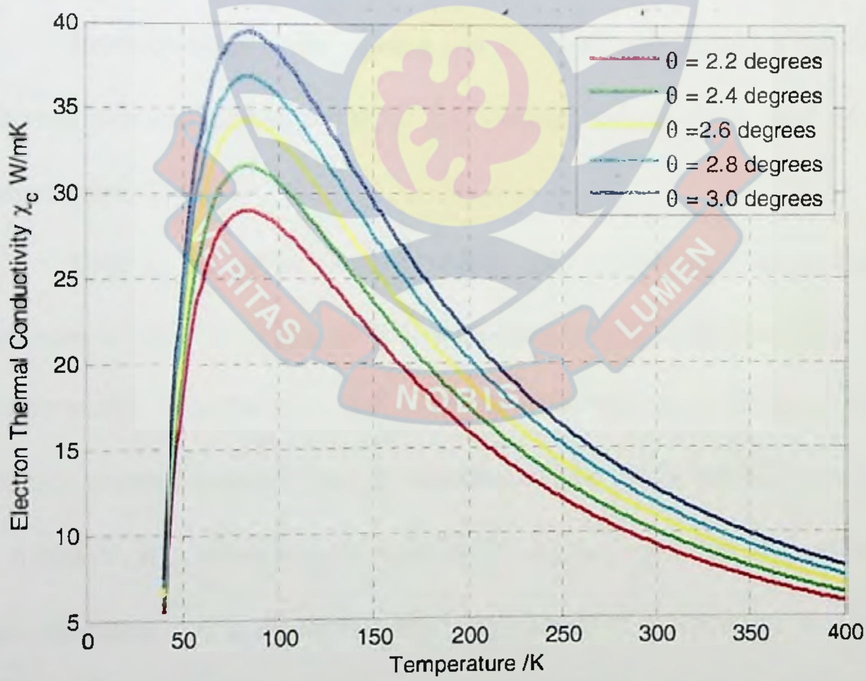


Figure 49: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $\Delta_z = 0.017$eV,. $E_s = 1.5 \times 10^7$V/m and GCA θ_h varied from 2.2^o to 3.0^o.

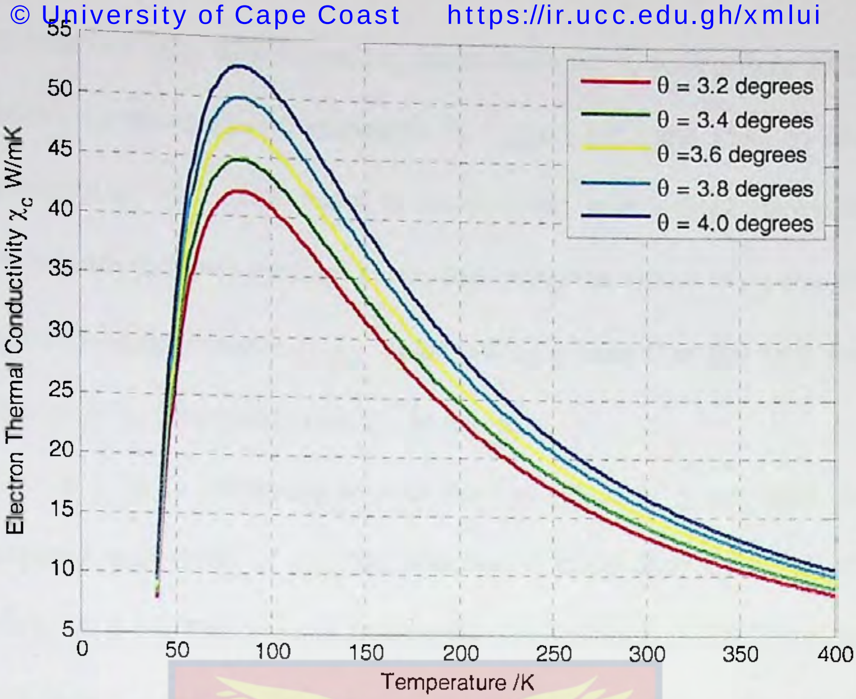


Figure 50: The dependence of χ_c on temperature T for $\Delta_s = 0.010$eV, $\Delta_z =$ 0.017eV,. $E_s = 1.5 \times 10^7$V/m and GCA θ_h varied from 3.2° to 4.0°.

Investigations were carried out to study the behavior of the axial electron thermal conductivity, χ_z for various values of Δ_z and increasing temperature, T.

Like χ_c, the relationship between χ_z and T is found to be nonlinear and indicates a positive slope at low temperatures and negative slope at high temperatures. Figures (51) and (52) illustrate the dependence of the axial electron thermal conductivity, χ_z, on temperature for Δ_z varied from 0.010eV to 0.026eV. It is interesting to note that as Δ_z increases, the peak values of χ_z also increases and it shifts towards large values of temperature T. However, when $\Delta_z = 0.026$eV, χ_z decreases rapidly at low temperatures up to about 80K where it turns and then conforms to the patterns shown for low values of Δ_z.

The behavior of χ_z with increasing temperature for Δ_z varied from 0.027eV to 0.048eV is sketched and presented as Figures (53) and (54). χ_z decreases exponentially with an increase in temperature, and at high temperatures it slowly tends to lower constant value. Increasing the values of Δ_z also provides a corresponding increase in χ_z. Values of Δ_z greater than 0.030eV make the behavior of χ_z to appear hyperbolic in nature.

It is quite interesting to note that the values of χ_z are much larger as compared with those of χ_c. This assertion is made clear by considering the ratio $\chi_z / \chi_c \approx 33$. This is quite substantial. The values $\chi_c = 110$ W/mK and $\chi_z = 3600$ W/mK used for the calculation are the peak values for which $\Delta_z = 0.010$eV in both cases.

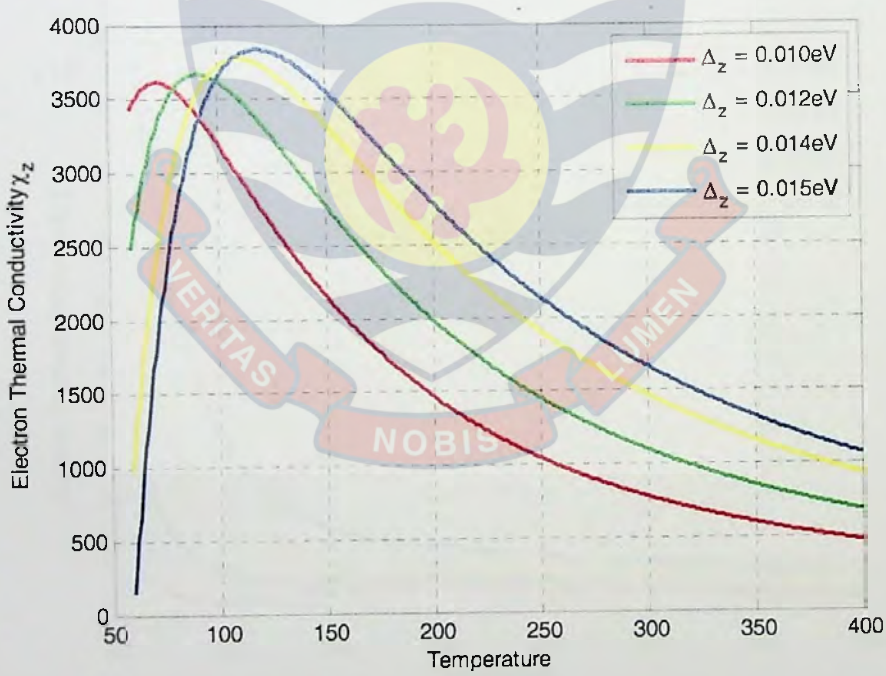


Figure 51: The dependence of χ_z on temperature T for $\Delta_s = 0.010$eV, $E_s = 1.5 \times 10^7$V/m and Δ_z varied from 0.010 to 0.015eV.

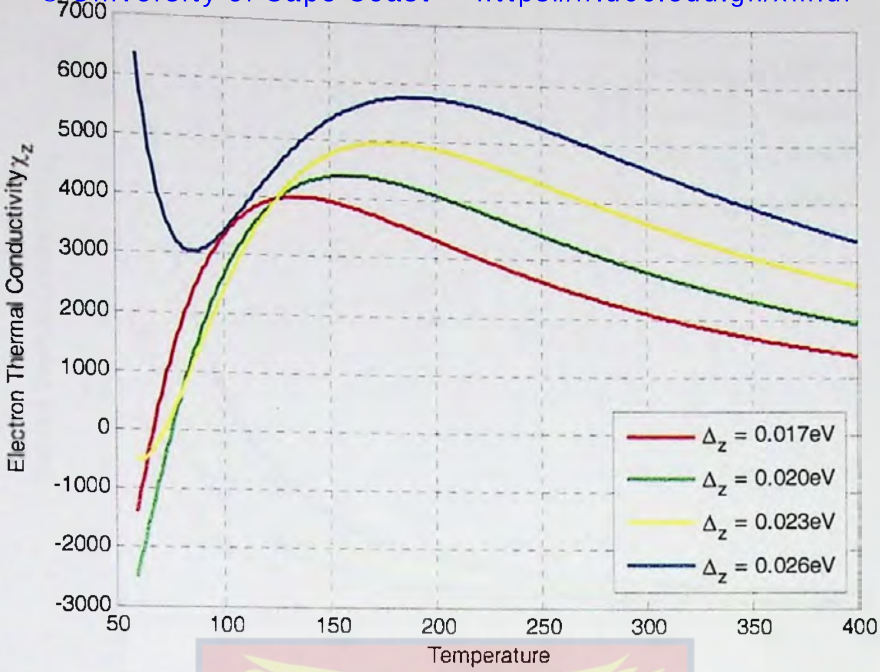


Figure 52: The dependence of χ_z on temperature T for $\Delta_s = 0.010eV$, $E_s = 1.5 \times 10^7 V/m$ and Δ_z varied from 0.017 to 0.026eV.

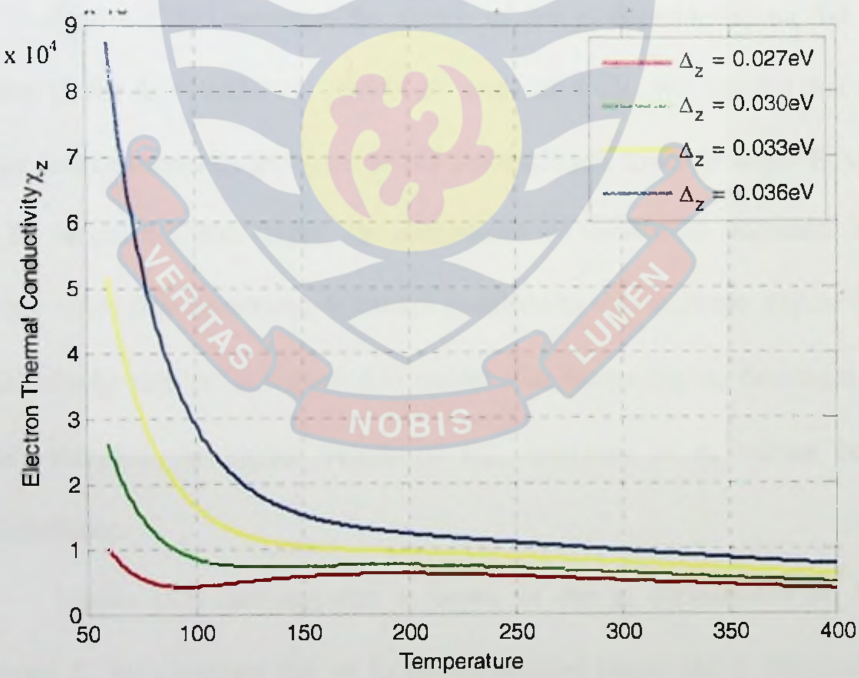


Figure 53: The dependence of χ_z on temperature T for $\Delta_s = 0.010eV$, $E_s = 1.5 \times 10^7 V/m$ and Δ_z varied from 0.027 to 0.036eV.

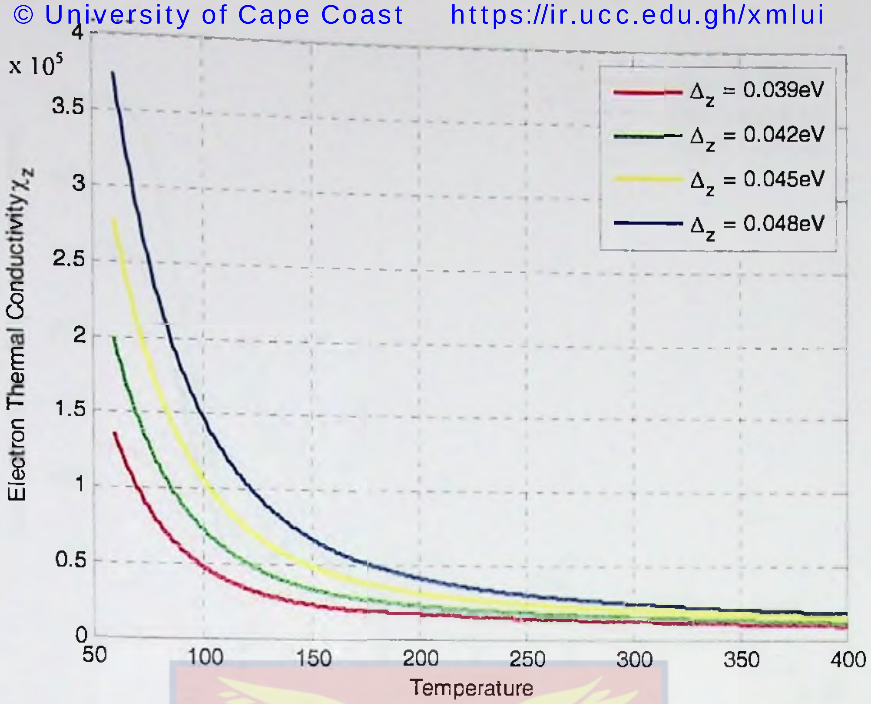


Figure 54: The dependence of χ_z on temperature T for $\Delta_s = 0.010$eV, $E_s = 1.5 \times 10^7$V/m and Δ_z varied from 0.039 to 0.048eV,.

Figure (55) illustrates the sketch of the χ_c dependence on the Laser source E_s for $\Delta_z = 0.010$ eV , 0.015 eV and 0.018 eV. We noticed that as the Laser source increases the χ_c drops off and oscillates towards larger E_s values. As E_s values become larger, the amplitudes of oscillation decrease. It was further noted that increasing Δ_s causes χ_c values to also increase. Figure (56) is qualitatively similar to Figure (55) except that increasing Δ_z decreases χ_c by small margins. At higher values of E_s, variations in Δ_z values become insignificant.

Figure (57) demonstrates a sketch of the χ_z dependence on E_s for varying Δ_z we observed that as E_s values become larger, the χ_z drops off and then oscillates. Like Figure (55), the amplitude of oscillation decreases towards larger values of E_s. Also, increasing Δ_z raises χ_z values too.

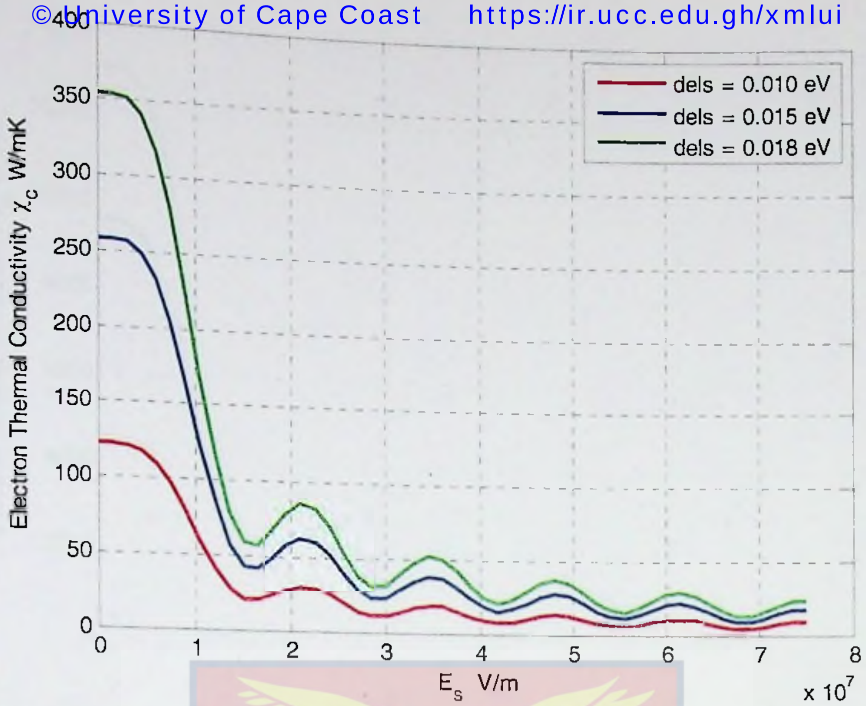


Figure 55: The dependence of χ_c on E_s at temperature T = 300K for Δ_z = 0.010eV, and Δ_s varied from 0.010 to 0.018eV.

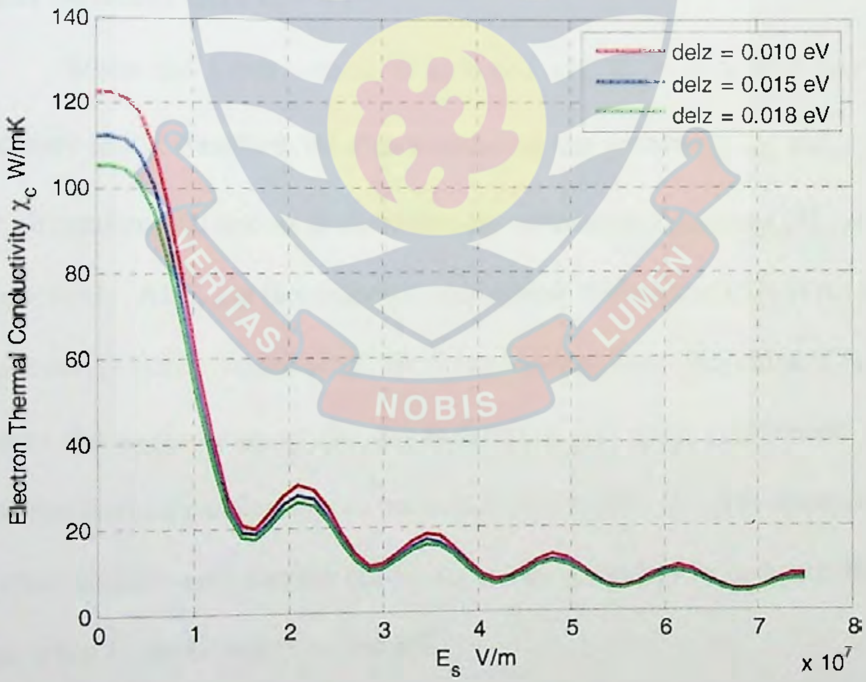


Figure 56: The dependence of χ_c on E_s at temperature T = 300K for Δ_s = 0.010eV and Δ_z varied from 0.010 to 0.018eV

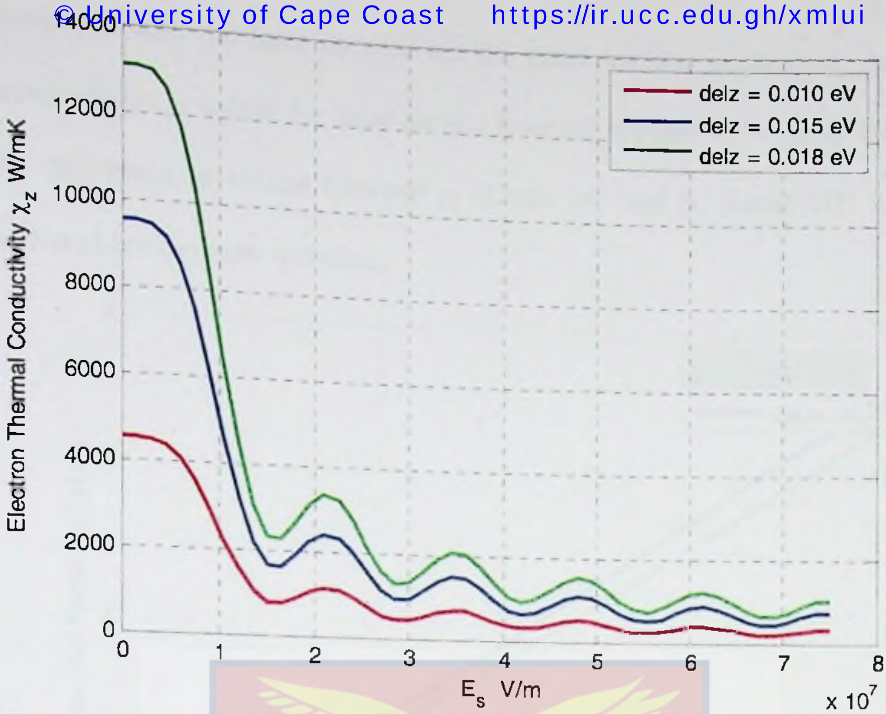


Figure 57: The dependence of χ_z on E_s at temperature T = 300K for $\Delta_s = 0.010$eV, and Δ_z varied from 0.010 to 0.018eV

Laser Switched Off ($E_s = 0$)

When the Laser source is switched off, $E_s = 0$, a = 0 and $J_n^2(a)$ becomes unity, therefore the expressions for the resistivity ρ_{cz} and ρ_{zz} along the circumferential and axial directions are reduced to Equations (91) and (92) respectively. Also, the thermopower expression in Equation (52) is reduced to Equation (93).The removal of the Laser source from the chiral CNT also causes the expressions of the circumferential and axial components of the electron thermal conductivity to become Equation (94) and (95) respectively. Further studies were carried out on ρ_c, ρ_z, α_z, χ_c and χ_z to compare for each case when Laser is switch on and off.

Figure (58) shows the behavior of the circumferential resistivity of the chiral CNT when Laser is switch on and also off. We noticed that when the laser source is switched off the values of ρ_c decrease in magnitude as compared with the laser on case but the trend remains unchanged. At lower temperatures ρ_c values for laser on and laser off appears to be close. However the difference in values between ρ_c (Laser on) and ρ_c (Laser off) tends to widen as temperature increases.

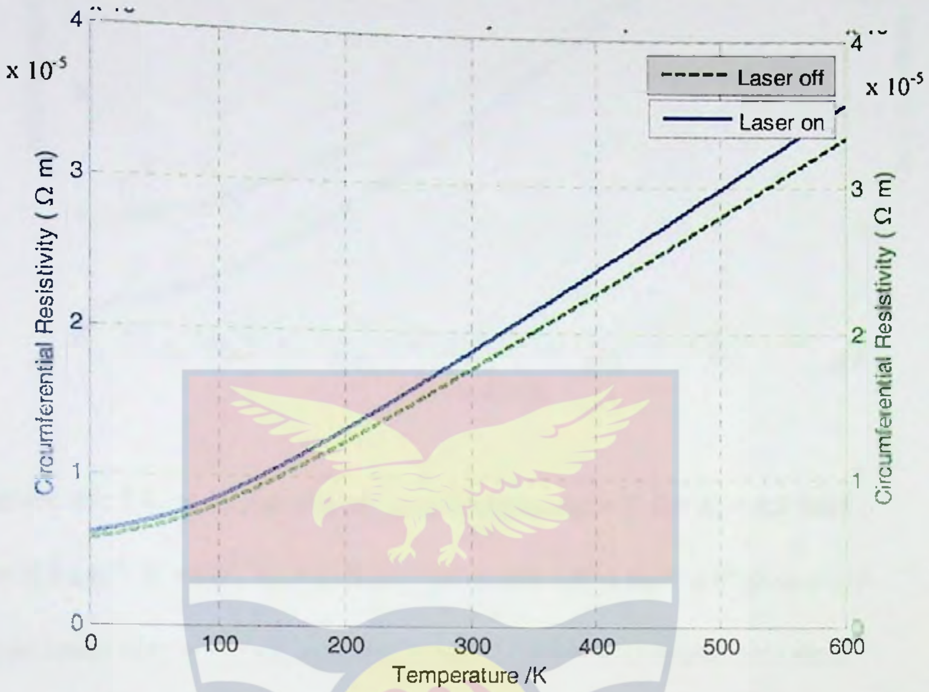


Figure 58: The dependence of ρ_c on temperature T for $\Delta_s = 0.018$eV, $\Delta_z = 0.024$eV,E =2 E_o. E_s =1. 5 x 10^7V/m and GCA $\theta_h = 4.0^o$ [*Laser off- Right hand side ordinate axis, Laser on- Left hand side ordinate axis*]

Comparison was made for ρ_z when Laser is on and also off as shown in Figure (59). Like ρ_c, we noted that when the laser source is switched off the values of ρ_z decrease in magnitude as compared with the laser on case but the trend remains unchanged. Laser transfers much energy to the carbon atoms within the walls of the CNT and set them vibrating at large amplitudes which scatter more electrons. For this reason, ρ_c and ρ_z values rise when laser is switched on.

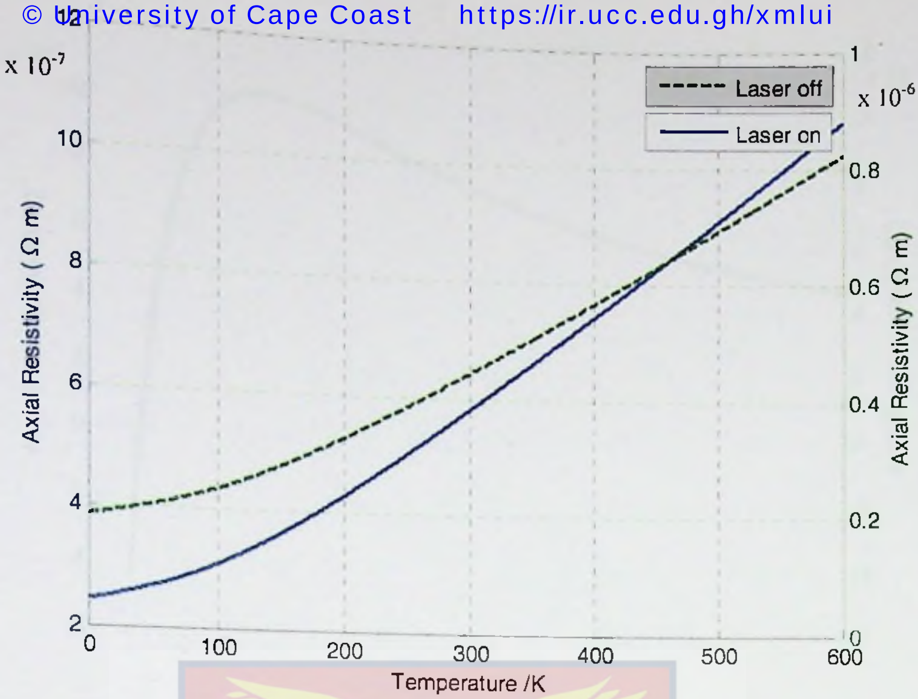


Figure 59: The dependence of ρ_z on temperature T for Δ_s = 0.018eV, Δ_z = 0.024eV,E =2 E_o. E_s =1. 5 x 10^7V/m and GCA θ_h = 4.0° [*Laser off- Right hand side ordinate axis, Laser on- Left hand side ordinate axis*]

The axial thermopower dependence on temperature in the presence and also absence of Laser was sketched and presented in Figure (60). In both cases, the thermopower was observed to exhibit the same characteristics of increasing rapidly to a maximum value and then start decreasing with increasing temperature. The overlapping of the two graphs show that there was no significant difference between the α_z (Laser off) and α_z (Laser on) . This results show that the laser source used have no effect on the thermopower values of the chiral CNT.

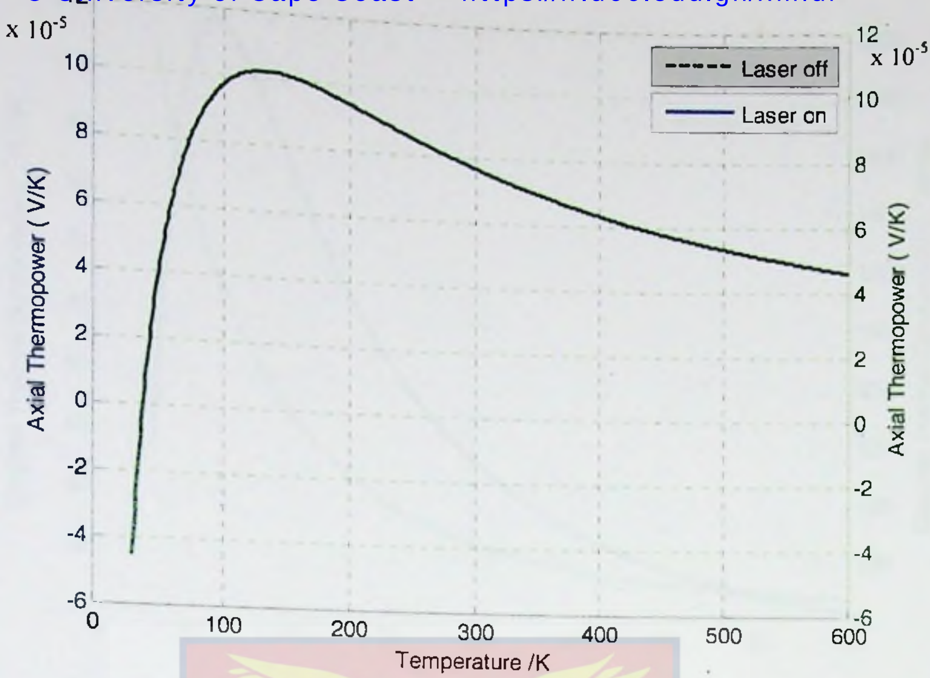


Figure 60: The dependence of α_z on temperature T for $\Delta_s = 0.018$eV,$\Delta_z = 0.024$eV,E =2 E_0. E_s =1. 5 x 10^7V/m and GCA $\theta_h = 4.0^o$ [*Laser off-Right hand side ordinate axis, Laser on- Left hand side ordinate axis*]

Figure (61) illustrates the behavior of the circumferential electron thermal conductivity, χ_c, of a chiral CNT when it is induced by Laser and also in the absence of Laser. In the presence of Laser, χ_c increases rapidly to a maximum value (≈109W/mK) and then start decreasing with increasing temperature. On the other hand when the Laser is switched off, χ_c decreases exponentially with increasing temperature. At temperatures below 70K the characteristic behavior of χ_c when Laser is induced in the chiral CNT becomes opposite to the case when Laser is switched off. We noticed that the χ_c values when Laser is absent are quite larger than the case when Laser is switched on.

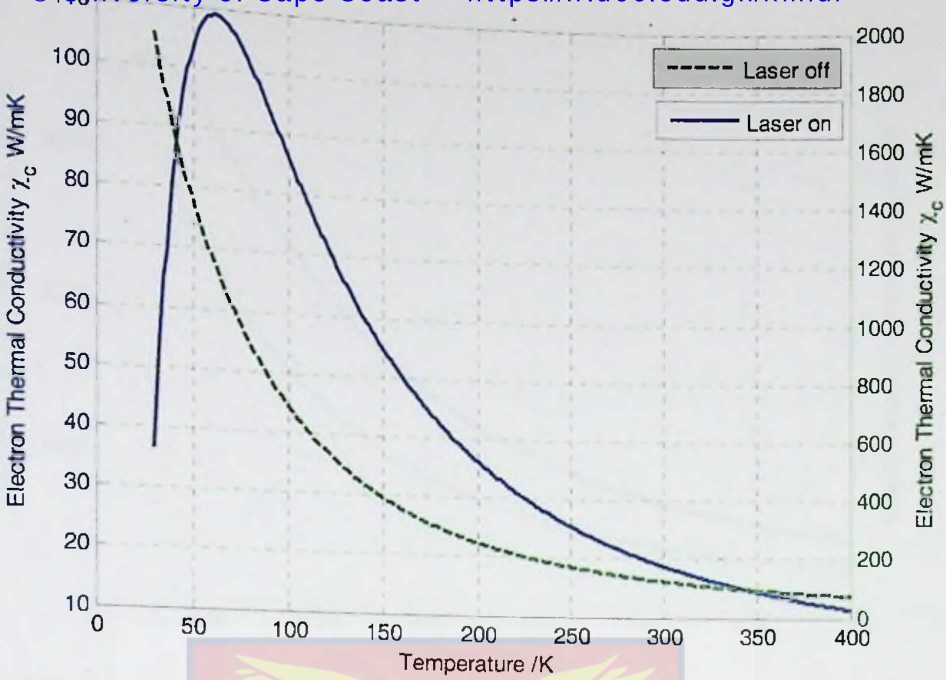


Figure 61: The dependence of χ_c on temperature T for $\Delta_s = 0.018$eV, $\Delta_z = 0.024$eV, $E_s = 1.5 \times 10^7$V/m and GCA $\theta_h = 4.0^o$ [*Laser off-Right hand side ordinate axis, Laser on- Left hand side ordinate axis*]

The behavior of χ_z was also studied for both cases when Laser was switched on and off as shown in Figure 62. When Laser is switched on, χ_z rises shortly to a turning point and then decrease exponentially with increasing temperature. On the other hand when Laser is absent, χ_z decreases exponentially with increasing temperature. The ratio χ_z (Laser off) to χ_z (Laser on) gave a value of 10; indicate that when Laser is switched off, χ_z values increases about ten times. The laser energizes the carbon atoms within the walls of the CNT and set them vibrating at large amplitudes which tend to scatter the electrons carrying thermal energy. For this reason, the presence of laser causes a reduction in χ_c and χ_z.

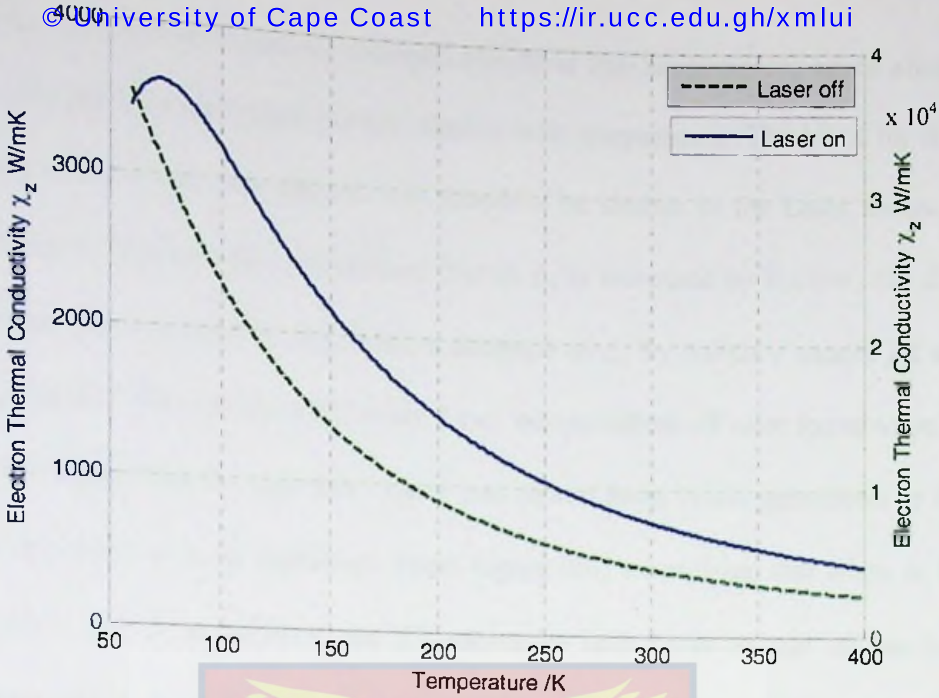


Figure 62: The dependence of χ_z on temperature T for $\Delta_s = 0.018$eV, $\Delta_z = 0.024$eV, E_s =1.5 x 107V/m and GCA $\theta_h = 4.0^o$ [*Laser off-Right hand side ordinate axis, Laser on- Left hand side ordinate axis*]

Thermoelectric Figure of Merit for Carbon Nano Tube (CNT)

In this section the thermoelectric figure of merit ZT was studied for both cases when Laser was switched on and off. The figure of merit expression used for our analysis is given by

$$ZT = \frac{\alpha^2 \sigma}{\chi} T \quad (96)$$

where α is the thermopower, $\sigma = \frac{1}{\rho}$ is the electrical conductivity and χ is the thermal conductivity of the chiral CNT. The value χ is the sum of the electron thermal conductivity and the lattice thermal conductivity of the chiral CNT. The relationship between the figure of merit ZT and temperature T is sketched for various fixed values of Δ_s and Δ_z. We observed in figures (63), (64), (65) and (66) that ZT changed slowly at low temperatures up to about 100K and then increased almost linearly with temperature. The trend for the case when Laser was present was found to be similar to the Laser absence situation. Interestingly, we noticed that as Δ_s is increased by 0.02eV, the ZT values also increase by 0.1. Also, a decrease in Δ_z by 0.002eV causes ZT to rise by 0.1. The values of ZT when Laser was switched off were found to be a little higher than the case when Laser was on and these values gets closer as Δ_s is increased or Δ_z is decreased. From Figure (66) we realized that when Δ_s is 0.18eV and Δ_z is 0.030eV, the ZT values for both Laser on and off are the same and at 300K the ZT = 1.3. For values of $\Delta_s > 0.18$eV or $\Delta_z < 0.030$eV, the ZT values rises but the graph for both Laser on and Laser off continue to overlap.

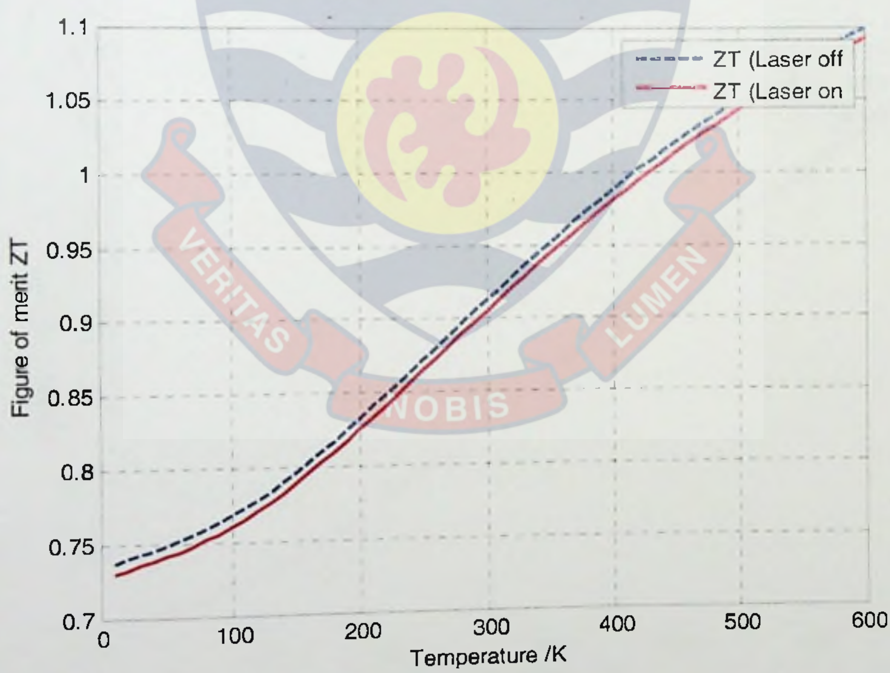


Figure 63: The dependence of ZT on temperature T for $\Delta_s = 0.10$eV, Δ_z is 0.030eV, $E_o = 2.507 \times 10^7$V/m, $E_s = 4.17 \times 10^8$V/m.

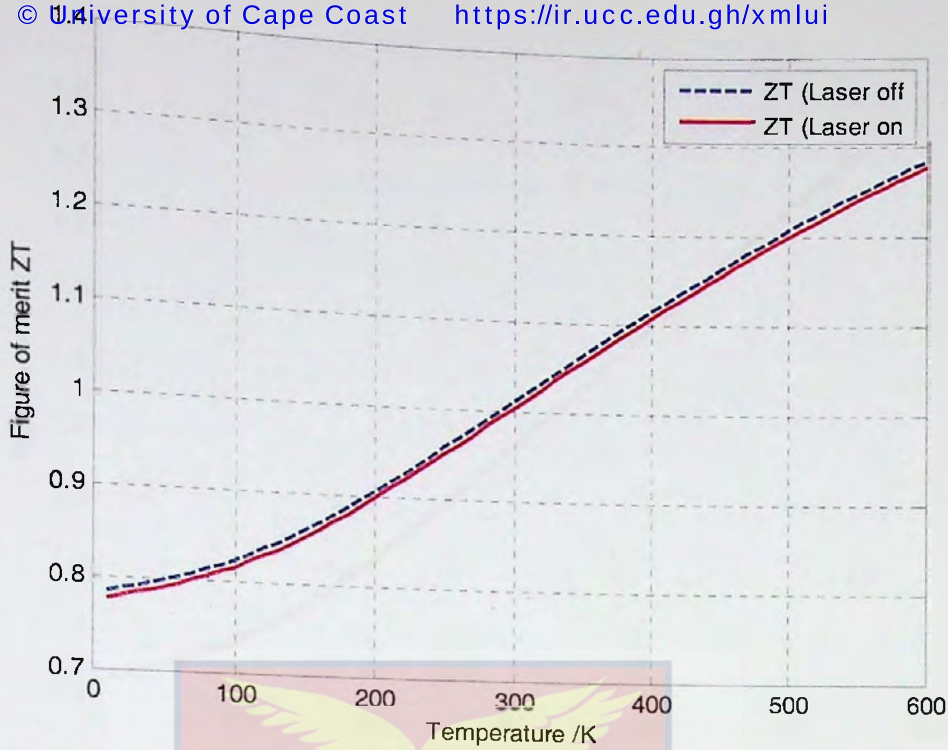


Figure 64: The dependence of ZT on temperature T for $\Delta_s = 0.12eV$, Δ_z is 0.030eV, $E_o = 2.507 \times 10^7 V/m$, $E_s = 4.17 \times 10^8 V/m$.

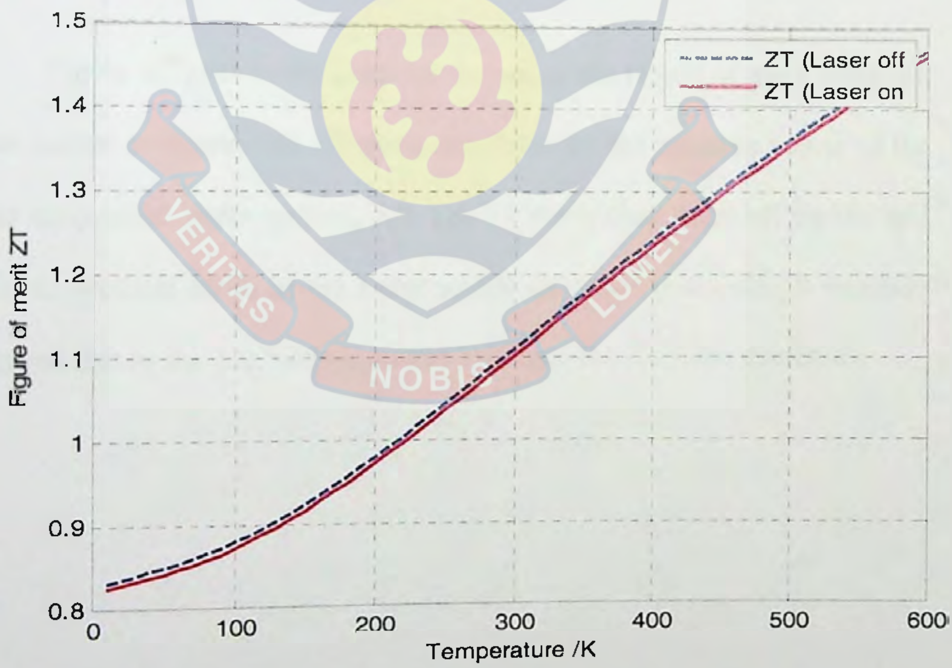


Figure 65: The dependence of ZT on temperature T for $\Delta_s = 0.14eV$, Δ_z is 0.030eV, $E_o = 2.507 \times 10^7 V/m$, $E_s = 4.17 \times 10^8 V/m$.

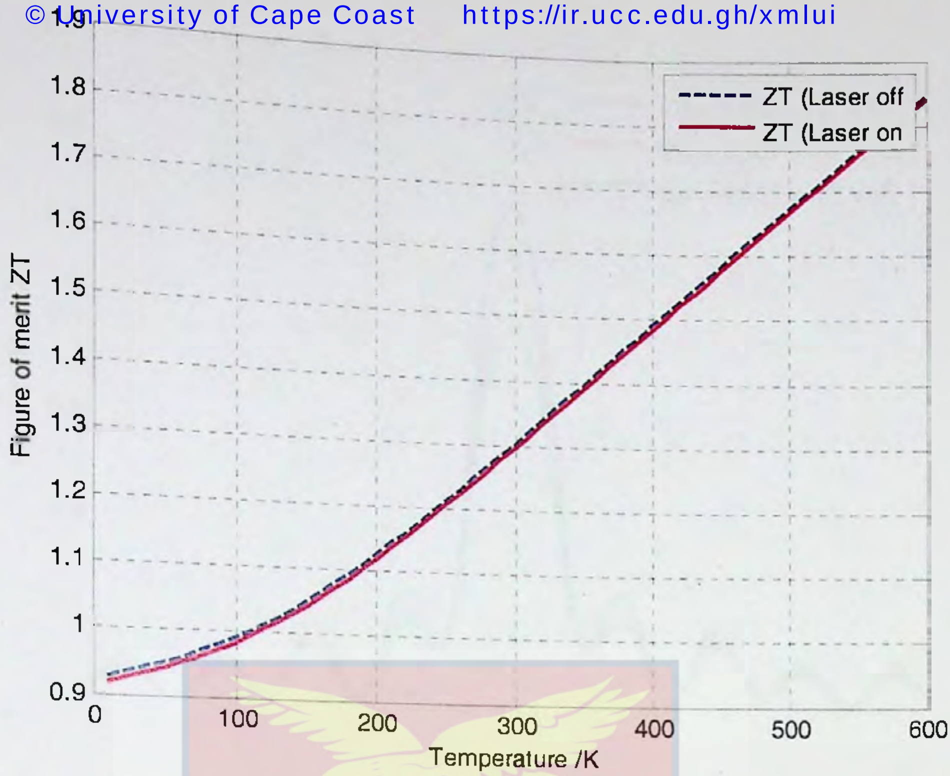


Figure 66: The dependence of ZT on temperature T for $\Delta_s = 0.18eV$, Δ_z is $0.030eV$, $E_o = 2.507 \times 10^7 V/m$, $E_s = 4.17 \times 10^8 V/m$.

Figure (67) shows the behavior pattern of the Figure of merit when the Laser source is varied. The ZT curve oscillates for the negative values of the Laser source and peaks up at $E_s = 0$. The ZT curve then drops off rapidly and begin to oscillate again as the Laser source increases positively. It was also observed that as the d. c. voltage source increases the ZT value decreases.

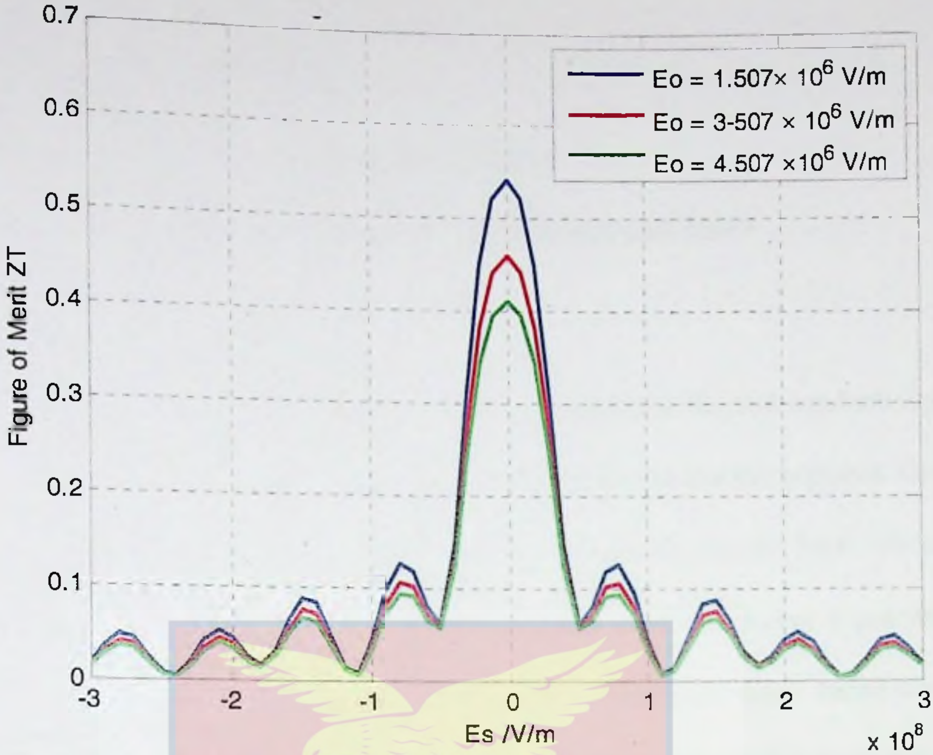


Figure 67: The dependence of ZT on Laser source E_s for $\Delta_s = 1.02eV$, Δ_z is 1.1eV, and varied values of $E_o = 1.507 \times 10^6 V/m$, $3.507 \times 10^6 V/m$, $4.507 \times 10^6 V/m$.

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATION

Conclusions

The resistivity ρ, thermopower α and the electron thermal conductivity χ of chiral CNT induced with monochromatic laser have been investigated. The chiral CNT parameters Δ_s Δ_z, θ_h, the d.c. electric field E_o and the laser source E_s were found to have influence on the resistivity ρ, thermopower α and the electron thermal conductivity χ of chiral CNT. Therefore these parameters affect the figure of merit ZT because ZT is a direct function of α^2 and inversely related to ρ and χ.

It was observed that increasing the d. c. field E_o, causes resistivity to increase which tends to affect ZT negatively. The results reveal that an increase in both Δ_s and θ_h causes a decrease in ρ which will in turn enhances ZT. Comparing the two situations when laser was switched on and also off, it became clear that laser made ρ values to rise. Also the resistivities ρ_c and ρ_z where found to be oscillating when the laser source was varied. The low ρ values recorded in our results indicate that the chiral CNT is a good conductor of electricity therefore it can exhibit metallic properties.

In the case of thermopower, the results show that the chiral CNT can exhibit semiconducting properties. It became clear that as Δ_z values increase beyond 0.040eV, the chiral CNT shifts from a p-type to an n-type semiconducting material. It was noted that an increase in both Δ_s and Δ_z causes a decrease in thermopower α, which will in turn reduce ZT. We noted that the presence of the laser source did not affect the thermopower values. However the behavior of thermopower with varying laser source E_s was found to be oscillatory.

The results obtained from the electron thermal conductivity show that a greater percentage of the electron and heat transport is along the axis of the chiral CNT axis. It was observed that an increase in Δ_z causes χ_c to decrease and χ_c to increase. Also an increase in θ_h made χ_c to rise but had no effect on χ_z. The parameters χ_c and χ_z were also found to be oscillating when the laser source E_s was varied. The results show that the laser source caused a drastic reduction in the χ values. The reduced values recorded for χ_c and χ_z is a clear indication that the laser retains heat at the junctions of the chiral CNT which helps to maintain a large temperature gradient.

Also we noted that the presence of the laser source lowered the figure of merit by small margin. The thermoelectric figure of merit is enhanced mainly by increasing Δ_s or decreasing Δ_z in the presence of the laser. At room temperature (300K) the value of ZT recorded for the chiral CNT in the presence of laser was greater than one.

Furthermore, it is realized that, when Δ_s is 0.18eV and Δ_z is 0.030eV, the ZT values for both laser-on and laser-off situations gets closer until they overlap. This observation is generally true for all the temperature ranges considered.

In view of our observations, we conclude that, Chiral CNTs should be induced with a monochromatic laser to enhance its usage as a thermoelement.

Recommendation

It is recommended that the findings of this study may be used to guide manufacturers of thermo devices in order to improve their products such as refrigerators and generators.

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Appendix A

Carrier Current Density in a Chiral Carbon Nanotube

In the linear approximation of ∇T and $\nabla\mu$, the solution to the Boltzmann kinetic equation is

$$f(p)=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)f_0\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)dt$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \quad \text{A1}$$

The current density j is defined as

$$j=e\sum_p v(p)f(p) \quad \text{A2}$$

Substituting Eqn. A1 into Eqn. A2 we have

$$j=e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v(p)f_0\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)$$

$$+e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v(p)\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \quad \text{A3}$$

Making the transformation $p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\rightarrow p$, Eqn. A3 becomes

$$j=e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)f_0(p)$$

$$+e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p \left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times\left\{v(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\}v\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \qquad \text{A4}$$

Resolving the current density along the tubular axis (z-axis) and the base helix we obtain

$$Z'=e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right)f_0(p)$$

$$+e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla_z T}{T}+\nabla_z\mu\right\}$$

$$\times\left\{v_z(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\}v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right) \qquad \text{A5}$$

and

$$S'=e\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p v_s\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)f_0(p)$$

$$+e\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\times\left\{v_s(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\}v_s\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \qquad \text{A6}$$

Making the transformation

$$\sum_p \to \frac{2}{(2\pi\hbar)^2}\int_{-\pi/d_s}^{\pi/d_s} dP_s\int_{-\pi/d_z}^{\pi/d_z} dP_z$$

Eqns. A5 and A6 become

$$Z'=\frac{2e\tau^{-1}}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s} dP_s\int_{-\pi/d_z}^{\pi/d_z} dP_z v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right)f_0(p)$$

$$+\frac{2e}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s} dP_s\int_{-\pi/d_z}^{\pi/d_z} dP_z\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla_z T}{T}+\nabla_z\mu\right\}$$

$$\times\left\{v_z(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\}v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right) \qquad \text{A7}$$

and

$$S' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z v_s\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)f_0(p)$$

$$+\frac{2e}{(2\pi\hbar)^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\times\left\{v_s(p)\frac{\partial f_0(p)}{\partial \varepsilon}\right\}v_s\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \qquad \text{A8}$$

respectively, where integrations are carried out over the first Brillouin zone.

Let's first consider S'. The energy ε(p) is given as

$$\varepsilon(p)=\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar} \qquad \text{A9}$$

and

$$v_s(p)=\frac{\partial\varepsilon(p)}{\partial P_s}=\frac{\Delta_s d_s}{\hbar}\sin\frac{P_s d_s}{\hbar} \qquad \text{A10}$$

$$v_s\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)=\frac{\partial\varepsilon}{\partial P_s}\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)$$

$$=\frac{\Delta_s d_s}{\hbar}\sin\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)$$

Expanding the trig function (sine)

$$=\frac{\Delta_s d_s}{\hbar}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\} \qquad \text{A11}$$

Substituting Eqns. A9, A10, A11 into Eqn. A8, we have

$$S' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right\} f_0(p)$$

$$+\frac{2e}{(2\pi\hbar)^2}\frac{\Delta_s^2 d_s^2}{\hbar^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

$$\times\left\{\left[\varepsilon_0 - \Delta_s\cos\frac{P_s d_s}{\hbar} - \Delta_z\cos\frac{P_z d_z}{\hbar} - \mu\right]\frac{\nabla_s T}{T} + \nabla_s\mu\right\}$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\frac{\partial f_0(p)}{\partial\varepsilon}\right\}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right\} \qquad \text{A12}$$

Now let

$$S_1' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)\right\} f_0(p) \qquad \text{A13}$$

$$S_2' = \frac{2e}{(2\pi\hbar)^2}\frac{\Delta_s^2 d_s^2}{\hbar^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

$$\times\left\{\left[\varepsilon_0 - \Delta_s\cos\frac{P_s d_s}{\hbar} - \Delta_z\cos\frac{P_z d_z}{\hbar} - \mu\right]\frac{\nabla_s T}{T} + \nabla_s\mu\right\}$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\frac{\partial f_0(p)}{\partial\varepsilon}\right\}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\} \qquad \text{A14}$$

So that $S' = S_1' + S_2'$. Let's consider S_1'. $f_0(p)$ is given by

$$f_0(p) = C\exp\left(\frac{\Delta_s\cos\frac{P_s d_s}{\hbar}+\Delta_z\cos\frac{P_z d_z}{\hbar}+\mu-\varepsilon_0}{kT}\right)$$

Where C is determined by the condition

$$n_0 = \frac{2}{(2\pi\hbar)^2}\int_{-\pi/d_s}^{\pi/d_s} dP_s\int_{-\pi/d_z}^{\pi/d_z} dP_z f_0(p)$$

n_0 is electron concentration. Thus

$$n_0 = \frac{2C}{(2\pi\hbar)^2}\int_{-\pi/d_s}^{\pi/d_s} dP_s\int_{-\pi/d_z}^{\pi/d_z} dP_z\exp\left(\frac{\Delta_s\cos\frac{P_s d_s}{\hbar}+\Delta_z\cos\frac{P_z d_z}{\hbar}+\mu-\varepsilon_0}{kT}\right)$$

$$n_0 = \frac{2C}{(2\pi\hbar)^2}\exp\left(\frac{\mu-\varepsilon_0}{kT}\right)\int_{-\pi/d_s}^{\pi/d_s} dP_s\exp\left(\frac{\Delta_s}{kT}\cos\frac{P_s d_s}{\hbar}\right)\int_{-\pi/d_z}^{\pi/d_z} dP_z\exp\left(\frac{\Delta_z}{kT}\cos\frac{P_z d_z}{\hbar}\right)$$

$$n_0 = \frac{2C}{(2\pi\hbar)^2}\exp\left(\frac{\mu-\varepsilon_0}{kT}\right)\int_{-\pi/d_s}^{\pi/d_s} dP_s\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}\right)\int_{-\pi/d_z}^{\pi/d_z} dP_z\exp\left(\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right) \qquad \text{A15}$$

where

$$\Delta_s^* = \frac{\Delta_s}{kT} \text{ and } \Delta_z^* = \frac{\Delta_z}{kT}$$

Now let's change the integration variables as follows

$$Z_s = P_s d_s \text{ and } Z_z = P_z d_z \qquad \text{A16}$$

Then

$$\frac{dZ_s}{dP_s} = d_s \quad \text{and} \quad \frac{dZ_z}{dP_z} = d_z$$

$$\frac{dZ_s}{d_s} = dP_s \quad \text{and} \quad \frac{dZ_z}{d_z} = dP_z \qquad \text{A17}$$

Substituting Eqns. A16 and A17 into Eqn. A15 we have

$$n_0 = \frac{8C}{(2\pi\hbar)^2 d_s d_z} \exp\left(\frac{\mu - \varepsilon_0}{kT}\right) \int_0^{\pi} dZ_s \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

From the definition of modified Bessel functions $I_n(x)$ of order n,

$$I_n(x) = \frac{1}{\pi}\int_0^{\pi} d\theta \cos n\theta \exp(x\cos\theta) \qquad \text{A18}$$

$$I_0(\Delta_s^*) = \frac{1}{\pi}\int_0^{\pi} dZ_s \exp(\Delta_s^* \cos Z_s) \qquad \text{A19}$$

Thus

$$n_0 = \frac{2C\hbar^2}{\hbar^2 d_s d_z} \exp\left(\frac{\mu - \varepsilon_0}{kT}\right) I_0(\Delta_s^*) I_0(\Delta_z^*)$$

$$C = \frac{d_s d_z n_0}{2 I_0(\Delta_s^*) I_0(\Delta_z^*)} \exp\left(-\frac{\mu - \varepsilon_0}{kT}\right) \qquad \text{A20}$$

Therefore

$$f_0(p) = \frac{d_s d_z n_0}{2 I_0(\Delta_s^*) I_0(\Delta_z^*)} \exp\left(-\frac{\mu - \varepsilon_0}{kT}\right) \exp\left(\frac{\Delta_s \cos\frac{P_s d_s}{\hbar} + \Delta_z \cos\frac{P_z d_z}{\hbar} + \mu - \varepsilon_0}{kT}\right)$$

$$f_0(p) = \frac{d_s d_z n_0}{2 I_0(\Delta_s^*) I_0(\Delta_z^*)} \exp\left(-\frac{\mu - \varepsilon_0}{kT}\right) \exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar} + \frac{\mu - \varepsilon_0}{kT}\right)$$

$$f_0(p) = \frac{d_s d_z n_0}{2 I_0(\Delta_s^*) I_0(\Delta_z^*)} \exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right) \qquad \text{A21}$$

Substituting Eqn. A21 into Eqn. A13 we get

$$S_1' = \frac{2e\tau^{-1}}{(2\pi\hbar)^2} \frac{\Delta_s d_s}{\hbar} \frac{d_s d_z n_0}{2 I_0(\Delta_s^*) I_0(\Delta_z^*)} \int_0^{\infty} \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\}\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)$$

$$S_1'=\frac{2e\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\frac{d_s d_z n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\}\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)$$

$$-\frac{2e\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\frac{d_s d_z n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z$$

$$\times\left\{\cos\frac{P_s d_s}{\hbar}\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\}\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)$$

The first term of this Equation is zero since it is an odd function of P_s integrated over the Brillouin zone $-\pi/d_s \le P_s \le \pi/d_s$. Thus S_1' becomes

$$S_1'=-\frac{2e\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\frac{4d_s d_z n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\int_0^{\pi/d_s}dP_s\int_0^{\pi/d_z}dP_z$$

$$\times\left\{\cos\frac{P_s d_s}{\hbar}\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\}\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)$$

$$S_1'=-\frac{e\tau^{-1}}{(\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\frac{d_s d_z n_0}{I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)dt$$

$$\times\int_0^{\pi/d_s}dP_s\cos\frac{P_s d_s}{\hbar}\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}\right)\int_0^{\pi/d_z}dP_z\exp\left(\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)$$

Changing the integration variables using Equations A16 and A17 we have

$$S_1' = -\frac{e\tau^{-1}}{(\pi\hbar)^2}\frac{\Delta_s d_s}{\hbar}\frac{d_s d_z n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''\right)dt$$

$$\times\frac{1}{d_s}\int_0^\pi dZ_s\cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\frac{1}{d_z}\int_0^\pi dZ_z\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$S_1' = -\frac{e\tau^{-1}}{\hbar^3}\frac{\Delta_s d_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''\right)dt$$

$$\times\frac{1}{\pi}\int_0^\pi dZ_s\cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^\pi dZ_z\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

From the definition of modified Bessel functions in A18

$$I_1(\Delta_s^*) = \frac{1}{\pi}\int_0^\pi \frac{dZ_s}{\hbar}\cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)$$

and

$$I_0(\Delta_z^*) = \frac{1}{\pi}\int_0^\pi dZ_s\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$S_1' = -\frac{e\tau^{-1}}{\hbar^3}\frac{\Delta_s d_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\hbar^2 I_1(\Delta_s^*)I_0(\Delta_z^*)$$

$$\times\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''\right)dt$$

$$S_1' = -\frac{e\tau^{-1}\Delta_s d_s n_0}{\hbar}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''\right)dt$$

The time integration is

$$\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''\right)dt = \sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\left(ed_sE_0/\hbar + nw\right)\tau^2}{1+\left(ed_sE_0/\hbar + nw\right)^2\tau^2}\right]$$

Where $a = \frac{ed_s E_s}{w\hbar}$

$$S_1' = -\frac{e\tau^{-1}\Delta_s d_s n_0}{\hbar}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\left(\frac{ed_s E_0}{\hbar} + nw\right)\tau^2}{1+\left(\frac{ed_s E_0}{\hbar} + nw\right)^2 \tau^2}\right]$$

$$S_1' = -\frac{e\tau\ \Delta_s d_s n_0}{\hbar}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{\left(\frac{ed_s E_0}{\hbar} + nw\right)}{\left[1+\left(\frac{ed_s E_0}{\hbar} + nw\right)^2 \tau^2\right]}$$

$$S_1' = -\frac{e^2\tau\ \Delta_s d_s^2 n_0}{\hbar^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{1}{1+\left(\frac{ed_s E_0}{\hbar} + nw\right)^2 \tau^2}\right]\left(E_0 + \frac{nw\hbar}{ed_s}\right) \qquad \text{A24}$$

Now let's define $\sigma_s(E)$ by

$$\sigma_s(E) = \frac{e^2\tau\Delta_s d_s^2 n_0}{\hbar^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{1}{1+\left(\frac{ed_s E_0}{\hbar} + nw\right)^2 \tau^2}\right] \qquad \text{A25}$$

Let $E_n = E_0 + \frac{nw\hbar}{ed_s}$

$$S_1' = -\sigma_s(E)\left(E_0 + \frac{nw\hbar}{ed_s}\right)$$

$$S_1' = -\sigma_s(E)E_n \qquad \text{A26}$$

Now we consider S_2' in Equation A14

$$S_2' = \frac{2e}{(2\pi\hbar)^2}\frac{\Delta_s^2 d_s^2}{\hbar^2}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s} dP_s\int_{-\pi/d_z}^{\pi/d_z} dP_z$$

$$\times\left\{\left[\varepsilon_0 - \Delta_s\cos\frac{P_s d_s}{\hbar} - \Delta_z\cos\frac{P_z d_z}{\hbar} - \mu\right]\frac{\nabla_s T}{T} + \nabla_s\mu\right\}$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\frac{\partial f_0(P)}{\partial\varepsilon}\right\}\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\} \qquad \text{A14}$$

From Equation A21

$$\frac{\partial f_0(P)}{\partial\varepsilon}=-\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}+\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right)$$

Using this equation S_2' becomes

$$S_2'=-\frac{2e}{(2\pi\hbar)^2}\frac{\Delta_s^2 d_s^2}{\hbar^2}\int_0^\infty\exp\left(-\frac{t}{\tau}\right)dt\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z$$

$$\times\left\{\left[\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}+\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right)\right\}$$

$$\times\left\{\sin\frac{P_s d_s}{\hbar}\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right.$$

$$\left.-\cos\frac{P_s d_s}{\hbar}\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)\right\}$$

$$S_2'=-\frac{2e\Delta_s^2 d_s^2}{(2\pi\hbar)^2\hbar^2}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty\exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)dt$$

$$\times\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\times\left\{\sin^2\frac{P_s d_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}+\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right)\right\}$$

$$+\frac{2e\Delta_s^2 d_s^2}{(2\pi\hbar)^2\hbar^2}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\sin\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt$$

$$\mathrm{x}\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\mathrm{x}\left\{\sin\frac{P_s d_s}{\hbar}\cos\frac{P_z d_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}+\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right)\right\} \qquad \text{A27}$$

Integrating over the Brillouin zone $-\pi/d_s \leq P_s \leq \pi/d_s$ makes the second term zero because it is an odd function of P_z. Thus,

$$S_2' = -\frac{2e\Delta_s^2 d_s^2}{(2\pi\hbar)^2\hbar^2}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt$$

$$\mathrm{x}\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\mathrm{x}\left\{\sin^2\frac{P_s d_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}+\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right)\right\}$$

$$= -\frac{2e\Delta_s^2 d_s^2}{(2\pi\hbar)^2\hbar^2}\frac{4d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt$$

$$\mathrm{x}\int_0^{\pi/d_s}dP_s\int_0^{\pi/d_z}dP_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\mathrm{x}\left\{\sin^2\frac{P_s d_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{P_s d_s}{\hbar}+\Delta_z^*\cos\frac{P_z d_z}{\hbar}\right)\right\}$$

$$= -\frac{e\Delta_s^2 d_s^2}{(\pi\hbar)^2\hbar^2}\frac{d_s d_z n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt$$

$$\mathrm{x}\int_0^{\pi/d_s}dP_s\int_0^{\pi/d_z}dP_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{P_s d_s}{\hbar}-\Delta_z\cos\frac{P_z d_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\mathrm{x}\left\{\sin^2\frac{P_s d_s}{\hbar}\exp\left(\Delta_s^{\bullet}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{P_z d_z}{\hbar}\right)\right\}$$

Changing the integration variables to Z_s and Z_z using Equations A16 and A17, we have

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{(\pi\hbar)^2\hbar^2}\frac{d_s d_z n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt$$

$$\mathrm{x}\frac{1}{d_s}\int_0^{\pi}dZ_s\frac{1}{d_z}\int_0^{\pi}dZ_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{Z_s}{\hbar}-\Delta_z\cos\frac{Z_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\mathrm{x}\left\{\sin^2\frac{Z_s}{\hbar}\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\right\}$$

Employing the trigonometry identity

$$\sin^2 x = \frac{1}{2}(1-\cos 2x)$$

We obtain,

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{(\pi\hbar)^2\hbar^2}\frac{n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt$$

$$\mathrm{x}\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{Z_s}{\hbar}-\Delta_z\cos\frac{Z_z}{\hbar}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\mathrm{x}\left\{\frac{1}{2}\left(1-\cos\frac{2Z_s}{\hbar}\right)\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\right\}$$

The time integration is

$$\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)dt = \sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]$$

where $a = \dfrac{ed_sE_s}{w\hbar}$

Therefore

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{(\pi\hbar)^2\hbar^2}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]$$

$$\times\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\left\{\left[\varepsilon_0-\Delta_s\cos\frac{Z_s}{\hbar}-\Delta_z\cos\frac{Z_z}{\hbar}-\mu\right]\frac{\nabla_sT}{T}+\nabla_s\mu\right\}$$

$$\times\left\{\frac{1}{2}\left(1-\cos\frac{2Z_s}{\hbar}\right)\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]$$

$$\times\left\{[\varepsilon_0-\mu]\frac{\nabla_sT}{T}+\nabla_s\mu\right\}\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\left\{\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$+\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]$$

$$\times\left\{[\varepsilon_0-\mu]\frac{\nabla_sT}{T}+\nabla_s\mu\right\}\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\left\{\left(\cos\frac{2Z_s}{\hbar}\right)\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$+\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_sT}{T}\right)$$

$$\times\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\left\{\cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$-\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_sT}{T}\right)$$

$$\text{x}\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{\cos\frac{Z_s}{\hbar}\cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$+\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_z n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(ed_sE_0/\hbar+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{\cos\frac{Z_z}{\hbar}\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$-\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_z n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(ed_sE_0/\hbar+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{\cos\frac{Z_z}{\hbar}\cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\right\} \qquad \text{A28}$$

Let the terms of Eqn. A28 be S_{21}, S_{22}, S_{23}, S_{24}, S_{25}, S_{26}

ie. $S_2' = S_{21} + S_{22} + S_{23} + S_{24} + S_{25} + S_{26}$

$$S_{21}' = -\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(ed_sE_0/\hbar+nw\right)^2\tau^2}\right]$$

$$\text{x}\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$=-\frac{e\Delta_s^2 d_s^2}{2\hbar^4}\frac{n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(ed_sE_0/\hbar+nw\right)^2\tau^2}\right]$$

$$\text{x}\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\frac{1}{\pi}\int_0^{\pi} dZ_s \exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^{\pi} dZ_z \exp\left(\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)$$

$$=-\frac{e\Delta_s^2 d_s^2}{2\hbar^4}\frac{n_0}{I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(ed_sE_0/\hbar+nw\right)^2\tau^2}\right]$$

$$\text{x}\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)$$

$$=-\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\} \qquad \text{A29}$$

$$S_{22}'=\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]$$

$$\text{x}\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z$$

$$\left\{\left(\cos\frac{2Z_s}{\hbar}\right)\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\right\}$$

$$S_{22}'=\frac{e\Delta_s^2 d_s^2}{2\hbar^4}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\text{x}\frac{1}{\pi}\int_0^{\pi}dZ_s\cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^{\pi}dZ_z\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$=\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_zE_0}{\hbar}+nw\right)^2\tau^2}\right]$$

$$\text{x}\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}I_2(\Delta_s^*)I_0(\Delta_z^*)$$

$$=\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{A30}$$

where

$$I_2\left(\Delta_s^*\right)=\frac{1}{\pi}\int_0^{\pi} dZ_s \cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \qquad \text{A31}$$

Eqn. A31 is a second order modified Bessel function. Modified Bessel functions obey the following recurrence relation

$$I_{n+1}(x)=I_{n-1}(x)-\frac{2n}{x}I_n(x) \qquad \text{A32}$$

Thus,

$$I_2\left(\Delta_s^*\right)=I_0\left(\Delta_s^*\right)-\frac{2}{\Delta_s^*}I_1\left(\Delta_s^*\right) \qquad \text{A33}$$

Substituting Eqn. A33 into A30, we have

$$=\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\frac{I_0\left(\Delta_s^*\right)-\frac{2}{\Delta_s^*}I_1\left(\Delta_s^*\right)}{I_0\left(\Delta_s^*\right)}$$

$$=\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\left(1-\frac{2}{\Delta_s^*}\frac{I_1\left(\Delta_s^*\right)}{I_0\left(\Delta_s^*\right)}\right)$$

$$S_{22}'=\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$-\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\left(\frac{2}{\Delta_s^*}\frac{I_1\left(\Delta_s^*\right)}{I_0\left(\Delta_s^*\right)}\right)$$

A34

$$S_{23}'=\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_s n_0}{I_0\left(\Delta_s^*\right)I_0\left(\Delta_z^*\right)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{\cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)\right\}$$

$$= \frac{e\Delta_s^2 d_s^2}{2\hbar^4}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\frac{1}{\pi}\int_0^{\pi} dZ_s \cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$= \frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_z T}{T}\right)I_1(\Delta_s^*)I_0(\Delta_z^*)$$

$$S_{23}' = \frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{\Delta_s n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_z T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{A35}$$

Let's consider S_{24}'

$$S_{24}' = -\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{\cos\frac{Z_s}{\hbar}\cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)\right\}$$

$$= -\frac{e\Delta_s^2 d_s^2}{2\hbar^4}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\frac{1}{\pi}\int_0^{\pi} dZ_s \cos\frac{Z_s}{\hbar}\cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$= -\frac{e\Delta_s^2 d_s^2}{2\hbar^4}\frac{\Delta_s n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\frac{1}{\pi}\int_0^\pi dZ_s\frac{1}{2}\left(\cos\frac{Z_s}{\hbar}+\cos\frac{3Z_s}{\hbar}\right)\exp\left(\Delta_s^\bullet\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^\pi dZ_z\exp\left(\Delta_z^\bullet\cos\frac{Z_z}{\hbar}\right)$$

$$=-\frac{e\Delta_s^2 d_s^2}{4\hbar^4}\frac{\Delta_s n_0}{I_0(\Delta_s^\bullet)I_0(\Delta_z^\bullet)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\frac{1}{\pi}\int_0^\pi dZ_s\cos\frac{Z_s}{\hbar}\exp\left(\Delta_s^\bullet\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^\pi dZ_z\exp\left(\Delta_z^\bullet\cos\frac{Z_z}{\hbar}\right)$$

$$-\frac{e\Delta_s^2 d_s^2}{4\hbar^4}\frac{\Delta_s n_0}{I_0(\Delta_s^\bullet)I_0(\Delta_z^\bullet)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\text{x}\frac{1}{\pi}\int_0^\pi dZ_s\cos\frac{3Z_s}{\hbar}\exp\left(\Delta_s^\bullet\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^\pi dZ_z\exp\left(\Delta_z^\bullet\cos\frac{Z_z}{\hbar}\right)$$

$$=-\frac{e\Delta_s^2 d_s^2}{4\hbar^2}\frac{\Delta_s n_0}{I_0(\Delta_s^\bullet)I_0(\Delta_z^\bullet)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)I_1(\Delta_s^\bullet)I_0(\Delta_z^\bullet)$$

$$-\frac{e\Delta_s^2 d_s^2}{4\hbar^2}\frac{\Delta_s n_0}{I_0(\Delta_s^\bullet)I_0(\Delta_z^\bullet)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)I_3(\Delta_s^\bullet)I_0(\Delta_z^\bullet)$$

$$=-\frac{e\Delta_s^2 d_s^2}{4\hbar^2}\frac{\Delta_s n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{I_1(\Delta_s^\bullet)+I_3(\Delta_s^\bullet)}{I_0(\Delta_s^\bullet)}\right\} \quad \text{A36}$$

where

$$I_3(\Delta_s^\bullet)=\frac{1}{\pi}\int_0^\pi dZ_s\cos\frac{3Z_s}{\hbar}\exp\left(\Delta_s^\bullet\cos\frac{Z_s}{\hbar}\right) \quad \text{A37}$$

Using the recurrence relation in Eqn. A32, $I_3(\Delta_s^\bullet)$ can be written as

$$I_3(\Delta_s^\bullet)=I_1(\Delta_s^\bullet)-\frac{4}{\Delta_s^\bullet}I_2(\Delta_s^\bullet) \quad \text{A38}$$

Using Eqn. A33

$$I_3(\Delta_s^*) = I_1(\Delta_s^*) - \frac{4}{\Delta_s^*}\left[I_0(\Delta_s^*) - \frac{2}{\Delta_s^*} I_1(\Delta_s^*)\right]$$

$$I_3(\Delta_s^*) = I_1(\Delta_s^*) - \frac{4}{\Delta_s^*} I_0(\Delta_s^*) - \frac{8}{\Delta_s^{*2}} I_1(\Delta_s^*) \qquad \text{A39}$$

Thus

$$\frac{I_1(\Delta_s^{*})+I_3(\Delta_s^{*})}{I_0(\Delta_s^*)} = \frac{I_1(\Delta_s^*)+I_1(\Delta_s^*) - \frac{4}{\Delta_s^*} I_0(\Delta_s^*) - \frac{8}{\Delta_s^{*2}} I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\frac{I_1(\Delta_s^*)+I_3(\Delta_s^*)}{I_0(\Delta_s^*)} = \frac{2I_1(\Delta_s^*)}{I_0(\Delta_s^*)} - \frac{4}{\Delta_s^*}\frac{I_0(\Delta_s^*)}{I_0(\Delta_s^*)} + \frac{8}{\Delta_s^{*2}}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{A40}$$

$$= -\frac{e\Delta_s^2 d_s^2}{4\hbar^2}\frac{\Delta_s n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{2I_1(\Delta_s^*)}{I_0(\Delta_s^*)} - \frac{4}{\Delta_s^*}\frac{I_0(\Delta_s^*)}{I_0(\Delta_s^*)} + \frac{8}{\Delta_s^{*2}}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}$$

$$= -\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{\Delta_s n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{e\Delta_s^2 d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$-\frac{2e\Delta_s^2 d_s^2}{\hbar^2\Delta_s^*}n_0\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{A41}$$

We now consider S_{25}'

$$S_{25}' = \frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_z n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\times \int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{ \cos\frac{Z_z}{\hbar} \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar} \right) \right\}$$

$$S_{25}' = \frac{e\Delta_s^2 d_s^2}{2\hbar^4} \frac{\Delta_z n_0}{I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\tau}{1 + \left(\frac{ed_s E_0}{\hbar} + nw \right)^2 \tau^2} \right] \left(\frac{\nabla_s T}{T} \right)$$

$$\times \frac{1}{\pi} \int_0^{\pi} dZ_s \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} \right) \frac{1}{\pi} \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar} \right)$$

$$S_{25}' = \frac{e\Delta_s^2 d_s^2}{2\hbar^2} \frac{\Delta_z n_0}{I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\tau}{1 + \left(\frac{ed_s E_0}{\hbar} + nw \right)^2 \tau^2} \right] \left(\frac{\nabla_z T}{T} \right) I_0(\Delta_s^*) I_1(\Delta_z^*)$$

$$S_{25}' = \frac{e\Delta_s^2 d_s^2}{2\hbar^2} \frac{\Delta_z n_0}{kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\tau}{1 + \left(\frac{ed_s E_0}{\hbar} + nw \right)^2 \tau^2} \right] \left(\frac{\nabla_s T}{T} \right) \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \qquad \text{A42}$$

We now consider S_{26}'

$$S_{26}' = -\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2 \hbar^2} \frac{\Delta_z n_0}{I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\tau}{1 + \left(\frac{ed_s E_0}{\hbar} + nw \right)^2 \tau^2} \right] \left(\frac{\nabla_s T}{T} \right)$$

$$\times \int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \left\{ \cos\frac{Z_z}{\hbar} \cos\frac{2Z_s}{\hbar} \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar} \right) \right\}$$

$$= -\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2 \hbar^2} \frac{\Delta_z n_0}{I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\tau}{1 + \left(\frac{ed_s E_0}{\hbar} + nw \right)^2 \tau^2} \right] \left(\frac{\nabla_s T}{T} \right)$$

$$\times \int_0^{\pi} dZ_s \cos\frac{2Z_s}{\hbar} \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} \right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar} \right)$$

$$= -\frac{e\Delta_s^2 d_s^2}{2(\pi\hbar)^2\hbar^2}\frac{\Delta_z n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$\mathrm{x}\frac{1}{\pi}\int_0^{\pi}dZ_s\cos\frac{2Z_s}{\hbar}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\frac{1}{\pi}\int_0^{\pi}dZ_z\cos\frac{Z_z}{\hbar}\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$= -\frac{e\Delta_s^2 d_s^2}{2(\hbar)^2}\frac{\Delta_z n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)I_2(\Delta_s^*)I_1(\Delta_z^*)$$

$$= -\frac{e\Delta_s^2 d_s^2}{2(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_2(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

Using Eqn. A33

$$\frac{I_2(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)} = \frac{\left[I_0(\Delta_s^*)-\frac{2}{\Delta_s^*}I_1(\Delta_s^*)\right]I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$= \frac{I_0(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)} - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$= \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)} \qquad \text{A44}$$

$$= -\frac{e\Delta_s^2 d_s^2}{2(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\right\}$$

$$S_{26} = -\frac{e\Delta_s^2 d_s^2}{2(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$+\frac{e\Delta_s^2 d_s^2}{(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\right\}$$

A45

Adding all the terms in S_2'. So we sum up Equations A29, A34, A35, A41, A42 and A45

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$+\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$-\frac{e\Delta_s^2 d_s^2}{\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\left(\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{\Delta_s n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$-\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{\Delta_s n_0}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{e\Delta_s^2 d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$-\frac{2e\Delta_s^2 d_s^2}{\hbar^2 \Delta_s^*}\frac{n_0}{}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{e\Delta_s^2 d_s^2}{2\hbar^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$-\frac{e\Delta_s^2 d_s^2}{2(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$+\frac{e\Delta_s^2 d_s^2}{(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\right\}$$

Simplifying, we have

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left\{[\varepsilon_0-\mu]\frac{\nabla_s T}{T}+\nabla_s \mu\right\}\left(\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{e\Delta_s^2 d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$-\frac{2e\Delta_s^2 d_s^2}{\hbar^2 \Delta_s^*}\frac{n_0}{}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{e\Delta_s^2 d_s^2}{(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_s E_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\right\}$$

$$S_2' = -\frac{e\Delta_s^2 d_s^2}{\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\nabla_s\mu$$

$$-\frac{e\Delta_s^2 d_s^2}{\hbar^2}\frac{n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right](\varepsilon_0-\mu)\left(\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\frac{\nabla_s T}{T}$$

$$+\frac{e\Delta_s^2 d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)$$

$$-\frac{2e\Delta_s^2 d_s^2}{\hbar^2\Delta_s^*}n_0\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{e\Delta_s^2 d_s^2}{(\hbar)^2}\frac{\Delta_z n_0}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{1}{\Delta_s^*}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\right\}$$

$$S_2' = -\frac{e\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\nabla_s\mu$$

$$-\frac{e\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right](\varepsilon_0-\mu)\left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\frac{\nabla_s T}{T}$$

$$+\frac{e\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\Delta_s\left(\frac{\nabla_s T}{T}\right)$$

$$-\frac{2e\Delta_s d_s^2 n_0}{\hbar^2\Delta_s^*}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\Delta_s\left(\frac{\nabla_s T}{T}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{e\Delta_s d_s^2\ \Delta_z n_0}{(\hbar)^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{\nabla_s T}{T}\right)\left\{\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\right\}$$

$$S_2'=-\frac{e^2\Delta_s d_s^2 n_0}{\hbar^2 e}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\nabla_s\mu$$

$$-\frac{e^2\Delta_s d_s^2 n_0 k}{\hbar^2 ke}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\text{x}\left\{(\varepsilon_0-\mu)-\Delta_s\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+\frac{2\Delta_s}{\Delta_s^*}-\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\frac{\nabla_s T}{T}$$

$$S_2'=-\frac{e^2\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\nabla_s\frac{\mu}{e}$$

$$-\frac{e^2\Delta_s d_s^2 n_0}{\hbar^2}\frac{k}{e}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\text{x}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S_2'=-\frac{e^2\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\nabla_s\frac{\mu}{e}$$

$$-\frac{e^2\Delta_s d_s^2 n_0}{\hbar^2}\frac{k}{e}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\text{x}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S_2' = -\frac{e^2\tau\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{1}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\nabla_s\frac{\mu}{e}$$

$$-\frac{e^2\tau\Delta_s d_s^2 n_0}{\hbar^2}\frac{k}{e}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{1}{1+\left(\frac{ed_sE_0}{\hbar}+nw\right)^2\tau^2}\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\text{x}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S_2' = -\sigma_s(E)\nabla_s\frac{\mu}{e}-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T \qquad \text{A46}$$

Where $\sigma_s\,(E)$ is defined by Eqn. A25. But S' = S_1'+ S_2', thus adding Eqns.

A26 to A46

we obtain

$$S' = -\sigma_s(E)E_n-\sigma_s(E)\nabla_s\frac{\mu}{e}-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S' = -\sigma_s(E)E_n-\sigma_s(E)\nabla_s\frac{\mu}{e}-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S' = -\sigma_s(E)\left(E_n+\nabla_s\frac{\mu}{e}\right)-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S' = -\sigma_s(E)\left(E_n + \nabla_s \frac{\mu}{e}\right) - \sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_s^* \frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^* \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T$$

$$S' = -\sigma_s(E)E_{sn}^* - \sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_s^* \frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^* \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T \qquad \text{A47}$$

Where we have defined E_{sn}^* as

$$E_{sn}^* = E_n + \nabla_s \frac{\mu}{e}$$

Going through similar steps described above, Z' is found to be

$$Z' = -\sigma_z(E)E_{zn}^* - \sigma_z(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_z^* \frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)} + 2 - \Delta_s^* \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\nabla_z T \qquad \text{A48}$$

The axial j_z and circumferential j_c components of the current density are given by

$$j_z = Z' + S' \sin\theta_h \qquad \text{A49}$$

$$j_c = S' \cos\theta_h \qquad \text{A50}$$

θ_h is the geometric chiral angle (GCA).

From Eqns. A47, A48, and A49, j_z is

$$j_z = -\sigma_z(E)E_{zn}^* - \sigma_s(E)\sin\theta_h E_{sn}^*$$

$$-\sigma_z(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_z^* \frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)} + 2 - \Delta_s^* \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\nabla_z T$$

$$-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0 - \mu}{kT}\right) - \Delta_s^* \frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)} + 2 - \Delta_z^* \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\sin\theta_h \nabla_s T \qquad \text{A51}$$

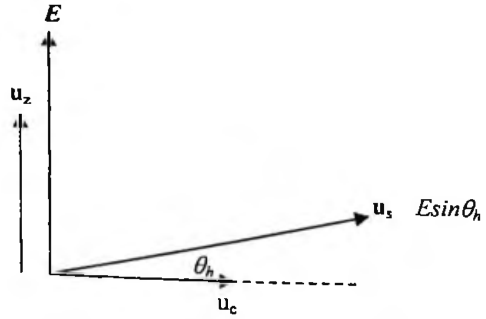

Figure A1: the magnitude of the component of *E* along the base helix E_s is $E\ sin\theta_h$.

From Figure A1,

$$E_s = E\sin\theta_h \qquad \text{A52}$$

$$\nabla_s T = \nabla_z T\sin\theta_h \qquad \text{A53}$$

$$E^*_{sn} = E^*_{zn}\sin\theta_h \qquad \text{A54}$$

Here, $E = E_z$ is the magnitude of the electric field ***E***. Therefore,

$$j_z = -\sigma_z(E)E^*_{zn} - \sigma_s(E)\sin\theta_h\sin\theta_h E^*_{zn}$$

$$-\sigma_z(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right) - \Delta^*_z\frac{I_0(\Delta^*_z)}{I_1(\Delta^*_z)} + 2 - \Delta^*_s\frac{I_1(\Delta^*_s)}{I_0(\Delta^*_s)}\right\}\nabla_z T$$

$$-\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right) - \Delta^*_s\frac{I_0(\Delta^*_s)}{I_1(\Delta^*_s)} + 2 - \Delta^*_z\frac{I_1(\Delta^*_z)}{I_0(\Delta^*_z)}\right\}\nabla_z T$$

$$j_z = -\sigma_z(E)E^*_{zn} - \sigma_s(E)\sin^2\theta_h E^*_{zn}$$

$$-\left\{\sigma_z(E)\frac{k}{e}\left[\left(\frac{\varepsilon_0-\mu}{kT}\right) - \Delta^*_z\frac{I_0(\Delta^*_z)}{I_1(\Delta^*_z)} + 2 - \Delta^*_s\frac{I_1(\Delta^*_s)}{I_0(\Delta^*_s)}\right]\right.$$

$$\left.+\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\left(\frac{\varepsilon_0-\mu}{kT}\right) - \Delta^*_s\frac{I_0(\Delta^*_s)}{I_1(\Delta^*_s)} + 2 - \Delta^*_z\frac{I_1(\Delta^*_z)}{I_0(\Delta^*_z)}\right]\right\}\nabla_z T$$

$$j_z = -\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\}E^*_{zn} - \left\{\sigma_z(E)\frac{k}{e}\left[\left(\frac{\varepsilon_0-\mu}{kT}\right) - \Delta^*_z\frac{I_0(\Delta^*_z)}{I_1(\Delta^*_z)} + 2 - \Delta^*_s\frac{I_1(\Delta^*_s)}{I_0(\Delta^*_s)}\right]\right.$$

$$+\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right]\Bigg\}\nabla_z T \qquad \text{A55}$$

From Eqns. A47 and A50, j_c is

$$j_c=-\sigma_s(E)\cos\theta_h E_{sn}^*-\sigma_s(E)\frac{k}{e}\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s T\cos\theta_h \qquad \text{A56}$$

Therefore using Eqns. A53 and A54, Eqn. A56 becomes

$$j_c=-\sigma_s(E)\cos\theta_h E_{zn}^*\sin\theta_h$$

$$-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_z T$$

$$j_c=-\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^*$$

$$-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)-\Delta_s^*\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}+2-\Delta_z^*\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_z T \qquad \text{A57}$$

Let us define

$$\xi=\frac{\varepsilon_0-\mu}{kT},\quad A_i=\frac{I_1(\Delta_i^*)}{I_0(\Delta_i^*)},\quad B_i=\frac{I_0(\Delta_i^*)}{I_1(\Delta_i^*)}-\frac{2}{\Delta_i^*},\quad i=s,z \qquad \text{A58}$$

Then Eqns. A55 and A57 become respectively

$$j_z=-\{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\}E_{zn}^*$$

$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi-\Delta_z^*B_z-\Delta_s^*A_s\right]+\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi-\Delta_s^*B_s-\Delta_z^*A_z\right]\right\}\nabla_z T \qquad \text{A59}$$

and

$$j_c=-\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^*-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\}\nabla_z T \qquad \text{A60}$$

The circumferential σ_{cs} and axial σ_{zz} components of the electrical conductivity are given by the coefficients of the electrical field $-E_{zn}^*$ in Eqns. A59 and A60 as follows

$$\sigma_{cz} = \sigma_s(E)\sin\theta_h\cos\theta_h \quad \text{A61}$$

$$\sigma_{zz} = \sigma_z(E) + \sigma_s(E)\sin^2\theta_h \quad \text{A62}$$

Resistivity, thermopower and power factor

The resistivities ρ_{cz} and ρ_{zz} along the circumferential and axial directions are respectively

$$\rho_c = \frac{1}{\sigma_{cz}}$$

$$\rho_c = \frac{1}{\sigma_s(E)\sin\theta_h\cos\theta_h} \quad \text{A63}$$

and

$$\rho_z = \frac{1}{\sigma_{zz}}$$

$$\rho_z = \frac{1}{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h} \quad \text{A64}$$

The differential thermoelectric power is defined as the ratio $\frac{|E_{zn}^{*}|}{|\nabla T|}$ in an open circuit (i.e. when j = 0). Thus setting j_c to zero in Eqn. A60, the thermoelectric power α_{cz} along the circumferential direction is obtained as follows

$$0 = -\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^{*} - \sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^{*}B_s - \Delta_z^{*}A_z\}\nabla_z T$$

$$\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^{*} = -\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^{*}B_s - \Delta_z^{*}A_z\}\nabla_z T$$

$$\frac{E_{zn}^{*}}{\nabla_z T} = -\frac{\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi - \Delta_s^{*}B_s - \Delta_z^{*}A_z\}}{\sigma_s(E)\sin\theta_h\cos\theta_h}$$

$$\alpha_{cz} = \left|\frac{E^{*}_{zn}}{\nabla_z T}\right| = \frac{k}{e}\left\{\xi - \Delta^{*}_{s}B_{s} - \Delta^{*}_{z}A_{z}\right\} \qquad \text{A65}$$

Similarly, the thermoelectric power α_{zz} along the axial direction is obtained from Eqn. A59 as follows (i.e. when $j_z = 0$)

$$0 = -\left\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\right\}E^{*}_{zn}$$

$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta^{*}_{z}B_{z} - \Delta^{*}_{s}A_{s}\right] + \sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta^{*}_{s}B_{s} - \Delta^{*}_{z}A_{z}\right]\right\}\nabla_z T$$

$$\left\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\right\}E^{*}_{zn} =$$

$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta^{*}_{z}B_{z} - \Delta^{*}_{s}A_{s}\right] + \sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta^{*}_{s}B_{s} - \Delta^{*}_{z}A_{z}\right]\right\}\nabla_z T$$

$$\frac{E^{*}_{zn}}{\nabla_z T} = -\frac{\left\{\sigma_z(E)\frac{k}{e}\left[\xi - \Delta^{*}_{z}B_{z} - \Delta^{*}_{s}A_{s}\right]\right.}{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h} + \frac{\left.\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta^{*}_{s}B_{s} - \Delta^{*}_{z}A_{z}\right]\right\}}{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h}$$

$$\alpha_{zz} = \left|\frac{E^{*}_{zn}}{\nabla_z T}\right| = \frac{\sigma_z(E)}{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta^{*}_{z}B_{z} - \Delta^{*}_{s}A_{s}\right]$$

$$+ \frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta^{*}_{s}B_{s} - \Delta^{*}_{z}A_{z}\right] \qquad \text{A66}$$

The electrical power factor P is defined as

$$P = \sigma\alpha^2 = \frac{\alpha^2}{\rho}$$

Therefore the power factor along the circumferential and axial directions are given respectively by

$$P_c = \frac{\alpha^2_{cz}}{\rho_c} \qquad \text{A69}$$

$$P_z = \frac{\alpha^2_{zz}}{\rho_z} \qquad \text{A70}$$

Appendix B

Thermal Current Density in a Chiral Carbon Nanotube

In the linear approximation of ∇T and $\nabla\mu$, the solution to the Boltzmann kinetic equation is given by Eqn. A1.

$$f(p)=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right) f_0\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right)dt$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''-\mu\right)\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times v\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right) \qquad \text{A1}$$

The thermal current density q is defined by

$$q=\sum_p\left[\varepsilon(p)-\mu\right]v(p)f(p) \qquad \text{B1}$$

Substituting Eq. A1 into Eq. B1, we have

$$q=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon(p)-\mu\right]v(p)f_0\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right)$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum\left[\varepsilon(p)-\mu\right]v(p)\left\{\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''-\mu\right)\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times v\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right)\frac{\partial f_0}{\partial\varepsilon}\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right) \qquad \text{B2}$$

Making the transformation $p-e\int\left[E_0+E\cos wt''\right]dt''\rightarrow p$, Eq. B2 becomes

$$q=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right)-\mu\right]$$

$$\text{x } v\left(p-e\int_{t-t'}^{t}\left[E_0+E\cos wt''\right]dt''\right) f_0(p)$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E\ \cos wt''\right]dt''\right)-\mu\right]\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla T}{T}+\nabla\mu\right\}$$

$$\times\left\{v(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v\left(p-e\int_{t-t'}^{t}\left[E_0+E\ \cos wt''\right]dt''\right) \qquad \text{B3}$$

Resolving the thermal current density along the tubular axis (Z – axis) and the base helix we obtain

$$Z'=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right)-\mu\right]$$

$$\text{x}\ \ v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right)f_0(p)$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right)-\mu\right]\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla_z T}{T}+\nabla_z\mu\right\}$$

$$\times\left\{v_z(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right) \qquad \text{B4}$$

and

$$S'=\tau^{-1}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)-\mu\right]$$

$$\text{x}\ \ v_s\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)f_0(p)$$

$$+\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt\sum_p\left[\varepsilon\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right)-\mu\right]\left\{\left[\varepsilon(p)-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\times\left\{v_s(p)\frac{\partial f_0(p)}{\partial\varepsilon}\right\}v_z\left(p-e\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right) \qquad \text{B5}$$

Making the transformation

$$\sum_p \to \frac{2}{(2\pi\hbar)^2} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z$$

Eqns. B4 and B5 respectively become

$$Z' = \frac{2\tau^{-1}}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \right) - \mu \right]$$

$$\times\ v_z\left(p - e\int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \right) f_0(p)$$

$$+ \frac{2}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \right) - \mu \right]$$

$$\left\{ [\varepsilon(p) - \mu] \frac{\nabla_z T}{T} + \nabla_z \mu \right\} \left\{ v_z(p) \frac{\partial f_0(p)}{\partial \varepsilon} \right\} v_z\left(p - e\int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \right) \qquad \text{B6}$$

and

$$S' = \frac{2\tau^{-1}}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right) - \mu \right]$$

$$\times\ v_s\left(p - e\int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right) f_0(p)$$

$$+ \frac{2}{(2\pi\hbar)^2} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left[\varepsilon\left(p - e\int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right) - \mu \right]$$

$$\left\{ [\varepsilon(p) - \mu] \frac{\nabla_s T}{T} + \nabla_s \mu \right\} \left\{ v_s(p) \frac{\partial f_0(p)}{\partial \varepsilon} \right\} v_s\left(p - e\int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right) \qquad \text{B7}$$

Where the integration is carried over the first Brillouin zone.

Let's consider S'. The energy $\varepsilon(p)$ is given by

$$\varepsilon(p) = \varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h} - \Delta_z \cos\frac{p_z d_z}{h} \qquad \text{B8}$$

and

$$\varepsilon\left(p - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right) = \varepsilon_0 - \Delta_s \cos\left(p_s - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right)\frac{d_s}{h}$$

$$-\Delta_z \cos\left(p_z - e\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt''\right)\frac{d_z}{h}$$

$$= \varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

$$-\Delta_s \sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

$$-\Delta_z \cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt''$$

$$-\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt'' \qquad \text{B9}$$

$$v_s(p) = \frac{\partial\varepsilon(p)}{\partial p_s} = \frac{\Delta_s d_s}{\hbar}\sin\frac{p_s d_s}{h} \qquad \text{B10}$$

$$v_s\left(p_s - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right) = \frac{\partial\varepsilon}{\partial p_s}\left(p_s - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right)$$

$$= \frac{\Delta_s d_s}{h}\sin\left(p_s - e\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right)\frac{d_s}{h}$$

Expanding the trig function

$$= \frac{\Delta_s d_s}{h}\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right.$$

$$\left.-\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right\} \qquad \text{B11}$$

Substituting Equations B8, B9, B10, B11 into B7

$$S' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{ \varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt'' \right.$$

$$-\Delta_s \sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

$$-\Delta_z \cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt''$$

$$\left. -\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt'' - \mu \right\}$$

$$\text{x} \left\{ \sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt'' \right.$$

$$\left. -\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt'' \right\} f_0(p)$$

$$+\frac{2}{(2\pi\hbar)^2}\frac{\Delta_s^2 d_s^2}{\hbar^2}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{ \varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt'' \right.$$

$$-\Delta_s \sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

$$-\Delta_z \cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt''$$

$$\left. -\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt'' - \mu \right\}$$

$$\times\left\{\left[\varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h} - \Delta_z \cos\frac{p_z d_z}{h} - \mu\right]\frac{\nabla_s T}{T} + \nabla_s \mu\right\}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\frac{\partial f_0(p)}{\partial \varepsilon}\right\}\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right.$$

$$\left. - \cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right\} \qquad \text{B12}$$

Now let S_1' and S_2' be equal to the terms of Eqn. B12 such that

$$S_1' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{\varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right.$$

$$- \Delta_s \sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''$$

$$- \Delta_z \cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt''$$

$$\left. - \Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt'' - \mu\right\}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right.$$

$$\left. - \cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right\} f_0(p) \qquad \text{B13}$$

and

$$S_2' = \frac{2}{(2\pi\hbar)^2}\frac{\Delta_s^{2} d_s^{2}}{\hbar^2}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{ \varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h} \cos\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right.$$

$$- \Delta_s \sin\frac{p_s d_s}{h} \sin\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$- \Delta_z \cos\frac{p_z d_z}{h} \cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt''$$

$$\left. - \Delta_z \sin\frac{p_z d_z}{h} \sin\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' - \mu \right\}$$

$$\text{x} \left\{ \left[\varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h} - \Delta_z \cos\frac{p_z d_z}{h} - \mu \right] \frac{\nabla_s T}{T} + \nabla_s \mu \right\}$$

$$\text{x} \left\{ \sin\frac{p_s d_s}{h} \frac{\partial f_0(p)}{\partial \varepsilon} \right\} \left\{ \sin\frac{p_s d_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right.$$

$$\left. - \cos\frac{p_s d_s}{h} \sin\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right\} \qquad \text{B14}$$

Thus Eqn. B12 becomes

$$S' = S_1' + S_2' \qquad \text{B15}$$

Let's consider S_1'

We substitute Equation A21 into B13

$$S_1' = \frac{2\tau^{-1}}{(2\pi\hbar)^2} \frac{\Delta_s d_s}{h} \frac{d_s d_s n_0}{2 I_0(\Delta_s^*) I_0(\Delta_z^*)} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_s}^{\pi/d_s} dP_z \left\{ \varepsilon_0 - \Delta_s \cos\frac{p_s d_s}{h} \cos\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \right.$$

$$- \Delta_s \sin\frac{p_s d_s}{h} \sin\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$- \Delta_z \cos\frac{p_z d_z}{h} \cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt''$$

$$-\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''-\mu\Bigg\}$$

$$\mathrm{x}\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right.$$

$$\left.-\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right\}\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)$$

B13a

$$S_1'=\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\mathrm{x}\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_s}^{\pi/d_s}dP_z\left\{\varepsilon_0-\mu-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right.$$

$$\left.-\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right\}\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''$$

$$\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)-\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\mathrm{x}\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_s}^{\pi/d_s}dP_z\left\{\varepsilon_0-\mu-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right.$$

$$\left.-\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right\}\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''$$

$$\exp\left(\Delta_s^{*}\cos\frac{P_s d_s}{\hbar}+\Delta_z^{*}\cos\frac{P_z d_z}{\hbar}\right)+\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\mathrm{x}\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_s}^{\pi/d_s}dP_z\left\{-\Delta_s\sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right.$$

$$\left.-\Delta_z\sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right\}\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''$$

$$\exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right) - \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{ -\Delta_s \sin\frac{p_s d_s}{h} \sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt'' \right.$$

$$\left. -\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z\cos wt'']dt''\right\}\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''$$

$$\exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right)$$

The first term of this equation is zero since it is an odd function of p_s that is integrated over the Brillouin zone $-\pi/d_s \le p_s \le \pi/d_s$. Thus

$$S_1' = -\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{ \varepsilon_0 - \mu - \Delta_s \cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt'' \right.$$

$$\left. -\Delta_z \cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z\cos wt'']dt''\right\}\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''$$

$$\exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right) + \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \left\{ -\Delta_s \sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''' \right.$$

$$\left. -\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z\cos wt'']dt''\right\}\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s\cos wt'']dt''$$

$$\exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right) - \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \Big\{ -\Delta_s \sin\frac{p_s d_s}{h} \sin\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$-\Delta_z \sin\frac{p_z d_z}{h} \sin\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \Big\} \cdot \cos\frac{p_s d_s}{h} \sin\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$\exp\left(\Delta_s^{*} \cos\frac{P_s d_s}{\hbar} + \Delta_z^{*} \cos\frac{P_z d_z}{\hbar} \right)$$

Simplifying gives,

$$S_1^{'} = -\frac{2\tau^{-1}}{(2\pi\hbar)^2} \frac{\Delta_s d_s}{h} \frac{d_s d_s n_0}{2I_0(\Delta_s^{*}) I_0(\Delta_z^{*})} \int_0^{\infty} \exp\left(-\frac{t}{\tau}\right) dt$$

$$\text{x} \int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \exp\left(\Delta_s^{*} \cos\frac{P_s d_s}{\hbar} + \Delta_z^{*} \cos\frac{P_z d_z}{\hbar} \right)$$

$$\text{x} \Big\{ -(\varepsilon_0 - \mu) \cos\frac{p_s d_s}{h} \sin\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$+\Delta_s \cos^2\frac{p_s d_s}{h} \cos\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt \sin\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$+\Delta_z \cos\frac{p_z d_z}{h} \cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt''$$

$$\text{x} \cos\frac{p_s d_s}{h} \sin\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$-\Delta_s \sin^2\frac{p_s d_s}{h} \sin\frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$-\Delta_z \sin\frac{p_z d_z}{h} \sin\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt''$$

$$\sin\frac{p_s d_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$+\Delta_s \sin\frac{p_s d_s}{h} \cos\frac{p_s d_s}{h} \sin^2\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$+\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt''$$

$$\left.\text{x}\ \cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right\} \qquad \text{B16}$$

Again, we set the terms (the last three terms of Eqn. B16) that contain integrals of odd functions of p_s and p_z over Brillouin zones $-\pi/d_s \le p_s \le \pi/d_s$ and $-\pi/d_z \le p_z \le \pi/d_z$ to zero.

$$S_1' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right)$$

$$\text{x}\left\{-(\varepsilon_0-\mu)\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right.$$

$$+\Delta_s \cos^2\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt \sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

$$+\Delta_z \cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z \cos wt''\right]dt''$$

$$\text{x}\ \cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

$$\left.-\Delta_s \sin^2\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt'' \cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''\right\}$$

$$S_1' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \exp\left(\Delta_s^* \cos\frac{P_s d_s}{\hbar} + \Delta_z^* \cos\frac{P_z d_z}{\hbar}\right)$$

$$\text{x}\left\{-(\varepsilon_0-\mu)\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right.$$

$$+\Delta_s\cos^2\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt\,\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$+\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''$$

$$\text{x}\quad\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$\left.-\Delta_s\sin^2\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right\}$$

Now the integration variables are changed to Z_s and Z_z using Eqns. A16 and A17 to get

$$S_1' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\ \frac{1}{d_s}\int_0^{\pi} dZ_s\frac{1}{d_z}\int_0^{\pi} dZ_z\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$\text{x}\left\{-(\varepsilon_0-\mu)\cos\frac{Z_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right.$$

$$+\Delta_s\cos^2\frac{Z_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt\,\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$+\Delta_z\cos\frac{Z_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\cos\frac{Z_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$\left.-\Delta_s\sin^2\frac{Z_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right\}$$

$$S_1' = \frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\frac{1}{d_s}\int_0^{\pi} dZ_s \frac{1}{d_z}\int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)$$

$$\text{x}\left\{-(\varepsilon_0-\mu)\cos\frac{Z_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right.$$

$$+\Delta_s\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt\left(\cos^2\frac{Z_s}{h}-\sin^2\frac{Z_s}{h}\right)$$

$$\left.+\Delta_z\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right\}$$

$$S_1^{'}=\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\ \frac{1}{d_s}\int_0^{\pi} dZ_s \frac{1}{d_z}\int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)$$

$$\text{x}\left\{-(\varepsilon_0-\mu)\cos\frac{Z_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right.$$

$$+\frac{\Delta_s}{2}\sin 2\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt\cos 2\frac{Z_s}{h}$$

$$+\frac{\Delta_z}{2}\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}\left[\sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''+\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)\right.$$

$$\left.\left.-\sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''-\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)\right]\right\}$$

Now let $S_1^{'}=S_{11}^{'}+S_{12}^{'}+S_{13}^{'}+S_{14}^{'}$, where

$$S_{11}^{'}=-\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta_s^{*})I_0(\Delta_z^{*})}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\ \frac{1}{d_s}\int_0^{\pi} dZ_s \frac{1}{d_z}\int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)$$

$$\times\ (\varepsilon_0-\mu)\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\cos\frac{Z_s}{h} \qquad \text{B17}$$

$$S'_{12}=\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta^*_s)I_0(\Delta^*_z)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\ \frac{1}{d_s}\int_0^\pi dZ_s\frac{1}{d_z}\int_0^\pi dZ_z\exp\left(\Delta^*_s\cos\frac{Z_s}{\hbar}+\Delta^*_z\cos\frac{Z_z}{\hbar}\right)$$

$$\times\frac{\Delta_s}{2}\sin 2\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt\cos 2\frac{Z_s}{h} \qquad \text{B18}$$

$$S'_{13}=\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta^*_s)I_0(\Delta^*_z)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\ \frac{1}{d_s}\int_0^\pi dZ_s\frac{1}{d_z}\int_0^\pi dZ_z\exp\left(\Delta^*_s\cos\frac{Z_s}{\hbar}+\Delta^*_z\cos\frac{Z_z}{\hbar}\right)\frac{\Delta_z}{2}\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}$$

$$\times\left[\sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''+\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)\right] \qquad \text{B19}$$

$$S'_{14}=-\frac{2\tau^{-1}}{(2\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{4d_s d_s n_0}{2I_0(\Delta^*_s)I_0(\Delta^*_z)}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\ \frac{1}{d_s}\int_0^\pi dZ_s\frac{1}{d_z}\int_0^\pi dZ_z\exp\left(\Delta^*_s\cos\frac{Z_s}{\hbar}+\Delta^*_z\cos\frac{Z_z}{\hbar}\right)$$

$$\times\frac{\Delta_z}{2}\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}\sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''-\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right)$$

B20

From Eqn. B17

$$S'_{11}=-\frac{\tau^{-1}}{(\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{n_0}{I_0(\Delta^*_s)I_0(\Delta^*_z)}(\varepsilon_0-\mu)\int_0^\infty dt\exp\left(-\frac{t}{\tau}\right)\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$\times\ \int_0^\pi dZ_s\cos\frac{Z_s}{h}\exp\left(\Delta^*_s\cos\frac{Z_s}{\hbar}\right)\int_0^\pi dZ_z\exp\left(\Delta^*_z\cos\frac{Z_z}{\hbar}\right)$$

The time integration is

$$\int_0^\infty dt \exp\left(-\frac{t}{\tau}\right)\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt'' = \sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\left(\frac{ed_s E_0}{\hbar} + nw\right)\tau^2}{1+\left(\frac{ed_s E_0}{\hbar} + nw\right)^2\tau^2}\right]$$

For weak electric fields,

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left[(ed_s E_0 + nw)\tau^2\left(1 - 0(ed_s E_0 + nw)^2\right)\right]$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left[(ed_s E_0 + nw)\tau^2\right] \qquad \text{B21}$$

Also, from the definition of modified Bessel functions in A18,

$$I_1(\Delta_s^*) = \frac{1}{\pi}\int_0^\pi dZ_s \cos\frac{Z_s}{h}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)$$

$$I_0(\Delta_z^*) = \frac{1}{\pi}\int_0^\pi dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

Therefore.

$$S_{11}' = -\frac{\tau^{-1}}{\hbar^2}\frac{\Delta_s d_s}{h}\frac{\hbar^2 n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}(\varepsilon_0 - \mu)I_1(\Delta_s^*)I_0(\Delta_z^*)\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\tau^2\right]$$

$$S_{11}' = -\frac{\tau\ \Delta_s d_s n_0}{h}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{B22}$$

From B18

$$S_{12}' = \frac{\tau^{-1}}{2(\pi\hbar)^2}\frac{\Delta_s^2 d_s}{h}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty dt \exp\left(-\frac{t}{\tau}\right)\sin 2\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt$$

$$\times \int_0^\pi dZ_s \cos 2\frac{Z_s}{h}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)\int_0^\pi dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

The time integration is,

$$\int_0^\infty dt \exp\left(-\frac{t}{\tau}\right)\sin 2\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt = \sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{2\left(ed_sE_0/\hbar + nw\right)\tau^2}{1+4\left(ed_sE_0/\hbar + nw\right)^2\tau^2}\right]$$

For weak electric fields, $\left(ed_sE_0/\hbar + nw\right)^2 \prec\prec 1$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left[2\left(ed_sE_0/\hbar + nw\right)\tau^2\left(1-0\left(ed_sE_0/\hbar + nw\right)^2\right)\right]$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left[2\left(ed_sE_0/\hbar + nw\right)\tau^2\right]$$

The integrals are expressed in terms of modified Bessel functions using

Eqns. A19 and A32

$$S_{12}' = \frac{\tau^{-1}}{2(\pi\hbar)^2}\frac{\Delta_s^2 d_z}{h}\frac{\hbar^2 n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[2\left(ed_sE_0/\hbar + nw\right)\tau^2\right]I_2(\Delta_s^*)I_0(\Delta_z^*)$$

$$S_{12}' = \frac{\tau^{-1}\Delta_s^2 d_s n_0}{2h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[2\left(ed_sE_0/\hbar + nw\right)\tau^2\right]\frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)} \quad \text{B23}$$

but

$$\frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)} = \frac{\left[I_0(\Delta_s^*) - \frac{2}{\Delta_s^*}I_1(\Delta_s^*)\right]}{I_0(\Delta_s^*)} = 1 - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$S_{12}' = \frac{\tau\ \Delta_s^2 d_s n_0}{h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(ed_sE_0/\hbar + nw\right)\right]\left(1 - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right) \quad \text{B24}$$

From Eqn. B19

$$S_{13}' = \frac{\tau^{-1}}{(\pi\hbar)^2}\frac{\Delta_s d_s}{h}\frac{\Delta_z}{2}\frac{n_0}{I_0(\Delta_s^*)I_0(\Delta_z^*)}\int_0^\infty dt \exp\left(-\frac{t}{\tau}\right)$$

$$\text{x}\ \sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0 + E_z\cos wt''\right]dt'' + \frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0 + E_s\cos wt''\right]dt''\right)$$

$$\times \int_0^{\pi} dZ_s \cos\frac{Z_s}{h} \exp\left(\Delta_s^{\bullet} \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{h} \exp\left(\Delta_z^{\bullet} \cos\frac{Z_z}{\hbar}\right)$$

Making use of Eqn. A18 to express the integrals in terms of Bessel functions

$$S_{13}' = \frac{\tau^{-1}}{(\pi\hbar)^2} \frac{\Delta_s d_s}{h} \frac{\Delta_z}{2} \frac{\hbar^2 n_0}{I_0(\Delta_s^{\bullet}) I_0(\Delta_z^{\bullet})} I_1(\Delta_s^{\bullet}) I_1(\Delta_z^{\bullet})$$

$$\text{x} \int_0^{\infty} dt \exp\left(-\frac{t}{\tau}\right) \sin\left(\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' + \frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''\right)$$

The time integration is

$$\int_0^{\infty} dt \exp\left(-\frac{t}{\tau}\right) \sin\left(\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' + \frac{ed_s}{h} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''\right)$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\tau^2}{1 + \left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]^2 \tau^2} \right]$$

For weak electric fields, $\left(\frac{ed_s E_0}{\hbar} + nw\right)^2 \prec\prec 1$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\right.$$

$$\left.\tau^2 \left(1 - 0\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]^2\right)\right]$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\tau^2\right]$$

B25

$$S_{13}' = \frac{\tau^{-1} \Delta_s \Delta_z d_s n_0}{2h} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\tau^2\right] \frac{I_1(\Delta_s^{\bullet}) I_1(\Delta_z^{\bullet})}{I_0(\Delta_s^{\bullet}) I_0(\Delta_z^{\bullet})}$$

$$S_{13}' = \frac{\tau \Delta_s \Delta_z d_s n_0}{2h} \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\right] \frac{I_1(\Delta_s^{\bullet}) I_1(\Delta_z^{\bullet})}{I_0(\Delta_s^{\bullet}) I_0(\Delta_z^{\bullet})}$$

B26

From Eqn. B20

$$S'_{14} = -\frac{\tau^{-1}}{(\pi\hbar)^2}\frac{\Delta_s d_s}{2h}\frac{\Delta_z n_0}{I_0(\Delta^*_s)I_0(\Delta^*_z)}\int_0^{\pi} dZ_s \cos\frac{Z_s}{h}\exp\left(\Delta^*_s \cos\frac{Z_s}{\hbar}\right)$$

$$\text{x} \int_0^{\pi} dZ_z \cos\frac{Z_z}{h}\exp\left(\Delta^*_z \cos\frac{Z_z}{\hbar}\right)$$

x

$$\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt \sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt'' - \frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right)$$

Making use of Eqn. A18 to express the integrals in terms of Bessel functions

$$S'_{14} = -\frac{\tau^{-1}\Delta_s d_s}{2\hbar}\frac{\Delta_z n_0}{I_0(\Delta^*_s)I_0(\Delta^*_z)}I_0(\Delta^*_s)I_0(\Delta^*_z)$$

$$\text{x} \int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt \sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt'' - \frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right)$$

The time integration is

$$\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt \sin\left(\frac{ed_z}{h}\int_{t-t'}^{t}[E_0 + E_z \cos wt'']dt'' - \frac{ed_s}{h}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\right)$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\tau^2}{1 + \left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]^2 \tau^2}\right]$$

For weak electric fields, $\left(\frac{ed_s E_0}{\hbar} + nw\right)^2 \prec\prec 1$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left\{\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\right.$$

$$\left.\tau^2\left(1 - 0\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]^2\right)\right\}$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\tau^2\right] \qquad B27$$

So,

$$S_{14}' = -\frac{\tau^{-1}\Delta_s d_s \Delta_z n_0}{2h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\tau^2\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$S_{14}' = -\frac{\tau\Delta_s d_s \Delta_z n_0}{2h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)} \qquad B28$$

Summing up Eqns. B22, B24, B26 and B28

$$S_1' = -\frac{\tau\ \Delta_s d_s n_0}{h}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{\tau\ \Delta_s^2 d_s n_0}{h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\left(1 - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{\tau\Delta_s\Delta_z d_s n_0}{2h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$-\frac{\tau\Delta_s d_s \Delta_z n_0}{2h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left[\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$S_1' = -\frac{\tau\ \Delta_s d_s n_0}{h}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{\tau\ \Delta_s^2 d_s n_0}{h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\left(1 - \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{\tau\Delta_s\Delta_z d_s n_0}{2h}\sum_{n=-\infty}^{\infty} J_n^2(a)\left\{\left(\frac{ed_z E_0}{\hbar} + nw\right) + \left(\frac{ed_s E_0}{\hbar} + nw\right)\right.$$

$$\left. -\left(\frac{ed_z E_0}{\hbar} + nw\right) - \left(\frac{ed_s E_0}{\hbar} + nw\right)\right\}\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$S_1' = -\frac{\tau\ \Delta_s d_s n_0}{\hbar}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\left(\frac{ed_s E_0}{\hbar} + nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{\tau\,\Delta_s^2 d_s n_0}{\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\left(1-\frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{\tau\Delta_s\Delta_z d_s n_0}{2\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)+\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$S_1^{'}=-\frac{\tau\,\Delta_s d_s n_0}{\hbar}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{\tau\,\Delta_s^2 d_s n_0}{\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\left(1-\frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{\tau\Delta_s\Delta_z d_s n_0}{2\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)2\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$

$$S_1^{'}=-\frac{\tau\,\Delta_s d_s n_0}{\hbar}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$+\frac{\tau\,\Delta_s^2 d_s n_0}{\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\left(1-\frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$+\frac{\tau\Delta_s\Delta_z d_s n_0}{\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\frac{I_1(\Delta_s^*)I_1(\Delta_z^*)}{I_0(\Delta_s^*)I_0(\Delta_z^*)}$$ B29

$$S_1^{'}=\frac{\tau\,\Delta_s d_s n_0}{\hbar}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)\right]\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\mathrm{x}\left\{-(\varepsilon_0-\mu)+\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)+\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}$$ B30

$$S_1^{'}=\frac{e\tau\,\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left(E_0+\frac{nw\hbar}{ed_s}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$\mathrm{x}\left\{-(\varepsilon_0-\mu)+\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)+\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}$$

$$S_1^{'}=\frac{e\tau\,\Delta_s d_s^2 n_0}{\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left(E_0+\frac{nw\hbar}{ed_s}\right)$$

$$\mathrm{x}\left\{-(\varepsilon_0-\mu)+\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)+\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\} \qquad \text{B31}$$

Let's define

$$\sigma_s(E)=\frac{e^2\tau\Delta_s d_s^{\,2}\, n_0}{(\hbar)^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{B32}$$

Then Eqn. B31 becomes

$$S_1'=\left[\frac{e^2\tau\;\Delta_s d_s^2 n_0}{e\hbar^2}\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right]$$

$$\mathrm{x}\left\{-(\varepsilon_0-\mu)+\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)+\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\left(E_0+\frac{nw\hbar}{ed_s}\right)$$

$$S_1'=\sigma_s(E)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{1}{e}\left\{-(\varepsilon_0-\mu)+\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)+\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\left(E_0+\frac{nw\hbar}{ed_s}\right)$$

We have defined E_n as

$$E_n=\left(E_0+\frac{nw\hbar}{ed_s}\right)$$

$$S_1'=-\sigma_s(E)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{1}{e}\left\{(\varepsilon_0-\mu)-\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}E_n \qquad \text{B33}$$

Now let us consider the term S_2' given by Eqn. B14

$$S_2'=\frac{2}{(2\pi\hbar)^2}\frac{\Delta_s^{\,2}d_z^{\,2}}{\hbar^2}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\mathrm{x}\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_s}^{\pi/d_s}dP_z\left\{\varepsilon_0-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right.$$

$$-\Delta_s\sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$-\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''$$

$$-\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''-\mu\Bigg\}$$

$$\times\left\{\left[\varepsilon_0-\Delta_s\cos\frac{p_s d_s}{h}-\Delta_z\cos\frac{p_z d_z}{h}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\left\{\sin\frac{p_s d_s}{h}\frac{\partial f_0(p)}{\partial\varepsilon}\right\}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''-\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\right\}$$

B14

Taking the derivative of Eqn. A21 with respect to ε, we obtain

$$\frac{\partial f_0(p)}{\partial\varepsilon}=-\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\exp\left(\Delta_s^*\cos\frac{p_s d_s}{\hbar}+\Delta_z^*\cos\frac{p_z d_z}{\hbar}\right) \qquad \text{B34}$$

Substituting Eqn. B34 into B14 gives

$$S_2'=-\frac{2}{(2\pi\hbar)^2}\frac{\Delta_s^{\,2}d_s^{\,2}}{\hbar^2}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_{-\pi/d_s}^{\pi/d_s}dP_s\int_{-\pi/d_z}^{\pi/d_z}dP_z\Bigg\{\varepsilon_0-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$-\Delta_s\sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$-\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''$$

$$-\Delta_z\sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''-\mu\Bigg\}$$

$$\times\left\{\left[\varepsilon_0-\Delta_s\cos\frac{p_s d_s}{h}-\Delta_z\cos\frac{p_z d_z}{h}-\mu\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\exp\left(\Delta_s^*\cos\frac{p_s d_s}{\hbar}+\Delta_z^*\cos\frac{p_z d_z}{\hbar}\right)\right\}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''-\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right\}$$

Rearranging gives

$$S_2' = -\frac{2}{(2\pi\hbar)^2}\frac{\Delta_s{}^2 d_s{}^2}{\hbar^2}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \exp\left(\Delta_s^*\cos\frac{p_s d_s}{\hbar}+\Delta_z^*\cos\frac{p_z d_z}{\hbar}\right)$$

$$\times\left\{\varepsilon_0-\mu-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right.$$

$$-\Delta_s\sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''$$

$$-\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''$$

$$\left.-\Delta_z\sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right\}$$

$$\times\left\{\left[\varepsilon_0-\mu-\Delta_s\cos\frac{p_s d_s}{h}-\Delta_z\cos\frac{p_z d_z}{h}\right]\frac{\nabla_s T}{T}+\nabla_s\mu\right\}\sin\frac{p_s d_s}{h}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''-\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right\}$$

$$S_2' = -\frac{2}{(2\pi\hbar)^2}\frac{\Delta_s{}^2 d_s{}^2}{\hbar^2}\frac{d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_{-\pi/d_s}^{\pi/d_s} dP_s \int_{-\pi/d_z}^{\pi/d_z} dP_z \exp\left(\Delta_s^*\cos\frac{p_s d_s}{\hbar}+\Delta_z^*\cos\frac{p_z d_z}{\hbar}\right)$$

$$\times\left\{(\varepsilon_0-\mu)^2\frac{\nabla_s T}{T}-(\varepsilon_0-\mu)\Delta_s\cos\frac{p_s d_s}{h}\frac{\nabla_s T}{T}\right.$$

$$-(\varepsilon_0-\mu)\Delta_z\cos\frac{p_z d_z}{h}\frac{\nabla_s T}{T}+(\varepsilon_0-\mu)\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s^2\cos^2\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s\Delta_z\cos\frac{p_s d_s}{h}\cos\frac{p_z d_z}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_s\sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s^2\sin\frac{p_s d_s}{h}\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s\Delta_z\sin\frac{p_s d_s}{h}\cos\frac{p_z d_z}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$-\Delta_s\sin\frac{p_s d_s}{h}\sin\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_z\Delta_s\cos\frac{p_z d_z}{h}\cos\frac{p_s d_s}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_z^2\cos^2\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$-\Delta_z\cos\frac{p_z d_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_z \sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s\Delta_z\frac{p_s d_s}{h}\sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\cos\frac{\nabla_s T}{T}$$

$$+\Delta_z^2\sin\frac{p_z d_z}{h}\cos\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$-\Delta_z\sin\frac{p_z d_z}{h}\sin\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\nabla_s\mu\Bigg\}\sin\frac{p_s d_s}{h}$$

$$\times\left\{\sin\frac{p_s d_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''-\cos\frac{p_s d_s}{h}\sin\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\right\}$$

Setting all the odd function terms of the above equation to zero, we have

$$S_2' = -\frac{2}{(2\pi\hbar)^2}\frac{\Delta_s^{\,2}d_s^{\,2}}{\hbar^2}\frac{4d_s d_z n_0}{2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_0^{\pi/d_s}dP_s\int_0^{\pi/d_z}dP_z\exp\left(\Delta_s^*\cos\frac{p_s d_s}{\hbar}+\Delta_z^*\cos\frac{p_z d_z}{\hbar}\right)$$

$$\text{x}\Bigg\{(\varepsilon_0-\mu)^2\frac{\nabla_s T}{T}-(\varepsilon_0-\mu)\Delta_s\cos\frac{p_s d_s}{h}\frac{\nabla_s T}{T}$$

$$-(\varepsilon_0-\mu)\Delta_z\cos\frac{p_z d_z}{h}\frac{\nabla_s T}{T}+(\varepsilon_0-\mu)\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s^2\cos^2\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$+\Delta_s\Lambda_z\cos\frac{p_s d_s}{h}\cos\frac{p_z d_z}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

$$-\Delta_s\cos\frac{p_s d_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_z\cos\frac{p_zd_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_sT}{T}$$

$$+\Delta_z\Delta_s\cos\frac{p_zd_z}{h}\cos\frac{p_sd_s}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_sT}{T}$$

$$+\Delta_z^2\cos^2\frac{p_zd_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_sT}{T}$$

$$-\Delta_z\cos\frac{p_zd_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\nabla_s\mu\Bigg\}$$

$$\times\sin^2\frac{p_sd_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

The integration variables are changed to Z_s and Z_z, using equations (A.16) and (A.17) as follows:

$$S_2'=-\frac{\Delta_s^{\,2}d_s^{\,2}d_sd_zn_0}{(\pi\hbar)^2\hbar^2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\frac{1}{d_sd_z}\int_0^\infty\exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_0^\pi dZ_s\int_0^\pi dZ_z\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$\text{x}\Bigg\{(\varepsilon_0-\mu)^2\frac{\nabla_sT}{T}-(\varepsilon_0-\mu)\Delta_s\cos\frac{Z_s}{h}\frac{\nabla_sT}{T}-(\varepsilon_0-\mu)\Delta_z\cos\frac{Z_z}{h}\frac{\nabla_sT}{T}$$

$$+(\varepsilon_0-\mu)\nabla_s\mu-(\varepsilon_0-\mu)\Delta_s\cos\frac{Z_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\frac{\nabla_sT}{T}$$

$$+\Delta_s^2\cos^2\frac{Z_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\frac{\nabla_sT}{T}$$

$$+\Delta_s\Delta_z\cos\frac{Z_s}{h}\cos\frac{Z_z}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\frac{\nabla_sT}{T}$$

$$-\Delta_s\cos\frac{Z_s}{h}\cos\frac{ed_s}{h}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\nabla_s\mu$$

$$-(\varepsilon_0-\mu)\Delta_z\cos\frac{Z_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_s T}{T}$$

$$+\Delta_z\Delta_s\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_s T}{T}$$

$$+\Delta_z^2\cos^2\frac{Z_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_s T}{T}$$

$$-\Delta_z\cos\frac{Z_z}{h}\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\nabla_s\mu\Bigg\}$$

$$\times\sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt'' \qquad \text{B35}$$

Let the terms of Equation (B35) be equal to U_1, U_2, U_3, …., U_{12} so that Equation (B35) can be expressed in the form

$$S_2' = U_1+U_2+U_3+\ldots+U_{12}$$

Then

$$U_1=-\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\frac{1}{d_s d_z}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_0^\pi dZ_s\int_0^\pi dZ_z\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)(\varepsilon_0-\mu)^2$$

$$\times\sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\frac{\nabla_s T}{T} \qquad \text{B36}$$

$$U_2=+\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\frac{1}{d_s d_z}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_0^\pi dZ_s\int_0^\pi dZ_z\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)(\varepsilon_0-\mu)\Delta_s\cos\frac{Z_s}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\frac{\nabla_s T}{T} \qquad \text{B37}$$

$$U_3 = +\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)(\varepsilon_0 - \mu)\Delta_z \cos\frac{Z_z}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \frac{\nabla_s T}{T} \qquad \text{B38}$$

$$U_4 = -\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)(\varepsilon_0 - \mu)$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \, \nabla_s \mu \qquad \text{B39}$$

$$U_5 = +\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)(\varepsilon_0 - \mu)\Delta_s \cos\frac{Z_s}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos^2\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \frac{\nabla_s T}{T} \qquad \text{B40}$$

$$U_6 = -\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) \Delta_s^2 \cos^2\frac{Z_s}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos^2\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \frac{\nabla_s T}{T} \qquad \text{B41}$$

$$U_7 = -\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)\Delta_s\Delta_z\cos\frac{Z_s}{h}\cos\frac{Z_z}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_s T}{T} \qquad \text{B42}$$

$$U_8=+\frac{\Delta_s^{\ 2}d_s^{\ 2}d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^{*})I_0(\Delta_z^{*})kT}\frac{1}{d_s d_z}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)\Delta_s\cos\frac{Z_s}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\,\nabla_s\mu \qquad \text{B43}$$

$$U_9=+\frac{\Delta_s^{\ 2}d_s^{\ 2}d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^{*})I_0(\Delta_z^{*})kT}\frac{1}{d_s d_z}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)(\varepsilon_0-\mu)\Delta_z\cos\frac{Z_z}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''$$

$$\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T} \qquad \text{B44}$$

$$U_{10}=-\frac{\Delta_s^{\ 2}d_s^{\ 2}d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^{*})I_0(\Delta_z^{*})kT}\frac{1}{d_s d_z}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}+\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)\Delta_z\Delta_s\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\cos\frac{ed_z}{h}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\frac{\nabla_s T}{T}$$

B45

$$U_{11} = -\frac{\Delta_s^{\ 2} d_s^{\ 2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) \Delta_z^2 \cos^2\frac{Z_z}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \frac{\nabla_s T}{T}$$

B46

$$U_{12} = +\frac{\Delta_s^{\ 2} d_s^{\ 2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) \Delta_z \cos\frac{Z_z}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \nabla_s \mu$$

B47

Let's evaluate each of the terms of Equation B35. The first term U_1, Eqn. B36 is

$$U_1 = -\frac{\Delta_s^{\ 2} d_s^{\ 2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) (\varepsilon_0 - \mu)^2$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \frac{\nabla_s T}{T}$$

The time dependent integral part in Eqn. B36, is

$$\int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\frac{\tau}{1 + \left({ed_s E_0}/{\hbar} + nw \right)^2 \tau^2} \right]$$

For weak electric fields, $\left(ed_s E_0 / \hbar + nw \right) << 1$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a) \left[\tau \left(1 - 0 \left(ed_s E_0 / \hbar + nw \right)^2 \right) \right]$$

$$= \sum_{n=-\infty}^{\infty} J_n^2(a) \tau \qquad \text{B48}$$

Therefore Eqn. B36 becomes

$$U_1 = -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu)^2 \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\text{x} \int_0^\pi dZ_s \sin^2 \frac{Z_s}{\hbar} \exp\left(\Delta_s^* \cos \frac{Z_s}{\hbar} \right) \int_0^\pi dZ_z \exp\left(\Delta_z^* \cos \frac{Z_z}{\hbar} \right)$$

$$= -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu)^2 \frac{\nabla_s T}{T} \sum_{n=-\infty}^{\infty} J_n^2(a)$$

$$\text{x} \int_0^\pi dZ_s \left\{ \frac{1}{2} \left(1 - \cos \frac{2Z_s}{h} \right) \right\} \exp\left(\Delta_s^* \cos \frac{Z_s}{\hbar} \right) \int_0^\pi dZ_z \exp\left(\Delta_z^* \cos \frac{Z_z}{\hbar} \right)$$

$$= -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0}{2(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu)^2 \frac{\nabla_s T}{T} \sum_{n=-\infty}^{\infty} J_n^2(a)$$

$$\times \left\{ \int_0^\pi dZ_s \exp\left(\Delta_s^* \cos \frac{Z_s}{\hbar} \right) \int_0^\pi dZ_z \exp\left(\Delta_z^* \cos \frac{Z_z}{\hbar} \right) \right.$$

$$\left. - \int_0^\pi dZ_s \cos \frac{2Z_s}{h} \exp\left(\Delta_s^* \cos \frac{Z_s}{\hbar} \right) \int_0^\pi dZ_z \exp\left(\Delta_z^* \cos \frac{Z_z}{\hbar} \right) \right\}$$

$$= -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \hbar^2}{2(\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu)^2 \frac{\nabla_s T}{T} \sum_{n=-\infty}^{\infty} J_n^2(a) \{ I_0(\Delta_s^*) I_0(\Delta_z^*) - I_2(\Delta_s^*) I_0(\Delta_z^*) \}$$

$$= -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0}{2(\hbar)^2 kT} (\varepsilon_0 - \mu)^2 \frac{\nabla_s T}{T} \sum_{n=-\infty}^{\infty} J_n^2(a) \left\{ 1 - \frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)} \right\}$$

The integrals have been expressed in terms of modified Bessel functions as I_0 and I_1.

$$= -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{2(\hbar)^2 kT}(\varepsilon_0 - \mu)^2 \frac{\nabla_s T}{T}\sum_{n=-\infty}^{\infty} J_n^2(a)\left\{1 - \frac{I_0(\Delta_s^*) - \frac{2}{\Delta_s^*} I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}$$

$$= -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{2(\hbar)^2 kT}(\varepsilon_0 - \mu)^2 \frac{\nabla_s T}{T}\sum_{n=-\infty}^{\infty} J_n^2(a)\left\{1 - 1 + \frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}$$

$$= -\frac{\tau\Delta_s\, d_s^{\,2} n_0 k}{(\hbar)^2}\frac{(\varepsilon_0 - \mu)^2}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\left\{\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\nabla_s T \qquad \text{B49}$$

Evaluating the next term of Eqn. B35 which is U_2,

$$U_2 = +\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\frac{1}{d_s d_z}\int_0^{\infty} \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times \int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)(\varepsilon_0 - \mu)\Delta_s \cos\frac{Z_s}{h}$$

$$\times \sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt'' \frac{\nabla_s T}{T}$$

$$U_2 = +\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0 \Delta_s}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\frac{1}{d_s d_z}(\varepsilon_0 - \mu)\frac{\nabla_s T}{T}$$

$$\times \int_0^{\infty} \exp\left(-\frac{t}{\tau}\right)dt \cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''$$

$$\times \int_0^{\pi} dZ_s \cos\frac{Z_s}{h}\sin^2\frac{Z_s}{h}\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)\int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right) \qquad \text{B50}$$

Using the identities,

$$\sin^2 x = \frac{1}{2}(1 - \cos 2x) \qquad \text{B51}$$

$$\cos x \cos y = \frac{1}{2}[\cos(x+y) + \cos(x-y)] \qquad \text{B52}$$

$\cos\left(\frac{Z_s}{\hbar}\right)\sin^2\left(\frac{Z_s}{\hbar}\right)$ is written as follows,

$$\cos\left(\frac{Z_s}{\hbar}\right)\sin^2\left(\frac{Z_s}{\hbar}\right) = \frac{1}{2}\cos\frac{Z_s}{\hbar}\left(1 - \cos\frac{2Z_s}{\hbar}\right)$$

$$= \frac{1}{2}\cos\frac{Z_s}{\hbar} - \frac{1}{2}\cos\frac{Z_s}{\hbar}\cos\frac{2Z_s}{\hbar}$$

$$= \frac{1}{2}\cos\frac{Z_s}{\hbar} - \frac{1}{4}\left(\cos\frac{Z_s}{\hbar} + \cos\frac{3Z_s}{\hbar}\right)$$

$$= \frac{1}{2}\cos\frac{Z_s}{\hbar} - \frac{1}{4}\cos\frac{Z_s}{\hbar} - \frac{1}{4}\cos\frac{3Z_s}{\hbar}$$

$$= \frac{1}{4}\left(\cos\frac{Z_s}{\hbar} - \cos\frac{3Z_s}{\hbar}\right) \qquad \text{B53}$$

Integration of Eqn. B50 with respect to time, using Eqn. B48, followed by substitution of Eqn. B53 gives,

$$U_2 = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s}{4(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{\nabla_s T}{T}$$

$$\times \int_0^{\pi} dZ_s \left(\cos\frac{Z_s}{\hbar} - \cos\frac{3Z_s}{\hbar}\right)\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)\int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_2 = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s \hbar^2}{4(\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{\nabla_s T}{T}$$

$$\times \{I_1(\Delta_s^*) - I_3(\Delta_s^*)\} I_0(\Delta_z^*)$$

$$U_2 = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s}{4(\hbar)^2 kT}(\varepsilon_0 - \mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{\nabla_s T}{T} \sum_{n=-\infty}^{\infty} J_n^2(a)\left\{\frac{I_1(\Delta_s^*) - I_3(\Delta_s^*)}{I_0(\Delta_s^*)}\right\} \qquad \text{B54}$$

Eqn B54 is expressed in terms of the modified Bessel functions I_0 and I_1.

Using the recurrence relation in Eqn A33, $I_3(\Delta_s^\bullet)$ can be written as

$$I_3(\Delta_s^\bullet) = I_1(\Delta_s^\bullet) - \frac{4}{\Delta_s^\bullet} I_0(\Delta_s^\bullet) + \frac{8}{\Delta_s^{\bullet 2}} I_1(\Delta_s^\bullet)$$

Therefore,

$$\left\{\frac{I_1(\Delta_s^\bullet) - I_3(\Delta_s^\bullet)}{I_0(\Delta_s^\bullet)}\right\} = \frac{I_1(\Delta_s^\bullet)}{I_0(\Delta_s^\bullet)} - \frac{I_1(\Delta_s^\bullet) - \frac{4}{\Delta_s^\bullet} I_0(\Delta_s^\bullet) + \frac{8}{\Delta_s^{\bullet 2}} I_1(\Delta_s^\bullet)}{I_0(\Delta_s^\bullet)}$$

$$= \frac{I_1(\Delta_s^\bullet)}{I_0(\Delta_s^\bullet)} - \frac{I_1(\Delta_s^\bullet)}{I_0(\Delta_s^\bullet)} + \frac{4 I_0(\Delta_s^\bullet)}{\Delta_s^\bullet I_0(\Delta_s^\bullet)} - \frac{8 I_1(\Delta_s^\bullet)}{\Delta_s^{\bullet 2} I_0(\Delta_s^\bullet)}$$

$$= \frac{4}{\Delta_s^\bullet} - \frac{8 I_1(\Delta_s^\bullet)}{\Delta_s^{\bullet 2} I_0(\Delta_s^\bullet)} \qquad \text{B55}$$

Substituting Eqn. B55 into Eqn. B54 gives,

$$U_2 = +\frac{\tau \Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s}{4(\hbar)^2 \hbar^2 kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \left(\frac{4}{\Delta_s^\bullet} - \frac{8 I_1(\Delta_s^\bullet)}{\Delta_s^{\bullet 2} I_0(\Delta_s^\bullet)}\right)$$

$$U_2 = +\frac{\tau \Delta_s^{\,2} d_s^{\,2} n_0 k}{(\hbar)^2} \left(\frac{\varepsilon_0 - \mu}{kT}\right) \sum_{n=-\infty}^{\infty} J_n^2(a) \left(1 - \frac{2 I_1(\Delta_s^\bullet)}{\Delta_s^\bullet I_0(\Delta_s^\bullet)}\right) \nabla_s T \qquad \text{B56}$$

The third term U_3 of Eqn. B35 is given by Eqn. B38

$$U_3 = +\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^\bullet) I_0(\Delta_z^\bullet) kT} \frac{1}{d_s d_z} \int_0^\infty \exp\left(-\frac{t}{\tau}\right) dt$$

$$\times \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^\bullet \cos\frac{Z_s}{\hbar} + \Delta_z^\bullet \cos\frac{Z_z}{\hbar}\right) (\varepsilon_0 - \mu) \Delta_z \cos\frac{Z_z}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{e d_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \frac{\nabla_s T}{T}$$

Integrating U_3 with respect to time using Eqn. B48 gives,

$$U_3 = +\frac{\tau \Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^\bullet) I_0(\Delta_z^\bullet) kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\times \int_0^{\pi} dZ_s \sin^2 \frac{Z_s}{h} \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$= + \frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\times \frac{1}{2} \int_0^{\pi} dZ_s \left(1 - \cos\frac{2Z_s}{h}\right) \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$= + \frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z}{2(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\times \int_0^{\pi} dZ_s \left(1 - \cos\frac{2Z_s}{h}\right) \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$= + \frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z}{2(\hbar)^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \{I_0(\Delta_s^*) - I_2(\Delta_s^*)\} I_1(\Delta_z^*)$$

$$= + \frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z}{2(\hbar)^2 kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \left\{\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} - \frac{I_2(\Delta_s^*) I_1(\Delta_z^*)}{I_0(\Delta_s^*) I_0(\Delta_z^*)}\right\} \qquad \text{B57}$$

Where as usual, the integrals have been expressed in terms of modified Bessel functions. Using the recurrence relation in Eqn A33, Eqn. B57 can be expressed in terms of I_0 and I_1 as follows:

$$\left\{\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} - \frac{I_2(\Delta_s^*) I_1(\Delta_z^*)}{I_0(\Delta_s^*) I_0(\Delta_z^*)}\right\} = \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1 - \frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$= \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1 - \frac{I_0(\Delta_s^*) - \frac{2}{\Delta_s^*} I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$= \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1 - 1 + \frac{2 I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right)$$

$$= \frac{2 I_1(\Delta_z^*)}{\Delta_s^* I_0(\Delta_z^*)} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{B58}$$

Substituting Eqn. B58 into Eqn. B57, we get

$$= +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z}{2(\hbar)^2 kT} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \frac{2 I_1(\Delta_z^*)}{\Delta_s^* I_0(\Delta_z^*)} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$U_3 = +\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z k}{(\hbar)^2} \left(\frac{\varepsilon_0 - \mu}{kT}\right) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \nabla_s T \qquad \text{B59}$$

The fourth term U_4 of Eqn. B35 is given by Eqn. B39.

$$U_4 = -\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^{\infty} \exp\left(-\frac{t}{\tau}\right) dt$$

$$\text{x} \int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) (\varepsilon_0 - \mu)$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{e d_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt'' \; \nabla_s \mu$$

Integrating U_4 with respect to time using Eqn. B48 gives,

$$U_4 = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) (\varepsilon_0 - \mu) \nabla_s \mu$$

$$\text{x} \int_0^{\pi} dZ_s \sin^2\frac{Z_s}{h} \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_4 = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) (\varepsilon_0 - \mu) \nabla_s \mu$$

$$\text{x} \; \frac{1}{2} \int_0^{\pi} dZ_s \left(1 - \cos\frac{2Z_s}{h}\right) \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_4 = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{2(\hbar)^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) (\varepsilon_0 - \mu) \nabla_s \mu \left\{I_0(\Delta_s^*) - I_2(\Delta_s^*)\right\} I_0(\Delta_z^*)$$

$$U_4 = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{2(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a) (\varepsilon_0 - \mu) \nabla_s \mu \left\{1 - \frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right\} \qquad \text{B60}$$

Where the integrals have been expressed in terms of modified Bessel functions.

Using the recurrence relation in Eqn A33, Eqn. B60 can be expressed in terms of I_0 and I_1 as follows:

$$\left\{1-\frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right\} = \left(1-\frac{I_0(\Delta_s^*)-\frac{2}{\Delta_s^*}I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right)$$

$$=\left(1-1+\frac{2I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right)$$

$$=\frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \qquad \text{B61}$$

Substituting Eqn. B61 into Eqn. B60, we get

$$U_4 = -\frac{\tau\Delta_s^{\,2} d_s^{\,2}\, n_0}{2(\hbar)^2 kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\,\nabla_s\mu\,\frac{2}{\Delta_s^*}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$$

$$U_4 = -\frac{\tau\Delta_s d_s^{\,2}\, n_0}{(\hbar)^2}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\nabla_s\mu \qquad \text{B62}$$

The next term U_5 of Eqn. B35 is given by Eqn. B40.

$$U_5 = +\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\frac{1}{d_s d_z}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x}\int_0^\pi dZ_s\int_0^\pi dZ_z \exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)(\varepsilon_0-\mu)\Delta_s\cos\frac{Z_s}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\,\frac{\nabla_s T}{T}$$

The time integral in U_5 is

$$\int_0^\infty dt\exp\left(-\frac{t}{\tau}\right)\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$=\frac{1}{2}\int_0^\infty dt\exp\left(-\frac{t}{\tau}\right)\left(1+\cos 2\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt'\right)$$

$$= \frac{1}{2}\int_0^\infty dt \exp\left(-\frac{t}{\tau}\right) + \frac{1}{2}\int_0^\infty dt \exp\left(-\frac{t}{\tau}\right)\cos 2\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0 + E_s \cos wt''\right]dt''$$

For weak electric fields, $\left(\frac{ed_sE_0}{\hbar} + nw\right) << 1$

$$= \frac{\tau}{2} + \frac{1}{2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left[\frac{\tau}{1 + 4\left(\frac{ed_sE_0}{\hbar} + nw\right)^2\tau^2}\right]$$

$$= \frac{1}{2}\left(\tau + \sum_{n=-\infty}^{\infty} J_n^2(a)\left[\tau\left(1 - 0\left(\frac{ed_sE_0}{\hbar} + nw\right)^2\right)\right]\right)$$

$$= \frac{1}{2}\left(\tau + \sum_{n=-\infty}^{\infty} J_n^2(a)\tau\right)$$

$$= \frac{1}{2}\tau\left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right) \qquad \text{B63}$$

Therefore integrating Eqn. B40 with respect to time using Eqn B63, we have

$$U_s = +\frac{\tau\Delta_s^{\ 2}d_s^{\ 2}n_0\Delta_s(\varepsilon_0 - \mu)}{2(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right)\frac{\nabla_s T}{T}$$

$$\text{x} \int_0^\pi dZ_s \cos\frac{Z_s}{h}\sin^2\frac{Z_s}{h}\int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

Using Eqn. B53, we have

$$U_s = +\frac{\tau\Delta_s^{\ 2}d_s^{\ 2}n_0\Delta_s(\varepsilon_0 - \mu)}{2(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right)\frac{\nabla_s T}{T}$$

$$\text{x} \ \frac{1}{4}\int_0^\pi dZ_s\left(\cos\frac{Z_s}{h} - \cos\frac{3Z_s}{h}\right)\exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right)\int_0^\pi dZ_z \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_s = +\frac{\tau\Delta_s^{\ 2}d_s^{\ 2}n_0\Delta_s(\varepsilon_0 - \mu)}{8(\hbar)^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right)\frac{\nabla_s T}{T}\left\{I_1(\Delta_s^*) - I_3(\Delta_s^*)\right\}I_0(\Delta_z^*)$$

$$U_5 = +\frac{\tau\Delta_s{}^2 d_s{}^2 n_0 \Delta_s(\varepsilon_0-\mu)}{8(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}\left\{\frac{I_1(\Delta_s^*)-I_3(\Delta_s^*)}{I_0(\Delta_s^*)}\right\} \quad \text{B64}$$

Where the integrals have been expressed in terms of modified Bessel functions.

By substituting Eqn B55 into, Eqn. B64, U_5 can be expressed in terms of I_0 and I_1 as follows:

$$U_5 = +\frac{\tau\Delta_s{}^2 d_s{}^2 n_0 \Delta_s(\varepsilon_0-\mu)}{8(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}\left\{\frac{4}{\Delta_s^*}-\frac{8I_1(\Delta_s^*)}{\Delta_s^{*2} I_0(\Delta_s^*)}\right\}$$

$$U_5 = +\frac{\tau\Delta_s{}^2 d_s{}^2 n_0 k}{2(\hbar)^2}\frac{(\varepsilon_0-\mu)}{kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left\{1-\frac{2I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right\}\nabla_s T \quad \text{B65}$$

The next term U_6 of Eqn. B35 is given by Eqn. B41. Integrating U_6 with respect to time using Eqn. B63, we have

$$U_6 = -\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\frac{1}{d_s d_z}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_0^\pi dZ_s\int_0^\pi dZ_z \exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\Delta_s^2\cos^2\frac{Z_s}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\,\frac{\nabla_s T}{T}$$

$$U_6 = -\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_s^2}{2(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}$$

$$\times\int_0^\pi dZ_s\sin^2\frac{Z_s}{h}\cos^2\frac{Z_s}{h}\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\int_0^\pi dZ_z\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right) \quad \text{B66}$$

But,

$$\sin^2\frac{Z_s}{h}\cos^2\frac{Z_s}{h} = \frac{1}{4}\sin^2\frac{2Z_s}{h}$$

$$=\frac{1}{4}\cdot\frac{1}{2}\left(1-\cos\frac{4Z_s}{\hbar}\right)$$

$$=\frac{1}{8}\left(1-\cos\frac{4Z_s}{\hbar}\right) \qquad \text{B67}$$

Substituting Eqn.B67 into Eqn.B66 gives

$$U_6=-\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_s^2}{2(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}$$

$$\text{x}\int_0^{\pi}dZ_s\frac{1}{8}\left(1-\cos\frac{4Z_s}{\hbar}\right)\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi}dZ_z\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$U_6=-\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_s^2}{16(\hbar)^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}\{I_0(\Delta_s^*)-I_4(\Delta_s^*)\}I_0(\Delta_z^*)$$

$$=-\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_s^2}{16(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}\frac{\{I_0(\Delta_s^*)-I_4(\Delta_s^*)\}}{I_0(\Delta_s^*)}$$

$$=-\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_s^2}{16(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_s T}{T}\left\{1-\frac{I_4(\Delta_s^*)}{I_0(\Delta_s^*)}\right\} \qquad \text{B68}$$

Where the integrals have been expressed in terms of modified Bessel functions.

According to Eqn. A33 the recurrence relation for $I_4(\Delta_s^*)$ is

$$I_4(\Delta_s^*)=I_2(\Delta_s^*)-\frac{6}{\Delta_s^*}I_3(\Delta_s^*)$$

Substituting Eqns. A33b and A37, this recurrence relation becomes

$$I_4(\Delta_s^*)=I_0(\Delta_s^*)-\frac{2I_1(\Delta_s^*)}{\Delta_s^*}-\frac{6}{\Delta_s^*}\left(I_1(\Delta_s^*)-\frac{4I_0(\Delta_s^*)}{\Delta_s^*}+\frac{8I_1(\Delta_s^*)}{\Delta_s^{*2}}\right)$$

$$I_4(\Delta_s^*)=I_0(\Delta_s^*)-\frac{8I_1(\Delta_s^*)}{\Delta_s^*}+\frac{24I_0(\Delta_s^*)}{\Delta_s^{*2}}-\frac{48I_1(\Delta_s^*)}{\Delta_s^{*3}} \qquad \text{B69}$$

Therefore

$$1-\frac{I_4(\Delta_s^*)}{I_0(\Delta_s^*)}=1-1+\frac{8I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}-\frac{24I_0(\Delta_s^*)}{\Delta_s^{*2}I_0(\Delta_s^*)}+\frac{48I_1(\Delta_s^*)}{\Delta_s^{*3}I_0(\Delta_s^*)}$$

$$=\frac{8}{\Delta_s^{\bullet}}\left(\frac{I_1(\Delta_s^{\bullet})}{I_0(\Delta_s^{\bullet})}-\frac{3}{\Delta_s^{\bullet}}+\frac{6I_1(\Delta_s^{\bullet})}{\Delta_s^{\bullet 2}I_0(\Delta_s^{\bullet})}\right) \quad \text{B70}$$

Substituting Eqn. B70 into Eqn. B68 gives

$$=-\frac{\tau\Delta_s^{2}d_s^{2}n_0\Delta_s^{2}}{16(\hbar)^2kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{8}{\Delta_s^{\bullet}}\left(\frac{I_1(\Delta_s^{\bullet})}{I_0(\Delta_s^{\bullet})}-\frac{3}{\Delta_s^{\bullet}}+\frac{6I_1(\Delta_s^{\bullet})}{\Delta_s^{\bullet 2}I_0(\Delta_s^{\bullet})}\right)\frac{\nabla_sT}{T}$$

$$=-\frac{\tau\Delta_s^{2}d_s^{2}n_0k\Delta_s^{\bullet}}{2(\hbar)^2}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_1(\Delta_s^{\bullet})}{I_0(\Delta_s^{\bullet})}-\frac{3}{\Delta_s^{\bullet}}+\frac{6I_1(\Delta_s^{\bullet})}{\Delta_s^{\bullet 2}I_0(\Delta_s^{\bullet})}\right)\nabla_sT \quad \text{B71}$$

The next term U_7 of Eqn. B35 is given by Eqn. B42. Integrating U_7 with respect to time, using Eqn. B63, we have

$$U_7=-\frac{\Delta_s^{2}d_s^{2}d_sd_zn_0}{(\pi\hbar)^2\hbar^2I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\frac{1}{d_sd_z}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}+\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)\Delta_s\Delta_z\cos\frac{Z_s}{h}\cos\frac{Z_z}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''\frac{\nabla_sT}{T}$$

$$U_7=-\frac{\tau\Delta_s^{2}d_s^{2}n_0\Delta_s\Delta_z}{2(\pi\hbar)^2\hbar^2I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_sT}{T}$$

$$\times\int_0^{\pi}dZ_s\cos\frac{Z_s}{h}\sin^2\frac{Z_s}{h}\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi}dZ_z\cos\frac{Z_z}{\hbar}\exp\left(\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)$$

Substituting Eqn. B53 and expressing the integrals in terms of modified Bessel functions, we get

$$U_7=-\frac{\tau\Delta_s^{2}d_s^{2}n_0\Delta_s\Delta_z}{2(\pi\hbar)^2\hbar^2I_0(\Delta_s^{\bullet})I_0(\Delta_z^{\bullet})kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\frac{\nabla_sT}{T}$$

x

$$\int_0^{\pi}dZ_s\frac{1}{4}\left(\cos\frac{Z_s}{\hbar}-\cos\frac{3Z_s}{\hbar}\right)\exp\left(\Delta_s^{\bullet}\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi}dZ_z\cos\frac{Z_z}{\hbar}\exp\left(\Delta_z^{\bullet}\cos\frac{Z_z}{\hbar}\right)$$

$$U_7 = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s \Delta_z}{8(\hbar)^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\frac{\nabla_s T}{T}\{I_1(\Delta_s^*) - I_3(\Delta_s^*)\} I_1(\Delta_z^*)$$

$$= -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s \Delta_z}{8(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\frac{\nabla_s T}{T}\left\{\frac{I_1(\Delta_s^*) - I_3(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \qquad \text{B72}$$

By substituting Eqn. B55 into Eqn. B72, U_7 can be expressed in terms I_0 and I_1 as follows

$$= -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s \Delta_z}{8(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\frac{\nabla_s T}{T}\left\{\frac{4}{\Delta_s^*} - \frac{8 I_1(\Delta_s^*)}{\Delta_s^{*2} I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$= -\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_s^{\,*} \Delta_z k}{2(\hbar)^2}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\left\{1 - \frac{2 I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\nabla_s T \qquad \text{B73}$$

The next term U_8 of Eqn. B35 is given by Eqn. B43. Integrating U_8 with respect to time, using Eqn. B63, we have

$$U_8 = +\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\frac{1}{d_s d_z}\int_0^\infty \exp\left(-\frac{t}{\tau}\right)dt$$

$$\text{x} \int_0^\pi dZ_s \int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right)\Delta_s \cos\frac{Z_s}{h}$$

$$\times \sin^2\frac{Z_s}{h}\cos^2\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0 + E_s \cos wt'']dt''\;\nabla_s \mu$$

$$U_8 = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s}{2(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\nabla_s \mu$$

$$\text{x} \int_0^\pi dZ_s \cos\frac{Z_s}{h}\sin^2\frac{Z_s}{h}\int_0^\pi dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) \qquad \text{B74}$$

Substituting Eqn. B53 into Eqn. B74 and expressing the integrals in terms of modified Bessel functions, we get

$$U_8 = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_s}{2(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\nabla_s \mu$$

$$x\int_0^{\pi} dZ_s \frac{1}{4}\left(\cos\frac{Z_s}{\hbar}-\cos\frac{3Z_s}{\hbar}\right)\exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi} dZ_z \exp\left(\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)$$

$$U_8=+\frac{\tau\Delta_s^{\,2}d_s^{\,2}n_0\Delta_s}{8(\hbar)^2 I_0(\Delta_s^{*})I_0(\Delta_z^{*})kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\nabla_s\mu\,\{I_1(\Delta_s^{*})-I_3(\Delta_s^{*})\}I_0(\Delta_z^{*})$$

$$U_8=+\frac{\tau\Delta_s^{\,2}d_s^{\,2}n_0\Delta_s}{8(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\nabla_s\mu\left\{\frac{I_1(\Delta_s^{*})-I_3(\Delta_s^{*})}{I_0(\Delta_s^{*})}\right\}$$

Substituting Eqn. B55, we have

$$U_8=+\frac{\tau\Delta_s^{\,2}d_s^{\,2}n_0\Delta_s}{8(\hbar)^2 kT}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\nabla_s\mu\left\{\frac{4}{\Delta_s^{*}}-\frac{8I_1(\Delta_s^{*})}{\Delta_s^{*2}I_0(\Delta_s^{*})}\right\}$$

$$U_8=+\frac{\tau\Delta_s^{\,2}d_s^{\,2}n_0}{2(\hbar)^2}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left\{1-\frac{2I_1(\Delta_s^{*})}{\Delta_s^{*}\,I_0(\Delta_s^{*})}\right\}\nabla_s\mu \qquad \text{B75}$$

The next term U_9 of Eqn. B35 is given by Eqn. B44 as follows

$$U_9=+\frac{\Delta_s^{\,2}d_s^{\,2}n_0\Delta_z}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^{*})I_0(\Delta_z^{*})kT}(\varepsilon_0-\mu)\frac{\nabla_s T}{T}$$

$$x\int_0^{\pi} dZ_s\sin^2\frac{Z_s}{\hbar}\exp\left(\Delta_s^{*}\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi} dZ_z\cos\frac{Z_z}{h}\exp\left(\Delta_z^{*}\cos\frac{Z_z}{\hbar}\right)$$

$$x\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\ \cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\ \cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt'' \qquad \text{B76}$$

The time dependent integral in Eqn. B76 is

$$\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt\ \cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''$$

$$=\frac{1}{2}\int_0^{\infty}dt\exp\left(-\frac{t}{\tau}\right)$$

$$\left[\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''+\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\right)\right.$$

$$+\cos\left(\frac{ed_s}{\hbar}\int_{t-t'}^{t}\left[E_0+E_s\cos wt''\right]dt''-\frac{ed_z}{\hbar}\int_{t-t'}^{t}\left[E_0+E_z\cos wt''\right]dt''\right)\Bigg]$$

$$=\frac{1}{2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left[\frac{\tau}{1+\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)+\left(\frac{ed_zE_0}{\hbar}+nw\right)\right]^2\tau^2}\right.$$

$$\left.+\frac{\tau}{1+\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)-\left(\frac{ed_zE_0}{\hbar}+nw\right)\right]^2\tau^2}\right]$$

For weak electric fields, $\left(\frac{ed_sE_0}{\hbar}+nw\right)<<1$

$$=\frac{1}{2}\sum_{n=-\infty}^{\infty}J_n^2(a)\left\{2\tau\left[1-0\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)+\left(\frac{ed_zE_0}{\hbar}+nw\right)\right]^2\right.\right.$$

$$\left.\left.-0\left[\left(\frac{ed_sE_0}{\hbar}+nw\right)-\left(\frac{ed_zE_0}{\hbar}+nw\right)\right]^2\right]\right\}$$

$$=\sum_{n=-\infty}^{\infty}J_n^2(a)\tau \qquad \text{B77}$$

Substituting Eqn. B77 into Eqn. B76 gives

$$U_9=+\frac{\tau\Delta_s^{\,2}d_s^{\,2}n_0\Delta_z}{(\pi\hbar)^2\hbar^2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_sT}{T}$$

$$\text{x}\int_0^{\pi}dZ_s\sin^2\frac{Z_s}{h}\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi}dZ_z\cos\frac{Z_z}{h}\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$U_9=+\frac{\tau\Delta_s^{\,2}d_s^{\,2}n_0\Delta_z}{(\pi\hbar)^2\hbar^2I_0(\Delta_s^*)I_0(\Delta_z^*)kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_sT}{T}$$

$$\text{x}\ \frac{1}{2}\int_0^{\pi}dZ_s\left(1-\cos\frac{2Z_s}{h}\right)\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}\right)\int_0^{\pi}dZ_z\cos\frac{Z_z}{h}\exp\left(\Delta_z^*\cos\frac{Z_z}{\hbar}\right)$$

$$U_9 = +\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_z}{2(\hbar)^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_s T}{T}\{I_0(\Delta_s^*)-I_2(\Delta_s^*)\}I_1(\Delta_z^*)$$

$$U_9 = +\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_z}{2(\hbar)^2 kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_s T}{T}\left\{\frac{I_0(\Delta_s^*)-I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$U_9 = +\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_z}{2(\hbar)^2 kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_s T}{T}\left\{1-\frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$U_9 = +\frac{2\tau\Delta_s\, d_s{}^2 n_0\Delta_z\Delta_s}{2(\hbar)^2\Delta_s^* kT}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_s T}{T}\left\{\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$U_9 = +\frac{\tau\Delta_s\, d_s{}^2 n_0\Delta_z}{(\hbar)^2}(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_s T}{T}\left\{\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$U_9 = +\frac{\tau\Delta_s\, d_s{}^2 n_0\Delta_z k}{(\hbar)^2}\left(\frac{\varepsilon_0-\mu}{kT}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\left\{\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\nabla_s T \qquad \text{B78}$$

where we have expressed all the integrals in terms of modified Bessel functions and made use of Eqn. B61. The next term U_{10} of Eqn. B35 is given by Eqn. B45 as follows

$$U_{10} = -\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\frac{1}{d_s d_z}\int_0^{\infty}\exp\left(-\frac{t}{\tau}\right)dt$$

$$\times\int_0^{\pi}dZ_s\int_0^{\pi}dZ_z\exp\left(\Delta_s^*\cos\frac{Z_s}{\hbar}+\Delta_z^*\cos\frac{Z_z}{\hbar}\right)\Delta_z\Delta_s\cos\frac{Z_z}{h}\cos\frac{Z_s}{h}$$

$$\times\sin^2\frac{Z_s}{h}\cos\frac{ed_s}{\hbar}\int_{t-t'}^{t}[E_0+E_s\cos wt'']dt''$$

$$\cos\frac{ed_z}{h}\int_{t-t'}^{t}[E_0+E_z\cos wt'']dt''\frac{\nabla_s T}{T}$$

Eqn. B45 is integrated with respect to time using Eqn. B77, followed by substitution of Eqn. B53 as follows

$$U_{10} = -\frac{\tau\Delta_s{}^2 d_s{}^2 n_0\Delta_z\Delta_s}{(\pi\hbar)^2\hbar^2 I_0(\Delta_s^*)I_0(\Delta_z^*)kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{\nabla_s T}{T}$$

$$\text{x} \int_0^{\pi} dZ_s \cos\frac{Z_s}{h} \sin^2\frac{Z_s}{h}\left(\Delta_s^{*} \cos\frac{Z_s}{\hbar}\right)\int_0^{\pi} dZ_z \cos\frac{Z_z}{h} \exp\left(\Delta_z^{*} \cos\frac{Z_z}{\hbar}\right)$$

$$U_{10} = -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z \Delta_s}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^{*}) I_0(\Delta_z^{*}) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\text{x} \ \frac{1}{4}\int_0^{\pi} dZ_s\left(\cos\frac{Z_s}{\hbar} - \cos\frac{3Z_s}{\hbar}\right)\exp\left(\Delta_s^{*} \cos\frac{Z_s}{\hbar}\right)\int_0^{\pi} dZ_z \cos\frac{Z_z}{h} \exp\left(\Delta_z^{*} \cos\frac{Z_z}{\hbar}\right)$$

$$U_{10} = -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z \Delta_s}{4(\hbar)^2 I_0(\Delta_s^{*}) I_0(\Delta_z^{*}) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \{I_1(\Delta_s^{*}) - I_3(\Delta_s^{*})\} I_1(\Delta_z^{*})$$

$$U_{10} = -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z \Delta_s}{4(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \left\{\frac{I_1(\Delta_s^{*}) - I_3(\Delta_s^{*})}{I_0(\Delta_s^{*})}\right\} \frac{I_1(\Delta_z^{*})}{I_0(\Delta_z^{*})} \qquad \text{B79}$$

Substituting Eqn. B55 into Eqn. B79 expresses the equation in terms of I_0 and I_1.

$$U_{10} = -\frac{\tau \Delta_s{}^2 d_s{}^2 n_0 \Delta_z \Delta_s}{4(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \left\{\frac{4}{\Delta_s^{*}} - \frac{8 I_1(\Delta_s^{*})}{\Delta_s^{*2} I_0(\Delta_s^{*})}\right\} \frac{I_1(\Delta_z^{*})}{I_0(\Delta_z^{*})}$$

$$U_{10} = -\frac{\tau \Delta_s \, d_s{}^2 n_0 \Delta_z \Delta_s{}^{*} k}{(\hbar)^2} \sum_{n=-\infty}^{\infty} J_n^2(a) \left\{1 - \frac{2 I_1(\Delta_s^{*})}{\Delta_s^{*} I_0(\Delta_s^{*})}\right\} \frac{I_1(\Delta_z^{*})}{I_0(\Delta_z^{*})} \nabla_s T \qquad \text{B80}$$

The next term U_{11} of Eqn. B35 is given by Eqn. B46 as follows

$$U_{11} = -\frac{\Delta_s{}^2 d_s{}^2 d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^{*}) I_0(\Delta_z^{*}) kT} \frac{1}{d_s d_z} \int_0^{\infty} \exp\left(-\frac{t}{\tau}\right) dt$$

$$\text{x} \int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^{*} \cos\frac{Z_s}{\hbar} + \Delta_z^{*} \cos\frac{Z_z}{\hbar}\right) \Delta_z^2 \cos^2\frac{Z_z}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt''] dt''$$

$$\cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt''] dt'' \frac{\nabla_s T}{T} \qquad \text{B81}$$

Eqn. B81 is integrated with respect to time using Eqn. B77

$$U_{11} = -\frac{\tau \Delta_s^{\ 2} d_s^{\ 2} n_0 \Delta_z^2}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\text{x} \int_0^\pi dZ_s \sin^2 \frac{Z_s}{h}\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^\pi dZ_z \cos^2 \frac{Z_z}{h} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

The following replacements are also made

$$\sin^2 \frac{Z_s}{h} = \frac{1}{2}\left(1 - \cos\frac{2Z_s}{h}\right) \quad \text{and} \quad \cos^2 \frac{Z_z}{h} = \frac{1}{2}\left(1 + \cos\frac{2Z_z}{h}\right)$$

$$U_{11} = -\frac{\tau \Delta_s^{\ 2} d_s^{\ 2} n_0 \Delta_z^2}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T}$$

$$\text{x} \int_0^\pi dZ_s \frac{1}{2}\left(1 - \cos\frac{2Z_s}{h}\right) \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^\pi dZ_z \frac{1}{2}\left(1 + \cos\frac{2Z_z}{h}\right) \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_{11} = -\frac{\tau \Delta_s^{\ 2} d_s^{\ 2} n_0 \Delta_z^2}{4(\hbar)^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \left(I_0(\Delta_s^*) - I_2(\Delta_s^*)\right)\left(I_0(\Delta_z^*) + I_2(\Delta_z^*)\right)$$

$$U_{11} = -\frac{\tau \Delta_s^{\ 2} d_s^{\ 2} n_0 \Delta_z^2}{4(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \left(1 - \frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right)\left(1 + \frac{I_2(\Delta_z^*)}{I_0(\Delta_z^*)}\right) \qquad \text{B82}$$

where we have expressed all the integrals in terms of modified Bessel functions.

Applying Eqn. A33

$$1 + \frac{I_2(\Delta_z^*)}{I_0(\Delta_z^*)} = 1 + \frac{I_0(\Delta_z^*) - \frac{2}{\Delta_z^*} I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$= 2 - \frac{2}{\Delta_z^*} \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$= 2\left(1 - \frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right) \qquad \text{B83}$$

Using Eqns. B61 and B83, Eqn. B82 can be expressed in terms of I_0 and I_1 as follows

$$U_{11} = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z^2}{4(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \frac{2}{\Delta_s^*} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} 2\left(1 - \frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)$$

$$U_{11} = -\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z^2}{(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{\nabla_s T}{T} \frac{1}{\Delta_s^*} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \left(1 - \frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)$$

$$U_{11} = -\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z \Delta_z^* k}{(\hbar)^2} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \left(1 - \frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right) \nabla_s T \qquad \text{B84}$$

The last term U_{12} of Eqn. B35 is given by Eqn. B47 as follows

$$U_{12} = +\frac{\Delta_s^{\,2} d_s^{\,2} d_s d_z n_0}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \frac{1}{d_s d_z} \int_0^{\infty} \exp\left(-\frac{t}{\tau}\right) dt$$

$$\text{x} \int_0^{\pi} dZ_s \int_0^{\pi} dZ_z \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar} + \Delta_z^* \cos\frac{Z_z}{\hbar}\right) \Delta_z \cos\frac{Z_z}{h}$$

$$\times \sin^2\frac{Z_s}{h} \cos\frac{ed_s}{\hbar} \int_{t-t'}^{t} [E_0 + E_s \cos wt'']dt'' \cos\frac{ed_z}{h} \int_{t-t'}^{t} [E_0 + E_z \cos wt'']dt'' \nabla_s \mu \qquad \text{B85}$$

Eqn. B85 is integrated with respect to time using Eqn. B77

$$U_{12} = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z}{(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \nabla_s \mu$$

$$\text{x} \int_0^{\pi} dZ_s \sin^2\frac{Z_s}{h} \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_{12} = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z}{2(\pi\hbar)^2 \hbar^2 I_0(\Delta_s^*) I_0(\Delta_z^*) kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \nabla_s \mu$$

$$\text{x} \int_0^{\pi} dZ_s \left(1 - \cos\frac{2Z_s}{h}\right) \exp\left(\Delta_s^* \cos\frac{Z_s}{\hbar}\right) \int_0^{\pi} dZ_z \cos\frac{Z_z}{\hbar} \exp\left(\Delta_z^* \cos\frac{Z_z}{\hbar}\right)$$

$$U_{12} = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z}{2(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a)\, \nabla_s \mu \left(1 - \frac{I_2(\Delta_s^*)}{I_0(\Delta_s^*)}\right) \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \qquad \text{B86}$$

Substituting Eqn. B61 into Eqn. B86, we have

$$U_{12} = +\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 \Delta_z}{2(\hbar)^2 kT} \sum_{n=-\infty}^{\infty} J_n^2(a)\, \nabla_s \mu \,\frac{2}{\Delta_s^*} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}$$

$$U_{12} = +\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z}{(\hbar)^2} \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \nabla_s \mu \qquad \text{B87}$$

Summing up all the terms U_1, U_2, ...U_{12} of Eqn. B35, we have

$$S_2^{'} = -\frac{\tau\Delta_s\, d_s^{\,2} n_0 k}{(\hbar)^2} \frac{(\varepsilon_0 - \mu)^2}{kT} \sum_{n=-\infty}^{\infty} J_n^2(a) \left\{\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\} \nabla_s T$$

$$+\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 k}{(\hbar)^2} \left(\frac{\varepsilon_0 - \mu}{kT}\right) \sum_{n=-\infty}^{\infty} J_n^2(a) \left(1 - \frac{2 I_1(\Delta_s^*)}{\Delta_s^*\, I_0(\Delta_s^*)}\right) \nabla_s T$$

$$+\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z k}{(\hbar)^2} \left(\frac{\varepsilon_0 - \mu}{kT}\right) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \nabla_s T$$

$$-\frac{\tau\Delta_s d_s^{\,2}\, n_0}{(\hbar)^2} (\varepsilon_0 - \mu) \sum_{n=-\infty}^{\infty} J_n^2(a) \frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} \nabla_s \mu$$

$$+\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 k}{2(\hbar)^2} \frac{(\varepsilon_0 - \mu)}{kT} \left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right) \left\{1 - \frac{2 I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right\} \nabla_s T$$

$$-\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0 k \Delta_s^*}{2(\hbar)^2} \left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right) \left(\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)} - \frac{3}{\Delta_s^*} + \frac{6 I_1(\Delta_s^*)}{\Delta_s^{*2} I_0(\Delta_s^*)}\right) \nabla_s T$$

$$-\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_s^* \Delta_z k}{2(\hbar)^2} \left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right) \left\{1 - \frac{2 I_1(\Delta_s^*)}{\Delta_s^*\, I_0(\Delta_s^*)}\right\} \frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)} \nabla_s T$$

$$+\frac{\tau\Delta_s^{\,2} d_s^{\,2} n_0}{2(\hbar)^2} \left(1 + \sum_{n=-\infty}^{\infty} J_n^2(a)\right) \left\{1 - \frac{2 I_1(\Delta_s^*)}{\Delta_s^*\, I_0(\Delta_s^*)}\right\} \nabla_s \mu$$

$$+\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z k}{(\hbar)^2}\left(\frac{\varepsilon_0-\mu}{kT}\right)\sum_{n=-\infty}^{\infty} J_n^2(a)\left\{\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\nabla_s T$$

$$-\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z \Delta_s^* k}{(\hbar)^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\left\{1-\frac{2I_1(\Delta_s^*)}{\Delta_s^*\, I_0(\Delta_s^*)}\right\}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\nabla_s T$$

$$-\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z \Delta_z^* k}{(\hbar)^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\nabla_s T$$

$$+\frac{\tau\Delta_s\, d_s^{\,2} n_0 \Delta_z}{(\hbar)^2}\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\nabla_s \mu$$

$$S_2' = -\frac{\tau\Delta_s d_s^{\,2}\, n_0}{(\hbar)^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty} J_n^2(a)\right.$$

$$\left.-\frac{\Delta_s}{2}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty} J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s \mu$$

$$-\frac{\tau\Delta_s\, d_s^{\,2} n_0 k}{(\hbar)^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty} J_n^2(a)\right.$$

$$-\Delta_s\left(\frac{\varepsilon_0-\mu}{kT}\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\sum_{n=-\infty}^{\infty} J_n^2(a)$$

$$-\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)$$

$$-\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty} J_n^2(a)$$

$$+\Delta_z\Delta_s^*\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T$$

$$S_2' = -\frac{\tau\Delta_s d_s^{\,2} n_0}{(\hbar)^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}\nabla_s\mu$$

$$-\frac{\tau\Delta_s d_s^{\,2} n_0 k}{(\hbar)^2}\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T$$

Let $\sigma_s(E)=\dfrac{e^2\tau\Delta_s d_s^{\,2} n_0}{(\hbar)^2}\dfrac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}$

$$S_2' = -\sigma_s(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}\nabla_s\frac{\mu}{e}$$

$$-\sigma_s(E)\frac{k}{e^2}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^*I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^*I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}\nabla_s T \qquad \text{B88}$$

Now, $S' = S_1' + S_2'$

$$S' = -\sigma_s(E)\frac{1}{e}\sum_{n=-\infty}^{\infty}J_n^2(a)\left\{(\varepsilon_0-\mu)-\Delta_s\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}E_n$$

$$-\sigma_s(E)\frac{1}{e}\left\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\right.$$

$$\left.-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}\nabla_s\frac{\mu}{e}$$

$$-\sigma_s(E)\frac{k}{e^2}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^*I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T \qquad \text{B89}$$

$$S^* = -\sigma_s(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\Delta_s\sum_{n=-\infty}^{\infty}J_n^2(a)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)$$

$$-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}E_n$$

$$-\sigma_s(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)$$

$$-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}\nabla_s\frac{\mu}{e}$$

$$-\sigma_s(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T$$

$$S=-\sigma_s(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)$$

$$-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}\left(E_n+\nabla_s\frac{\mu}{e}\right)$$

$$-\sigma_s(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^{*}\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T$$

$$S'=-\sigma_s(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}E_{sn}^*$$

$$-\sigma_s(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^{*}\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T$$

$$S'=-\sigma_s(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}E_{sn}^*$$

$$-\sigma_s(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\ \nabla_s T \qquad \text{B90}$$

Where we have defined E_{sn}^* as

$$E_{sn}^* = E_n + \nabla_s \frac{\mu}{e}$$

Now going through the same steps as above, Z' is found to be

$$Z' = -\sigma_z(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)-\Delta_s\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\Bigg\}E_{zn}^*$$

$$-\sigma_z(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_s\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_z\Delta_z^*}{2}\left(1-\frac{3I_0(\Delta_z^*)}{\Delta_z^* I_1(\Delta_z^*)}+\frac{6}{\Delta_z^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_z\Delta_s}{2}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_s\Delta_s^*\left(1-\frac{I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_z T \qquad \text{B91}$$

The axial and circumferential components of the thermal current density are respectively given by

$$q_z = Z' + S'\sin\theta_h \qquad \text{B92}$$

$$q_c = S'\cos\theta_h \qquad \text{B93}$$

Therefore in order to obtain the axial thermal current density, Eqn. B90 and B91are substituted into Eqn. B92 as follows

$$q_z = -\sigma_z(E)\frac{1}{e}\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)-\Delta_s\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\Bigg\}E_{zn}^*$$

$$-\sigma_z(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_s\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_z\Delta_z^*}{2}\left(1-\frac{3I_0(\Delta_z^*)}{\Delta_z^* I_1(\Delta_z^*)}+\frac{6}{\Delta_z^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_z^*\Delta_s}{2}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_s\Delta_s^*\left(1-\frac{I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_z T$$

$$-\sigma_s(E)\frac{1}{e}\left\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\right.$$

$$\left.-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}E_{sn}^*\sin\theta_h$$

$$-\sigma_s(E)\frac{k}{e^2}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^*I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^*I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}\nabla_s T\sin\theta_h \qquad \text{B94}$$

Also, from Figure A1, we see that

$$E_s = E\sin\theta_h \qquad \text{B95}$$

$$\nabla_s T = \nabla_z T\sin\theta_h \qquad \text{B96}$$

So, substitution of Eqns. B95 and B96 into Eqn. B94 gives

$$q_z = -\sigma_z(E)\frac{1}{e}\left\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$\left.-\frac{\Delta_z}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)-\Delta_s\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\right\}E_{zn}^*$$

$$-\sigma_z(E)\frac{k}{e^2}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_z}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_s\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_z\Delta_z^*}{2}\left(1-\frac{3I_0(\Delta_z^*)}{\Delta_z^* I_1(\Delta_z^*)}+\frac{6}{\Delta_z^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_z^*\Delta_s}{2}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\Delta_s\Delta_s^*\left(1-\frac{I_1(\Delta_s^*)}{\Delta_s^* I_0(\Delta_s^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}\nabla_z T$$

$$-\sigma_s(E)\frac{1}{e}\left\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\right.$$

$$\left.-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}E_{zn}^*\sin^2\theta_h$$

$$-\sigma_s(E)\frac{k}{e^2}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^{*}\left(1-\frac{I_1(\Delta_z^{*})}{\Delta_z^{*}I_0(\Delta_z^{*})}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_z T\sin^2\theta_h$$

The terms of the above equation are rearranged, and then multiplied and divided by kT as follows

$$q_z=-\frac{1}{e}\Bigg\{\sigma_z(E)\Bigg[(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_z^{*})}{I_1(\Delta_z^{*})}-\frac{2}{\Delta_z^{*}}\right)-\Delta_s\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^{*})}{I_0(\Delta_s^{*})}\Bigg]$$

$$+\sigma_s(E)\sin^2\theta_h\Bigg[(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^{*})}{I_1(\Delta_s^{*})}-\frac{2}{\Delta_s^{*}}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^{*})}{I_0(\Delta_z^{*})}\Bigg]\Bigg\}E_{zn}^{*}$$

$$-\frac{k}{e^2}\Bigg\{\sigma_z(E)\Bigg[\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_z^{*})}{I_1(\Delta_z^{*})}-\frac{2}{\Delta_z^{*}}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_s\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_s^{*})}{I_0(\Delta_s^{*})}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_z\Delta_z^{*}}{2}\left(1-\frac{3I_0(\Delta_z^{*})}{\Delta_z^{*}I_1(\Delta_z^{*})}+\frac{6}{\Delta_z^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_z^{*}\Delta_s}{2}\left(\frac{I_0(\Delta_z^{*})}{I_1(\Delta_z^{*})}-\frac{2}{\Delta_z^{*}}\right)\frac{I_1(\Delta_s^{*})}{I_0(\Delta_s^{*})}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_s\Delta_s^{*}\left(1-\frac{I_1(\Delta_s^{*})}{\Delta_s^{*}I_0(\Delta_s^{*})}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg]$$

$$+\sigma_s(E)\sin^2\theta_h\Bigg[\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^*I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^*I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg]\Bigg\}\nabla_z T$$

$$q_z=-\frac{kT}{e}\Bigg\{\sigma_z(E)\Bigg[\left(\frac{\varepsilon_0-\mu}{kT}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z^*}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)-\Delta_s^*\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\Bigg]$$

$$+\sigma_s(E)\sin^2\theta_h\Bigg[\left(\frac{\varepsilon_0-\mu}{kT}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s^*}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z^*\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg]\Bigg\}E_{zn}^*$$

$$-\frac{k^2T}{e^2}\Bigg\{\sigma_z(E)\Bigg[\left(\frac{\varepsilon_0-\mu}{kT}\right)^2\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_z^*}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_z^*)}{I_1(\Delta_z^*)}-\frac{2}{\Delta_z^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_s^*\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_s^*)}{I_0(\Delta_s^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{(\Delta_z^*)^2}{2}\left(1-\frac{3I_0(\Delta_z^*)}{\Delta_z^*I_1(\Delta_z^*)}+\frac{6}{\Delta_z^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_z^{\bullet}\Delta_s^{\bullet}}{2}\left(\frac{I_0(\Delta_z^{\bullet})}{I_1(\Delta_z^{\bullet})}-\frac{2}{\Delta_z^{\bullet}}\right)\frac{I_1(\Delta_s^{\bullet})}{I_0(\Delta_s^{\bullet})}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+(\Delta_s^{\bullet})^2\left(1-\frac{I_1(\Delta_s^{\bullet})}{\Delta_s^{\bullet}I_0(\Delta_s^{\bullet})}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\left(\frac{\varepsilon_0-\mu}{kT}\right)^2\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s^{\bullet}}{2}\left(\frac{\varepsilon_0-\mu}{kT}\right)\left(\frac{I_0(\Delta_s^{\bullet})}{I_1(\Delta_s^{\bullet})}-\frac{2}{\Delta_s^{\bullet}}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z^{\bullet}\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^{\bullet})}{I_0(\Delta_z^{\bullet})}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{(\Delta_s^{\bullet})^2}{2}\left(1-\frac{3I_0(\Delta_s^{\bullet})}{\Delta_s^{\bullet}I_1(\Delta_s^{\bullet})}+\frac{6}{\Delta_s^{\bullet 2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^{\bullet}\Delta_z^{\bullet}}{2}\left(\frac{I_0(\Delta_s^{\bullet})}{I_1(\Delta_s^{\bullet})}-\frac{2}{\Delta_s^{\bullet}}\right)\frac{I_1(\Delta_z^{\bullet})}{I_0(\Delta_z^{\bullet})}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+(\Delta_z^{\bullet})^2\left(1-\frac{I_1(\Delta_z^{\bullet})}{\Delta_z^{\bullet}I_0(\Delta_z^{\bullet})}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\Bigg\}\nabla_z T \qquad \text{B97}$$

If we define C_i as

$$C_i=1-\frac{3I_0(\Delta_s^{\bullet})}{\Delta_s^{\bullet}I_1(\Delta_s^{\bullet})}+\frac{6}{\Delta_s^{\bullet 2}},\quad i=s,z \qquad \text{B98}$$

And use the definitions of ξ, A_i and B_i given in Eqn. A58, Eqn. B97 is rewritten as follows

$$q_z=-\frac{kT}{e}\left\{\sigma_z(E)\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{\bullet}}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^{\bullet}A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{\bullet}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{\bullet}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}E_{zn}^{\bullet}$$

$$-\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^*}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.$$

$$-2\Delta_s^*\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_z^*)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_z^*\Delta_s^*}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.\left.+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}\nabla_zT \qquad \text{B99}$$

In order to obtain circumferential thermal current density, Eqn. B90 is substituted into Eqn. B93

$$q_c=-\sigma_s(E)\frac{1}{e}\left\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\right.$$

$$\left.-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}E_{sn}^*\cos\theta_h$$

$$-\sigma_s(E)\frac{k}{e^2}\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^*I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T\cos\theta_h$$

$$q_c=-\sigma_s(E)\frac{1}{e}\cos\theta_h\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}E_{sn}^*$$

$$-\sigma_s(E)\frac{k}{e^2}\Bigg\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_s T\cos\theta_h$$

Using Eqns. B95 and B96, we have

$$q_c=-\sigma_s(E)\frac{1}{e}\sin\theta_h\cos\theta_h\Bigg\{(\varepsilon_0-\mu)\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$-\frac{\Delta_s}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\Bigg\}E_{zn}^*$$

$$-\sigma_s(E)\frac{k}{e^2}\sin\theta_h\cos\theta_h\left\{\frac{(\varepsilon_0-\mu)^2}{kT}\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{\Delta_s\Delta_s^*}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^*\Delta_z}{2}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\Delta_z\Delta_z^*\left(1-\frac{I_1(\Delta_z^*)}{\Delta_z^* I_0(\Delta_z^*)}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}\nabla_z T \qquad \text{B100}$$

Multiplying and dividing Eqn. B100 by *kT*, we get

$$q_c=-\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$\left.-\frac{\Delta_s^*}{2}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)-\Delta_z^*\sum_{n=-\infty}^{\infty}J_n^2(a)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\right\}E_{zn}^*$$

$$-\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\left\{\left(\frac{\varepsilon_0-\mu}{kT}\right)^2\sum_{n=-\infty}^{\infty}J_n^2(a)\right.$$

$$-\frac{\Delta_s^*}{2}\frac{(\varepsilon_0-\mu)}{kT}\left(\frac{I_0(\Delta_s^*)}{I_1(\Delta_s^*)}-\frac{2}{\Delta_s^*}\right)\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z^*\left(\frac{\varepsilon_0-\mu}{kT}\right)\frac{I_1(\Delta_z^*)}{I_0(\Delta_z^*)}\sum_{n=-\infty}^{\infty}J_n^2(a)$$

$$+\frac{(\Delta_s^*)^2}{2}\left(1-\frac{3I_0(\Delta_s^*)}{\Delta_s^* I_1(\Delta_s^*)}+\frac{6}{\Delta_s^{*2}}\right)\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^{\bullet}\Delta_z^{\bullet}}{2}\left(\frac{I_0(\Delta_s^{\bullet})}{I_1(\Delta_s^{\bullet})}-\frac{2}{\Delta_s^{\bullet}}\right)\frac{I_1(\Delta_z^{\bullet})}{I_0(\Delta_z^{\bullet})}\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+(\Delta_z^{\bullet})^2\left(1-\frac{I_1(\Delta_z^{\bullet})}{\Delta_z^{\bullet}I_0(\Delta_z^{\bullet})}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_z T \qquad \text{B101}$$

Using the definitions in Eqns. A58 and B98, Eqn. 101 is rewritten as

$$q_c=-\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{\bullet}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{\bullet}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}E_{zn}^{\bullet}$$

$$-\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\Bigg\{\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{\bullet}}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z^{\bullet}\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^{\bullet})^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^{\bullet}\Delta_z^{\bullet}}{2}B_sA_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^{\bullet})^2\left(1-\frac{A_z}{\Delta_z^{\bullet}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\}\nabla_z T \qquad \text{B102}$$

Let χ_{ec} and χ_{ez} be the circumferential and axial components of the electron thermal conductivity respectively

$$\chi_{ec}=\sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\Bigg\{\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{\bullet}}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_z^{\bullet}\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^{\bullet})^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_s^{\bullet}\Delta_z^{\bullet}}{2}B_sA_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^{\bullet})^2\left(1-\frac{A_z}{\Delta_z^{\bullet}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg\} \qquad \text{B103}$$

$$\chi_{ez}=\frac{k^2T}{e^2}\Bigg\{\sigma_z(E)\Bigg[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{\bullet}}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$-2\Delta_s^{\bullet}\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_z^{\bullet})^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$+\frac{\Delta_z^{\bullet}\Delta_s^{\bullet}}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_s^{\bullet})^2\left(1-\frac{A_s}{\Delta_s^{\bullet}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\Bigg]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\Bigg\} \qquad \text{B104}$$

Onsagar Relations

$$j_c=-\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^*-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\}\nabla_z T \qquad \text{B105}$$

and

$$j_z=-\{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\}E_{zn}^*$$

$$-\left\{\sigma_z(E)\frac{k}{e}\left[\xi-\Delta_z^*B_z-\Delta_s^*A_s\right]+\sigma_s(E)\frac{k}{e}\sin^2\theta_h\left[\xi-\Delta_s^*B_s-\Delta_z^*A_z\right]\right\}\nabla_z T \qquad \text{B106}$$

Using Eqns. A61 and A65, Eqn. B105 can be written as

$$j_c=\sigma_{cz}E_{zn}^*-\sigma_{cz}\alpha_{cz}\nabla_z T \qquad \text{B107}$$

Similarly, using Eqns. A62 and A66, Eqn. B106 can be written as

$$j_z=\sigma_{zz}E_{zn}^*-\sigma_{zz}\alpha_{zz}\nabla_z T \qquad \text{B108}$$

We now make E_{zn}^* the subject in Eqn. A60

$$j_c=-\sigma_s(E)\sin\theta_h\cos\theta_h E_{zn}^*-\sigma_s(E)\frac{k}{e}\sin\theta_h\cos\theta_h\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\}\nabla_z T$$

$$E_{zn}^*=-\frac{j_c}{\sigma_s(E)\sin\theta_h\cos\theta_h}-\frac{k}{e}\{\xi-\Delta_s^*B_s-\Delta_z^*A_z\}\nabla_z T \qquad \text{B109}$$

Eqn. B109 is substituted into Eqn. B102

$$q_c=\sigma_s(E)\frac{kT}{e}\sin\theta_h\cos\theta_h\left\{\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-\Delta_z^{\bullet} A_z \sum_{n=-\infty}^{\infty} J_n^2(a) \Bigg\} \frac{j_c}{\sigma_s(E)\sin\theta_h \cos\theta_h}$$

$$+\sigma_s(E)\frac{kT}{e}\sin\theta_h \cos\theta_h \left\{ \xi \sum_{n=-\infty}^{\infty} J_n^2(a) - \frac{\Delta_s^{\bullet}}{2} B_s \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\right.$$

$$\left. -\Delta_z^{\bullet} A_z \sum_{n=-\infty}^{\infty} J_n^2(a) \right\} \frac{k}{e}\{\xi - \Delta_s^{\bullet} B_s - \Delta_z^{\bullet} A_z\} \nabla_z T$$

$$-\sigma_s(E)\frac{k^2 T}{e^2}\sin\theta_h \cos\theta_h \left\{ \xi^2 \sum_{n=-\infty}^{\infty} J_n^2(a) - \frac{\Delta_s^{\bullet}}{2}\xi B_s \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\right.$$

$$-2\Delta_z^{\bullet}\xi A_z \sum_{n=-\infty}^{\infty} J_n^2(a) + \frac{(\Delta_s^{\bullet})^2}{2} C_s \left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)$$

$$\left. +\frac{\Delta_s^{\bullet}\Delta_z^{\bullet}}{2} B_s A_z \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right) + (\Delta_z^{\bullet})^2 \left(1-\frac{A_z}{\Delta_z^{\bullet}}\right) \sum_{n=-\infty}^{\infty} J_n^2(a) \right\} \nabla_z T$$

$$q_c = \frac{kT}{e}\left\{ \xi \sum_{n=-\infty}^{\infty} J_n^2(a) - \frac{\Delta_s^{\bullet}}{2} B_s \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right) - \Delta_z^{\bullet} A_z \sum_{n=-\infty}^{\infty} J_n^2(a) \right\} j_c$$

$$-\sigma_s(E)\frac{k^2 T}{e^2}\sin\theta_h \cos\theta_h \left[\left\{ \xi^2 \sum_{n=-\infty}^{\infty} J_n^2(a) - \frac{\Delta_s^{\bullet}}{2}\xi B_s \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right)\right.\right.$$

$$-2\Delta_z^{\bullet}\xi A_z \sum_{n=-\infty}^{\infty} J_n^2(a) + \frac{(\Delta_s^{\bullet})^2}{2} C_s \left(1+\sum_{n=-\infty}^{\infty} J_n^2(a)\right)$$

$$\left. +\frac{\Delta_s^{\bullet}\Delta_z^{\bullet}}{2} B_s A_z \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right) + (\Delta_z^{\bullet})^2 \left(1-\frac{A_z}{\Delta_z^{\bullet}}\right) \sum_{n=-\infty}^{\infty} J_n^2(a) \right\}$$

$$\left. -\left\{ \xi \sum_{n=-\infty}^{\infty} J_n^2(a) - \frac{\Delta_s^{\bullet}}{2} B_s \left(1+3\sum_{n=-\infty}^{\infty} J_n^2(a)\right) - \Delta_z^{\bullet} A_z \sum_{n=-\infty}^{\infty} J_n^2(a) \right\} \{\xi - \Delta_s^{\bullet} B_s - \Delta_z^{\bullet} A_z\} \right] \nabla_z T$$

B110

We now make $E_{zn}^{\bullet}$ the subject in Eqn. B106

$$j_z = -\{\sigma_z(E) + \sigma_s(E)\sin^2\theta_h\} E_{zn}^{\bullet}$$

$$-\left\{ \sigma_z(E)\frac{k}{e}\left[\xi - \Delta_z^{\bullet} B_z - \Delta_s^{\bullet} A_s\right] + \sigma_s(E)\frac{k}{e}\sin^2\theta_h \left[\xi - \Delta_s^{\bullet} B_s - \Delta_z^{\bullet} A_z\right]\right\} \nabla_z T$$

$$E^{\bullet}_{zn} = -\frac{j_z}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h} - \left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\left[\xi - \Delta^{\bullet}_z B_z - \Delta^{\bullet}_s A_s\right]\right.$$

$$\left. + \frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\frac{k}{e}\sin^2\theta_h\left[\xi - \Delta^{\bullet}_s B_s - \Delta^{\bullet}_z A_z\right]\right\}\nabla_z T \qquad \text{B111}$$

Eqn. B111 is substituted into Eqn. B99

$$q_z = \frac{kT}{e}\left\{\sigma_z(E)\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta^{\bullet}_z}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta^{\bullet}_s A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta^{\bullet}_s}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$\left.\left. - \Delta^{\bullet}_z A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}\frac{j_z}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}$$

$$+\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta^{\bullet}_z}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta^{\bullet}_s A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta^{\bullet}_s}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta^{\bullet}_z A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi - \Delta^{\bullet}_z B_z - \Delta^{\bullet}_s A_s\right]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi - \Delta^{\bullet}_s B_s - \Delta^{\bullet}_z A_z\right]\right\}\nabla_z T$$

$$-\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta^{\bullet}_z}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.$$

$$-2\Delta^{\bullet}_s\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a) + \frac{\left(\Delta^{\bullet}_z\right)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta^{\bullet}_z\Delta^{\bullet}_s}{2}A_s B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + \left(\Delta^{\bullet}_s\right)^2\left(1-\frac{A_s}{\Delta^{\bullet}_s}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.\left.+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}\nabla_zT$$

Simplifying we get

$$q_z=\frac{kT}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^*}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^*A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^*A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}j_z$$

$$-\frac{k^2T}{e^2}\left(\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^*}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.\right.$$

$$-2\Delta_s^*\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_z^*)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_z^*\Delta_s^*}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.\left.+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$-\left\{\sigma_z(E)\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^*}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^*A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\sigma_s(E)\sin^2\theta_h\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^*}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^*A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi-\Delta_z^{*}B_z-\Delta_s^{*}A_s\right]\right.$$

$$\left.\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi-\Delta_s^{*}B_s-\Delta_z^{*}A_z\right]\right\}\right)\nabla_z T$$

$$q_z=\frac{kT}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{*}}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^{*}A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{*}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{*}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}j_z$$

$$-\left(\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{*}}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.\right.$$

$$-2\Delta_s^{*}\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{\left(\Delta_z^{*}\right)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_z^{*}\Delta_s^{*}}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+\left(\Delta_s^{*}\right)^2\left(1-\frac{A_s}{\Delta_s^{*}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{*}}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^{*}\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{\left(\Delta_s^{*}\right)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.\left.+\frac{\Delta_s^{*}\Delta_z^{*}}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+\left(\Delta_z^{*}\right)^2\left(1-\frac{A_z}{\Delta_z^{*}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$-\frac{k^2T}{e^2}\left(\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\right)\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)\right.\right.$$

$$\left.-\frac{\Delta_z^{*}}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^{*}A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{*}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{*}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi-\Delta_z^{*}B_z-\Delta_s^{*}A_s\right]\right.$$

$$\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi-\Delta_s^{*}B_s-\Delta_z^{*}A_z\right]\right\}\right)\nabla_z T$$

$$q_z=\frac{kT}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{*}}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^{*}A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{*}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{*}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}j_z$$

$$-\left(\frac{k^2T}{e^2}\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{*}}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.\right.$$

$$-2\Delta_s^{*}\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_z^{*})^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_z^{*}\Delta_s^{*}}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_s^{*})^2\left(1-\frac{A_s}{\Delta_s^{*}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{*}}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^{*}\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a)+\frac{(\Delta_s^{*})^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.\left.+\frac{\Delta_s^{*}\Delta_z^{*}}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)+(\Delta_z^{*})^2\left(1-\frac{A_z}{\Delta_z^{*}}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$-\frac{k^2T}{e^2}\left(\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\right)\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)\right.\right.$$

$$\left.-\frac{\Delta_z^{*}}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^{*}A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{*}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{*}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$\times\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi-\Delta_z^{\bullet}B_z-\Delta_s^{\bullet}A_s\right]\right.$$

$$\left.\left.+\frac{\sigma_s(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\sin^2\theta_h\left[\xi-\Delta_s^{\bullet}B_s-\Delta_z^{\bullet}A_z\right]\right\}\right)\nabla_z T \qquad \text{B112}$$

Eqns. 110 and 112 are in the form of the Onsagar relations given by

$$q_c=\Pi_{cz}j_c-\mathrm{X}_{cz}\nabla_z T \qquad \text{B113}$$

and

$$q_z=\Pi_{zz}j_c-\mathrm{X}_{zz}\nabla_z T \qquad \text{B114}$$

Where X is the electron thermal conductivity when the carrier current density j is zero and Π, the Peltier coefficient, is given by $\Pi=\alpha T$. As usual α is the thermopower.

Comparing Eqn. B110 and Eqn.B112, we obtain the circumferential component of the Peltier coefficient Π as follows

$$\Pi_{cz}=\frac{k}{e}\left\{\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{\bullet}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{\bullet}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}T$$

Again comparing Eqn. B112 and Eqn. B114, we obtain the axial component of Π as follows

$$\Pi_{zz}=\frac{k}{e}\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_z^{\bullet}}{2}B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_s^{\bullet}A_s\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right.$$

$$\left.+\frac{\sigma_s(E)\sin^2\theta_h}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)-\frac{\Delta_s^{\bullet}}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)-\Delta_z^{\bullet}A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}T$$

Now, comparing Eqns. B110 and B113, the circumferential component of the electron thermal conductivity X_{cz} (when j = 0) is as follows

$$X_{cz} = \sigma_s(E)\frac{k^2T}{e^2}\sin\theta_h\cos\theta_h\left[\left\{\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a) + \frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_s^*\Delta_z^*}{2}B_sA_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + (\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}$$

$$\left.-\left\{\xi\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_s^*}{2}B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) - \Delta_z^*A_z\sum_{n=-\infty}^{\infty}J_n^2(a)\right\}\left\{\xi - \Delta_s^*B_s - \Delta_z^*A_z\right\}\right]$$

Also, comparing Eqns. B112 and B114, the circumferential component of the electron thermal conductivity X_{zz} (when j = 0) is as follows

$$X_{zz} = \left(\frac{k^2T}{e^2}\right)\left\{\sigma_z(E)\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_z^*}{2}\xi B_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.\right.$$

$$-2\Delta_s^*\xi A_s\sum_{n=-\infty}^{\infty}J_n^2(a) + \frac{(\Delta_z^*)^2}{2}C_z\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.+\frac{\Delta_z^*\Delta_s^*}{2}A_sB_z\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + (\Delta_s^*)^2\left(1-\frac{A_s}{\Delta_s^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]$$

$$+\sigma_s(E)\sin^2\theta_h\left[\xi^2\sum_{n=-\infty}^{\infty}J_n^2(a) - \frac{\Delta_s^*}{2}\xi B_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right)\right.$$

$$-2\Delta_z^*\xi A_z\sum_{n=-\infty}^{\infty}J_n^2(a) + \frac{(\Delta_s^*)^2}{2}C_s\left(1+\sum_{n=-\infty}^{\infty}J_n^2(a)\right)$$

$$\left.\left.+\frac{\Delta_s^*\Delta_z^*}{2}A_zB_s\left(1+3\sum_{n=-\infty}^{\infty}J_n^2(a)\right) + (\Delta_z^*)^2\left(1-\frac{A_z}{\Delta_z^*}\right)\sum_{n=-\infty}^{\infty}J_n^2(a)\right]\right\}$$

$$-\frac{k^2T}{e^2}\left(\sigma_z(E)+\sigma_s(E)\sin^2\theta_h\right)\left\{\frac{\sigma_z(E)}{\sigma_z(E)+\sigma_s(E)\sin^2\theta_h}\left[\xi\sum_{n=-\infty}^{\infty}J_n^2(a)\right.\right.$$

$$
-\frac{\dot{\Delta}_z}{2} B_z \left(1 + 3 \sum_{n=-\infty}^{\infty} J_n^2(a) \right) - \dot{\Delta}_s A_s \sum_{n=-\infty}^{\infty} J_n^2(a) \Bigg]
$$

$$
+ \frac{\sigma_s(E) \sin^2 \theta_h}{\sigma_z(E) + \sigma_s(E) \sin^2 \theta_h} \left[\xi \sum_{n=-\infty}^{\infty} J_n^2(a) - \frac{\dot{\Delta}_s}{2} B_s \left(1 + 3 \sum_{n=-\infty}^{\infty} J_n^2(a) \right) \right.
$$

$$
\left. \left. - \dot{\Delta}_z A_z \sum_{n=-\infty}^{\infty} J_n^2(a) \right] \right\} \times \left\{ \frac{\sigma_z(E)}{\sigma_z(E) + \sigma_s(E) \sin^2 \theta_h} \left[\xi - \dot{\Delta}_z B_z - \dot{\Delta}_s A_s \right] \right.
$$

$$
\left. + \frac{\sigma_s(E)}{\sigma_z(E) + \sigma_s(E) \sin^2 \theta_h} \sin^2 \theta_h \left[\xi - \dot{\Delta}_s B_s - \dot{\Delta}_z A_z \right] \right\} \Bigg)
$$