MODEL CALCULATIONS OF PLASMA EXCITATIONS

FOR

ARRAYS OF CYLINDRICAL NANOTUBLES

By

Tibab Zare McNeish

A dissertation submitted to the Graduate Faculty in Physics
in Partial fulfillment for the requirements for the degree of
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ABSTRACT

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Tibab Zare McNeish

Adviser: Professor Godfrey A. Gumbs

In this thesis we attempt to do calculations of the collective plasma excitations for an electron gas confined to the surface of cylindrical nanotubules in various spatial configurations. We present a self-consistent formalism of the dispersion relation for the plasmons and for the particle-hole modes as functions of the wave vector q_z along the axis of the nanotube(s). These results have been obtained in the random phase approximation (RPA) for nanotubules of arbitrary radii, R_i.

In our formalism, a magnetic field is at times directed along the axis of the nanotube and its spectra analyzed. We propose a general method for calculating the oscillator strength of the plasma excitations; determined the contribution of the plasmon and particle-hole excitations to the absorption coefficient, and investigated and tried to explain the Rashba effect within the context of cylindrical geometry on the nanotubules.

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LIST OF SYMBOLS

$\chi \equiv$ Polarization response function.

$R_j \equiv$ Radius of the nanotube.

$m^* \equiv$ Effective mass of the electron.

$m \equiv$ Angular momentum transfer, $(l - l')$.

$e \equiv$ Fundamental electron charge.

$\varepsilon_b \equiv$ Background dielectric constant.

$\varepsilon_s \equiv$ $4\pi(\varepsilon_0 \varepsilon_b)$.

$\varepsilon_F \equiv$ Fermi energy.

$f_0(\varepsilon_\alpha) \equiv$ Fermi distribution function at zero temperature.

$\alpha \equiv$ Energy band index (Whilst appearing as subscript)

$k_F \equiv$ Fermi wave vector.

$\vec{q}_\perp \equiv$ Fixed in plane momentum.

$\omega \equiv$ Plasmon frequency.

$\omega_c \equiv$ Cyclotron frequency.

$\varphi_{ij}, \vartheta_j \equiv$ Azimuth angles.

$\vec{\rho}_{ij}, \vec{\rho}'_{ij} \equiv$ In-plane position vectors, which relates the origin of one nanotube with respect to a point on the lateral surface of a another.

$L_z \equiv$ Length of nanotube.

$\varphi^{app} \equiv$ Screened potential.

$J_m \equiv$ m^{th}-order Bessel function.

$I_m \equiv$ m^{th}-order modified Bessel function of the first kind.

$K_m \equiv$ m[th]-order modified Bessel function of the second kind.

$G_{N_{x,y}} \equiv$ Reciprocal lattice vector.

$\beta_{abs} \equiv$ Absorption coefficient.

$\vec{\alpha} \equiv$ Rashba parameter.

$\alpha' \equiv$ Modified Rashba parameter.

$g_s \equiv$ Spin moment gyromagnetic ratio $\left(= \frac{-e}{m^* c} \right)$ in c.g.s. units.

LIST OF FIGURES

DEDICATION

I would like to dedicate this work to those of you who have helped in the realization of this, my dream. Your kind words of encouragement and continual support are, but only a few the many intangible ways in which you've enriched my life. To wit my children: Ammon, Amara, Anika and Amanda. My parents, Dorothy Maria McNeish, Eric Lloyd McNeish (deceased). My siblings: Princess Desta, Mikael Makonnen (deceased), Paul Clarence, Kwame Jomo (deceased) and Kamau Jawara. My grand parents Edna Morgrage-Jones, Moses Jones and Edith Maxwell, all deceased. My aunts: Cello Chong and Pauline Scott. My Uncles: Creech-Roy and Arthur Jones. To my many cousins, this is for you also, especially Mrs. Elaine Thomas. A handful of dear friends: Mrs. Alida Gupton, Mrs. Patricia Harris, Drs. Carlos Morrison, Dale McLachlan, and George Bennett; Leroy Jemison, Lincoln Hendricks, Wayne Thompson, Prof. Godfrey Gumbs, Prof. Yonatan Abranyos and Gary Mantle.

Chapter 1

Introduction and Literature Survey

In recent years, there have been considerable experimental and theoretical studies on carbon nanotubes [1, 2, 3, and 4]. In particular, the optical and electronic transport properties have been investigated. Experimentalists have been able to produce these tubes individually on a surface or in axially aligned clusters. There are potential device applications for these seemingly one-dimensional (1D) structures.

The novel electronic properties of carbon nanotubes (Hereafter referred to as nanotubes.) are due to the quantum confinement of electrons on a graphite sheet which is rolled up in a right circular cylinder of radius between $10\,\mathring{A}$ and $100\,\mathring{A}$. Around the lateral surface of the nanotube, periodic boundary conditions arise. For example, if a zigzag nanotube has ten hexagons around its lateral surface, the eleventh hexagon will coincide with the first. Traversing the circumference once produces a phase shift of 2π. As a result of this quantum confinement, electrons can only propagate on the surface in a direction parallel to the axis of the cylinder or around its circumference. The resulting number of 1D conduction and valence bands effectively depends on the standing waves that are set up around the circumference of the nanotube. Based on these facts and by temporarily suppressing effects from the lattice geometry, we develop a simple model that allows us to calculate the dispersion relation for an electron gas on the surface of a nanotube. This model is then applied to concentric nanotubules; two tubules separated by a finite distance on a line with their axes perpendicular to the line; a right-triangular triad of tubules with their axes perpendicular to the in-plane vertices of the triangle, and an infinite 2D array of tubules.

There are a few papers dealing with the excitation spectrum of quasi-1D structures. For instance, Williams and Bloch [7] have calculated the dispersion relation of plasmons and particle-hole modes for electrons confined within a cylindrical tube of finite radius in the RPA. These authors showed that the plasmon modes are not Landau damped and that in the long wavelength limit these modes

have Eigen frequencies ranging continuously from the usual three-dimensional plasma frequency for propagation along the axis of the chain to zero frequency for propagation perpendicular to it. The plasmons in this model were always above the particle-hole modes. The effect, which these modes have on the optical properties, was again discussed by Williams and Bloch [7]. Their results showed that the longitudinal dielectric response and elementary excitations are qualitatively different from their counterparts in isotropic three-dimensional metals.

Other papers include plasmon excitations of an electron gas within a quantum well wire by Huang [8] and Das Sarma and Hwang [9]. Acoustic plasmons for HgAsF in the long-wavelength limit were studied by Gumbs and Griffin [5], as well as by Mohan [11]. Although these references treat 1D systems rather extensively, the phenomena of surface plasmons on the surface of an effective 1D system, i.e., a cylindrical nanotube, remained largely unexplored. Huang [8], for instance, was able to determine the angular intersubband plasmon modes, as well as the fact that the collective modes were decoupled from the intrasubband mode due to the quantized angular motion of the electrons confined within the single quantum well wire. He also found that intersubband modes (when angular quantization is accounted for) have excitation energies outside the single-particle excitation continuum and that these modes escape Landau damping. Again, as in the case of the paper by Williams and Bloch [7], the plasmon modes lie above the particle-hole modes in the excitation spectrum. In the paper by Gumbs and Griffin [5], the authors looked at the acoustic plasmons in mercury chain compounds arranged perpendicular to each other and neglecting the effects of the chain lattice geometry. We have a single nanotube as our basis model. The quest of Gumbs and Griffin was sparked by a prediction in Mohan's thesis. Mohan did a study within the RPA of a coupled array in which the electrons are restricted to move in the channels of such an array. From the study, Mohan predicted a new plasmon mode in which the charge fluctuations in the two arrays are out of phase with each other. We emphasize that Mohan treatment was for a model when the electrons are within the channels, whereas we do not. Das Sarma and Hwang [9] calculated in considerable detail, the RPA dynamical response of an electron gas confined within a narrow channel when only one subband is considered.

For a while, there was paucity on the study of collective excitations of these 1D structures. Then there was the advent of two papers by Gumbs, et al [14] & [15]. In the first of these papers the authors showed amongst other things, that for a linear periodic array of nanotubes, the inter-tubule Coulomb interaction couples the modes of distinct angular *momenta*, m in individual nanotubes and shifts the $+m$ or $-m$ degeneracy of the single- nanotube modes. In the second, they looked at the effects on plasmon modes and drift-induced instabilities in a pair of coupled nanotubes. It was found that the phase velocity of high frequency plasmons is inversely proportional to the wave vector and that low frequency un-damped plasmon excitations may have a phase velocity smaller than the Fermi velocity.

We use standard many-body techniques to calculate the dielectric response function of an electron gas on a nanotube [5] in the RPA. Our analysis is initially restricted to a single nanotube but is soon extended to a configurationally diverse array of nanotubes in determining their excitation spectra. We propose to show in some cases that the plasmon excitations are unattenuated and lie below the particle-hole modes provided their longitudinal wave vector q_z exceeds a critical value, q_c. Our calculations in part, show that q_c depends not only critically, on the radius, R of the tube, but also on the parameter, λ which is a measure of the strength of the screened electron-electron interaction.

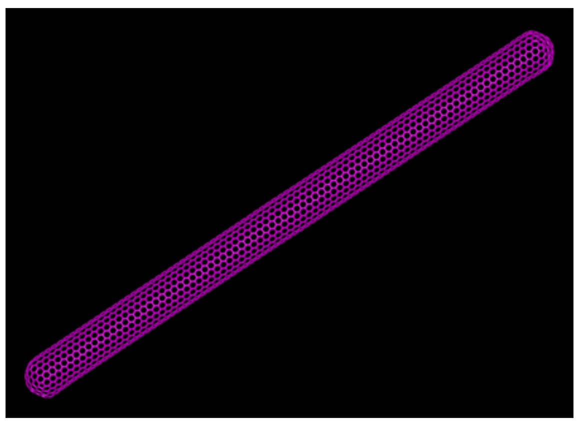


Fig 1

Finite Extent, Single-Walled Nanotubule (with Lattice).

Before we begin an analysis of our problem, we must first state what it is we seek to investigate, what type of model best facilitates the scope of our investigation and the tools at our disposal with which we attempt perform the operation.

We wish to examine the behavior of a surface restricted electron gas and its subsequent Coulomb interactions on a nano-sized cylindrical surface of effectively infinite extent. The actual lattice structure of the carbon nanotube, i.e., atomic, bond angles, chiarality, etc. are ignored. In such a setting, there are bound to be oscillations which manifest themselves through aggregate electron-electron propulsion and through their attendant energy-dependent elementary excitations. The aforementioned correlations give rise to collective oscillations within the plasma, which are termed plasmons. Phonons are the collective lattice vibrations, but which we will not treat such a case in this thesis. We also examine what happens when the plasmons are perturbed by an external transient electromagnetic field. The electron's spin and its relationship to 2D confinement are also explored with novel consequences.

Chapter 2

Spectroscopy: Light Absorption

2.1. Theoretical Formalism

The absorption coefficient is defined as the ratio of the energy absorbed per unit volume and unit time to the incident flux [18], [19].

$$\beta_{abs} \equiv \frac{N\hbar\omega}{2n\varepsilon_0 c(\vec{E}_{ext}\cdot\vec{E}_{ext})}W(\omega) \qquad (2.1.1)$$

Wherein $N =$ number of particles per unit volume, $n =$ refractive index of the medium, $\vec{E}_{ext} =$ constant(uniform) external electric field vector, $W(\omega) =$ transition probability per unit time, $\omega =$ frequency, $\varepsilon_0 =$ permittivity of free space and $c =$ speed of light.

By introducing perturbation Hamiltonian induced by light of frequency, ω and characterized by an electric dipole interaction

$$H' = \int d\vec{r} n_{ind}(\vec{r},t)e\varphi_{ext}(\vec{r}) \qquad (2.1.2)$$

where

$$\varphi_{ext}(\vec{r}) = -\vec{r}\cdot\vec{E}_{ext} \quad , \qquad (2.1.3)$$

we may calculate the transition probability via Fermi's golden rule. Please note that the external scalar potential, $\varphi_{ext}(\vec{r})$ assumes an entirely dissimilar form than that of Eqn (2.1.3) when the electric field vector is variable (non-uniform). We will address such matters subsequently in this chapter.

Electron Transition Probability and Fermi's Golden Rule

The following is a schoolboy's review of transition probability. The review is appropriate in that one may use this tool in determining the absorption coefficient. Consider the perturbation,

$$H^1(t) = H^1 e^{-i\omega t} \tag{2.1.4}$$

Additionally, let us expose the system to this perturbation and say that we wait for a long time. That is, we let $t = \pm T/2$ where $T \to \infty$. The amplitude for transition from states $\left|i^0\right\rangle$ to $\left|f^0\right\rangle$ is

$$C_f^1(\omega) = \frac{-2\pi i}{\hbar} H_{fi}^1 \delta(\omega_{fi} - \omega) \tag{2.1.5}$$

We can now define the probability of transition as

$$P_{i\to f} = \left|C_f^1(\omega)\right|^2 = \frac{4\pi^2}{\hbar^2}\left|H_{fi}^1\right|^2 \delta(\omega_{fi} - \omega)\delta(\omega_{fi} - \omega) \tag{2.1.6}$$

However,

$$\begin{aligned}\delta(\omega_{fi} - \omega)\delta(\omega_{fi} - \omega) &= \lim_{T\to\infty} \delta(\omega_{fi} - \omega)\frac{1}{2\pi}\int_{-T/2}^{T/2} dte^{i(\omega_{fi}-\omega)} \\ &= \frac{1}{2\pi}\lim_{T\to\infty} \delta(\omega_{fi} - \omega)\int_{-T/2}^{T/2} dt\delta_{\omega_{fi},\omega} \\ &= \delta(\omega_{fi} - \omega)\lim_{T\to\infty}\frac{T}{2\pi} \end{aligned} \tag{2.1.7}$$

Back-substitute Eqn. (2.1.7) into Eqn. (2.1.6) and we get

$$\begin{aligned} P_{i\to f} &= \frac{4\pi^2}{\hbar^2}\left|H_{fi}^1\right|^2 \delta(\omega_{fi} - \omega)\frac{T}{2\pi} \\ &= \frac{2\pi}{\hbar^2}\left|H^1{}_{fi}\right|^2 \delta(\omega_{fi} - \omega)T \end{aligned} \tag{2.1.8}$$

If we divide both sides of Eqn. (2.1.8) by $T \neq 0$, we obtain the average rate of first order transition (or transition probability per unit time).

$$W_{i\to f}^{1^{st.order}}(\omega) = \frac{P_{i\to f}}{T}$$

$$= \frac{2\pi}{\hbar^2}\left|H^1{}_{fi}\right|^2 \delta(\omega_{fi} - \omega)$$

$$= \frac{2\pi}{\hbar^2}\left|H^1{}_{fi}\right|^2 \delta(\omega_f - \omega_i - \omega)$$

$$= \frac{2\pi}{\hbar^2}\left|H^1{}_{fi}\right|^2 \delta\left(\frac{E_f^0}{\hbar} - \frac{E_i^0}{\hbar} - \frac{\hbar}{\hbar}\omega\right)$$

$$= \frac{2\pi}{\hbar^2}\left|H^1{}_{fi}\right|^2 \delta\left(\left(\frac{1}{\hbar}\right)\left(E_f^0 - E_i^0 - \hbar\omega\right)\right) \tag{2.1.9}$$

Using Eqn. (5.3.1.178), we may re-write the delta function in Eqn. (6.1.2.197) as

$$\delta\left(\left(\frac{1}{\hbar}\right)\left(E_f^0 - E_i^0 - \hbar\omega\right)\right) = \frac{1}{\left|\frac{1}{\hbar}\right|}\delta\left(E_f^0 - E_i^0 - \hbar\omega\right) = \hbar\delta\left(E_f^0 - E_i^0 - \hbar\omega\right) \tag{2.1.10}$$

We may now back-substitute Eqn. (2.1.10) into Eqn. (2.1.9) thereby obtaining

$$W_{i\to f}^{1^{st.order}}(\omega) = \frac{2\pi}{\hbar}\left|H^1_{fi}\right|^2 \delta\left(E_f^0 - E_i^0 - \hbar\omega\right) \tag{2.1.11}$$

However,

$$\left|H^1{}_{fi}\right|^2 \equiv \left|\left\langle f^0\left|H^1\right|i^0\right\rangle\right|^2 \tag{2.1.12}$$

Therefore, the transition probability for first order transitions due to absorption is

$$W_{i\to f}^{1^{st.order}}(\omega) = \frac{2\pi}{\hbar}\left|\left\langle f^0\left|H^1\right|i^0\right\rangle\right|^2 \delta\left(E_f^0 - E_i^0 - \hbar\omega\right) \tag{2.1.13}$$

Summed over the final state, f Eqn. (2.1.13) becomes

$$W_{i\to f}^{1^{st.order}}(\omega) = \frac{2\pi}{\hbar}\sum_f\left|\left\langle f^0\left|H^1\right|i^0\right\rangle\right|^2 \delta\left(E_f^0 - E_i^0 - \hbar\omega\right) \tag{2.1.14}$$

Using the completeness relation [20]

$$\sum_f \left|\langle f|i\rangle\right|^2 = \sum_f \langle f|i\rangle\langle i|f\rangle \qquad (2.1.15)$$

one may re-write the square of the matrix elements of H^1 as

$$\sum_f \left|\left\langle f^0\middle|H^1\middle|i^0\right\rangle\right|^2 = \sum_f \left\langle f^0\middle|H^1\middle|i^0\right\rangle\left\langle i^0\middle|H^1\middle|f^0\right\rangle \qquad (2.1.16)$$

We may also note that

$$\delta\left(E_f^0 - E_i^0 - \hbar\omega\right) = \Re e\left\{\lim_{\tau\to\infty}\frac{1}{\pi}\int_{-\infty}^{0} dt e^{i\frac{t}{\hbar}\left(E_f^0 - E_i^0 - \hbar\omega - \frac{i\hbar}{\tau}\right)}\right\} \qquad (2.1.17)$$

Back-substituting Eqns. (2.1.16) and (2.1.17) into Eqn. (2.1.15) yields

$$W_{i\to f}^{1^{st.order}}(\omega) = \frac{2}{\hbar}\Re e\int_{-\infty}^{0} dt \sum_f \left\langle i^0\middle|H^1(0)\middle|f^0\right\rangle\left\langle f^0\middle|H^1\middle|i^0\right\rangle e^{\frac{iE_f^0 t}{\hbar}} e^{\frac{-iE_i^0 t}{\hbar}} e^{i\frac{t}{\hbar}\left(-\hbar\omega - \frac{i\hbar}{\tau}\right)} \qquad (2.1.18)$$

Now, when

$$H^0\psi_f = E_f^0\psi_f \Rightarrow H^0 = E_f^0 \text{ and similarly , } H^0\psi_i = E_i^0\psi_i \Rightarrow H^0 = E_i^0 \qquad (2.1.19)$$

Back-substituting Eqns. (6.1.2.207) into Eqn. (6.1.2.206) yields

$$W_{i\to f}^{1^{st.order}}(\omega) = \frac{2}{\hbar}\Re e\int_{-\infty}^{0} dt \sum_f \left\langle i^0\middle|H^1(0)\middle|f^0\right\rangle\left\langle f^0\middle|H^1\middle|i^0\right\rangle e^{\frac{iH^0 t}{\hbar}} e^{\frac{-iH^0 t}{\hbar}} e^{-it\left(\omega + \frac{i}{\tau}\right)}$$

$$= \frac{2}{\hbar}\Re e\int_{-\infty}^{0} dt \sum_f \left\langle i^0\middle|H^1(0)\middle|f^0\right\rangle\left\langle f^0\middle|H^1(t)\middle|i^0\right\rangle e^{-it\left(\omega + \frac{i}{\tau}\right)}$$

$$\therefore \quad W_{i\to f}^{1^{st.order}}(\omega) = \frac{2}{\hbar}\Re e\int_{-\infty}^{0} dt \sum_f \left\langle i^0\middle|H^1(0)H^1(t)\middle|i^0\right\rangle e^{-it\left(\omega + \frac{i}{\tau}\right)} \qquad (2.1.20)$$

where

$$H^1(t) = e^{\frac{iH^0 t}{\hbar}} H^1 e^{\frac{-iH^0 t}{\hbar}} \qquad (2.1.21)$$

We can now express the transition probability in terms of the explicit representations of the eigenfunctions that arise from the problem under investigation.

Equations (2.1.2) and (2.1.3) permit us to write the mean of $H^1(0)H^1(t)$ as

$$\left\langle H^1(0)H^1(t)\right\rangle = Tr\left[\rho_0 H^1(0)H^1(t)\right]$$

$$= \iint d\vec{r}d\vec{r}' \left\langle n_{ind}(\vec{r},t=0)n_{ind}(\vec{r}',t)\right\rangle e\varphi_{ext}(\vec{r})e\varphi_{ext}(\vec{r}')$$

$$= \int d\vec{r}'\delta n_{ind}(\vec{r}',t)e\vec{r}\cdot\vec{E}_{ext} \tag{2.1.22}$$

This allows us to apply the familiar *fluctuation dissipation* theorem from Fourier analysis

$$\int_{-\infty}^{\infty} e^{-i\omega t}\left\langle A(0)B(t)\right\rangle = i\hbar\left[1+\rho_{photon}(\omega)\right]\int_{-\infty}^{\infty} e^{-i\omega t}\Phi_{AB}(t) \tag{2.1.23}$$

where

$$\rho_{photon}(\omega) = \frac{1}{\left.\left\{e^{\frac{\hbar\omega}{k_B T}}-1\right\}\right|_{T\neq 0}} \tag{2.1.24}$$

$$\Phi_{AB}(t) = \frac{\left\langle\left[A,B(t)\right]\right\rangle}{i\hbar} \tag{2.1.25}$$

to Eqn. (2.1.22). We then back substitute the results into Eqn. (2.1.20). The subsequent result is then back-substituted into Eqn. (2.1.1), which is the equation for the absorption coefficient, in light of a uniform electric field vector.

$$\beta_{abs} \equiv \frac{N\hbar\omega}{2n\varepsilon_0 c(\vec{E}_{ext}\cdot\vec{E}_{ext})}\frac{2}{\hbar}\Re e\left[i\hbar\left[1+\rho_{photon}(\omega)\right]\int_{-\infty}^{\infty} dte^{-i\omega t}\left(e\int d\vec{r}\delta n_{ind}(\vec{r},t)\vec{r}\cdot\vec{E}_{ext}\right)\right] \tag{2.1.26}$$

One may investigate what happens to the above form of the absorption coefficient when we back-substitute in q-space, the Eigen functions for our system, as well as the appropriate form for the change in the induced electron density $\delta n_{ind}(\vec{q},t)$ (See Eqn. 3.1.55 wherein we can let $a_x \to \infty$ resulting in a single nanotube system.) throughout the preceding general formalism. We will however take another approach to the question of absorption. The path to which will be outlined in the succeeding section.

2.2 The Absorption Coefficient for a SWNT- An Alternate Approach.

We present a calculation for the absorption coefficient when an incident beam of light of frequency, ω interacts weakly with a single, as well as a multi-walled nanotube. The perturbation in each instance will involve uniform and non-uniform electric fields, respectively.

In calculating the rate at which energy is absorbed by the quantum system, we'll make use of linear response theory. The formalism developed for the multi-walled geometry will subsequently be applied to two tubules.

Beginning with Fermi's Golden Rule and applying the fluctuation dissipation theorem, the absorption coefficient is defined as the ratio of the energy absorbed per unit volume and unit time to the incident flux. A general formalism for calculating the absorption coefficient, $\beta_{abs}(\omega)$ suggests that it may be expressed in terms of the real, $\Re e$ and imaginary, $\Im m$ parts of the Lorentz ratio, $\alpha_L(\omega)$. This is defined as the ratio of the Fourier coefficients of the absorbed energy at frequency, ω of a probative field, to that of the square of its accompanying amplitude and is defined as

$$\beta_{abs}(\omega) = \frac{\omega}{n(\omega)\varepsilon_b c}\left[1+\rho_{ph}(\omega)\right]\Im m(\alpha_L(\omega)) \tag{2.2.27}$$

Where

$$\rho_{ph}(\omega) = \left[1+e^{\frac{\hbar\omega}{K_b T}}\right] \tag{2.2.28}$$

is the photon distribution function, the refractive index is

$$n(\omega) = \left\{\frac{1}{2}\left(\varepsilon_b + \Re e(\alpha_L(\omega))\right) + ((\varepsilon_b + \Re e(\alpha_L(\omega)))^2 + (\Im m(\alpha_L(\omega)))^2)^{\frac{1}{2}}\right\}^{\frac{1}{2}} \tag{2.2.29}$$

and

$$\alpha_L(\omega) = \frac{-e}{\left|\vec{E}_{ext}\right|}\int d\vec{r}\,\delta n_{ind}(\vec{r},\omega)\vec{r}\cdot\hat{e}_0 \tag{2.2.30}$$

Here,

$$\hat{e}_0 \equiv \frac{\vec{E}_{ext}}{\left|\vec{E}_{ext}\right|} \tag{2.2.31}$$

is a unit vector in the same direction of the uniform external electric field, $\vec{E}_{ext}$ and $-e\vec{r}$ is the electron dipole moment.

For the case in which the perturbing $\vec{E}_{ext}$-field is non-uniform, one may replace the dipole term in Eqn.(2.2.30) with an external potential in the form of a Fourier series expansion

$$\alpha_L(\omega) = -e\int d\vec{r}\,\delta n_{ind}(\vec{r},\omega)\frac{\varphi_{ext}(\vec{r})}{\left|\nabla\varphi_{ext}(\vec{r})\right|} \tag{2.2.32}$$

Explicit details of this calculation and its consequences will be postponed until the latter quarter of section 2.3.

Now, in addition, the induced electron charge density fluctuations, $\delta n_{ind}(\vec{r},\omega)$, arise due both to the external electric field and the electric field associated with the induced potential, from any undergraduate course on Electricity and Magnetism, one may recall that provided the electric field is non-rotational, $\vec{E}_{ind} = -\nabla\varphi_{ind}$. Thus in linear response theory (a.k.a. the Random Phase Approximation with perturbation) within the random phase approximation, we have

$$\delta n_{ind}(\vec{r},\omega) = -e\int d\vec{r}'\chi^0(\vec{r},\vec{r}')\Phi_{tot}(\vec{r}',\omega) \tag{2.2.33}$$

We define $\Phi_{tot}(\vec{r}',\omega)$, as the sum of the external and induced potentials respectively. Explicitly,

$$\Phi_{tot}(\vec{r},\omega) = \varphi_{ind}(\vec{r}) + \varphi_{ext}(\vec{r}) \tag{2.2.34}$$

The response function is given by

$$\chi^0(\vec{r},\vec{r}') = \sum_{\alpha\alpha'}\left[\frac{f_0(\varepsilon_{\alpha'}) - f_0(\varepsilon_\alpha)}{\hbar\omega + \varepsilon_\alpha - \varepsilon_{\alpha'}}\right]\Psi^\dagger_\alpha(\vec{r}')\Psi_{\alpha'}(\vec{r}')\Psi^\dagger_{\alpha'}(\vec{r})\Psi_\alpha(\vec{r})$$

$$\equiv \sum_{\alpha\alpha'}\Pi^0_{\alpha\alpha'}(\omega)\Psi^\dagger_\alpha(\vec{r}')\Psi_{\alpha'}(\vec{r}')\Psi^\dagger_{\alpha'}(\vec{r})\Psi_\alpha(\vec{r}) \tag{2.2.35}$$

Where,

$$\Pi^0_{\alpha\alpha'}(\omega) = \left[\frac{f_0(\varepsilon_{\alpha'}) - f_0(\varepsilon_\alpha)}{\hbar\omega + \varepsilon_\alpha - \varepsilon_{\alpha'}}\right] \tag{2.2.36}$$

By back-substituting equation (2.2.35) into equation (2.2.33), and further back-substituting the result into equation (8.1.338), we obtain for the latter equation

$$\alpha_L(\omega) = -e^2\sum_{\alpha\alpha'}\left[\frac{f_0(\varepsilon_{\alpha'}) - f_0(\varepsilon_\alpha)}{\hbar\omega + \varepsilon_\alpha - \varepsilon_{\alpha'}}\right]\Big\{\int d\vec{r}'\Psi_{\alpha'}(\vec{r}')\vec{r}'\Psi^\dagger_\alpha(\vec{r}')\cdot\hat{e}_0 -$$

$$-\int d\vec{r}'\Psi_{\alpha'}(\vec{r}')\varphi_{ind}(\vec{r}';\omega)\Psi^\dagger_\alpha(\vec{r}')\frac{1}{E_{ext}}\Big\}\int d\vec{r}\Psi^\dagger_{\alpha'}(\vec{r})\vec{r}\Psi_\alpha(\vec{r})\cdot\hat{e}_0 \tag{2.2.37}$$

Where

$$E_{ext} \equiv \left|\vec{E}_{ext}\right| \tag{2.2.38}$$

If with regard to equation (2.2.37) we further define the following set of equations

$$\int d\vec{r}'\Psi_{\alpha'}(\vec{r}')\vec{r}'\Psi^\dagger_\alpha(\vec{r}') \equiv \vec{r}'_{\alpha\alpha'} \tag{2.2.39}$$

$$\int d\vec{r}\Psi^\dagger_{\alpha'}(\vec{r})\vec{r}\Psi_\alpha(\vec{r}) \equiv \vec{r}_{\alpha\alpha'} \tag{2.2.40}$$

$$\int d\vec{r}'\Psi_{\alpha'}(\vec{r}')\varphi_{ind}(\vec{r}';\omega)\Psi^\dagger_\alpha(\vec{r}') \equiv V'_{\alpha\alpha'}(\omega) \tag{2.2.41}$$

As the dipole transition matrix elements and the matrix elements associated with the induced potential respectively, we can back-substitute them along with equation (2.2.36), into equation (2.2.37), to obtain the following compact expression for the absorption coefficient for a SWNT

$$\alpha_L(\omega) = -e^2 \sum_{\alpha\alpha'} \Pi^0_{\alpha\alpha'}(\omega) \left\{ \vec{r}'_{\alpha\alpha'} \cdot \hat{e}_0 - \frac{V'_{\alpha\alpha'}(\omega)}{E_{ext}} \right\} \left(\vec{r}_{\alpha\alpha'} \cdot \hat{e}_0 \right) \tag{2.2.42}$$

The above expression for the absorption coefficient is in close agreement with that obtained by Prof. Gumbs with two exceptions: (1) in the sign of the second term and (2) the extra charge multiplicity on the electron.

2.3 The Case of Two Concentric Nanotubes

In light of an external potential, $\varphi_{ext}(\vec{r})$ the induced potential, $\varphi_{ind}(\vec{r})$ is the general solution of Poisson's equation

$$\nabla^2 \varphi_{ind} = \frac{4\pi}{\varepsilon_s} \left[\delta n_{ind}(\vec{r}, \omega) + \int d\vec{r} \chi^0 \varphi_{ext}(\vec{r}) \right] \tag{2.3.43}$$

The induced electrostatic potential, $\varphi_{ind}(\vec{r}(r, \varphi, z); \omega)$ where, $r \neq |\vec{r}|$ can be Fourier-transformed with respect to the independent variables φ and z respectively yielding,

$$\varphi_{ind}(r, \varphi, z; \omega) = \sum_{q_z, L} \varphi_L(r, q_z; \omega) e^{iq_z z} e^{iL\varphi}\ , \quad L, n \in \mathbb{Z}, \text{zero inclusive,} \tag{2.3.44}$$

When one back-substitutes the general solution above into Poisson's equation in momentum space, q_z, we obtain, *via* reasoning akin to what was done in section 2

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial \varphi_L(r, q_z, \omega)}{\partial r} \right) - \frac{L}{r^2} \varphi_L(r, q_z, \omega) - q_z^2 \varphi_L(r, q_z, \omega) = \sum_{j=1}^{2} \left(A_L^j(q_z) + B_L^j(q_z) \right) \delta(r - R_j) \tag{2.3.45}$$

The two summands on the right hand side of the above equation will be defined shortly. Based on our geometry, the particular solution to the above equation assumes the piece-wise form

$$\varphi_L(r,q_z,\omega) \equiv \begin{cases} D_1 I_L(q_z,r), r < R_1 \\ D_2 K_L(q_z,r), r > R_2 \\ D_3 I_L(q_z,r) + D_4 K_L(q_z,r), R_1 \le r \le R_2 \end{cases} \tag{2.3.46}$$

When one imposes the boundary and continuity conditions demanded by the preceding Eigen functions, we obtain the following system of deceptively linear-looking equations

$$\left\{ \begin{array}{l} I_L(q_z,R_1)D_1 + 0\cdot D_2 - I_L(q_z,R_1)D_3 - K_L(q_z,R_1)D_4 = 0 \\ 0\cdot D_1 - K_L(q_z,R_2)D_2 + I_L(q_z,R_2)D_3 + K_L(q_z,R_2)D_4 = 0 \\ -I_L'(q_z,R_1)D_1 + 0\cdot D_2 + I_L'(q_z,R_1)D_3 + K_L'(q_z,R_1)D_4 = \dfrac{A_L^1(q_z,\omega_p) + B_L^1(q_z,\omega_p)}{q_z} \\ 0\cdot D_1 + K_L'(q_z,R_2)D_2 - I_L'(q_z,R_2)D_3 - K_L'(q_z,R_2)D_4 = \dfrac{A_L^2(q_z,\omega_p) + B_L^2(q_z,\omega_p)}{q_z} \end{array} \right\}$$

(2.3.47)

Herein, the variable coefficients, $\left\{D_j\right\}_{j=1}^{4}$, will be subsequently determined.

Equation (2.3.47) may also be re-written in the rather familiar matrix notation

$$\begin{bmatrix} I_L(q_z,R_1) & 0 & -I_L(q_z,R_1) & -K_L(q_z,R_1) \\ 0 & -K_L(q_z,R_2) & I_L(q_z,R_2) & K_L(q_z,R_2) \\ -I_L'(q_z,R_1) & 0 & I_L'(q_z,R_1) & K_L'(q_z,R_1) \\ 0 & K_L'(q_z,R_2) & -I_L'(q_z,R_2) & -K_L'(q_z,R_2) \end{bmatrix} \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \dfrac{A_L^1(q_z,\omega) + B_L^1(q_z,\omega_p)}{q_z} \\ \dfrac{A_L^2(q_z,\omega) + B_L^2(q_z,\omega_p)}{q_z} \end{bmatrix}$$

(2.3.48)

With regard to the aforementioned variable coefficients, one finds that after some lengthy algebra

$$D_1 = \left(A_L^2(q_z,\omega) + B_L^2(q_z,\omega_p)\right) K_L(q_z,R_2)R_2 + \left(A_L^1(q_z,\omega) + B_L^1(q_z,\omega_p)\right) K_L(q_z,R_1)R_1$$

(2.3.49)

$$D_2 = \left(A_L^2(q_z,\omega) + B_L^2(q_z,\omega_p)\right) I_L(q_z,R_2)R_2 + \left(A_L^1(q_z,\omega) + B_L^1(q_z,\omega_p)\right) I_L(q_z,R_1)R_1 \tag{2.3.50}$$

$$D_3 = \left(A_L^2(q_z,\omega) + B_L^2(q_z,\omega_p)\right) K_L(q_z,R_2)R_2 \tag{2.3.51}$$

and

$$D_4 = \left(A_L^1(q_z,\omega) + B_L^1(q_z,\omega_p)\right) I_L(q_z,R_1)R_1 \tag{2.3.52}$$

We are now ready to 'back-substitute' these coefficients into the expressions for the piece-wise defined induced electrostatic potential, *id est.* equation (2.3.47). The behavior of the potential at points $r = 0$ and $0 < r < R_1$ were excluded. Why? You may ask? In the former case, the Bessel functions become singular there and in the latter case, the electrons are restricted to the outer surfaces of the nanotubes. That said, the potential assumes the regional forms

$$\varphi_L(r = R_1, q_z, \omega) = \left(A_L^1(q_z,\omega) + B_L^1(q_z,\omega_p)\right) I_L(q_z,R_1)K_L(q_z,R_1)R_1 \tag{2.3.53}$$

$$\varphi_L(r = R_2, q_z, \omega) = \left(A_L^2(q_z,\omega) + B_L^2(q_z,\omega_p)\right) I_L(q_z,R_2)K_L(q_z,R_2)R_2 \tag{2.3.54}$$

$$\varphi_L(R_1 < r = R_3 < R_2, q_z, \omega) = \left(A_L^1(q_z,\omega) + B_L^1(q_z,\omega_p)\right) R_1 I_L(q_z,R_1)K_L(q_z,R_3) + \\ + \left(A_L^2(q_z,\omega) + B_L^2(q_z,\omega_p)\right) R_2 I_L(q_z,R_3)K_L(q_z,R_2) \tag{2.3.55}$$

Wherein, for $B_L^{(j)}(q_z,\omega_p) \neq 0$,

$$A_L^{(1)}(q_z,\omega) =$$

$$\left[\frac{V_{12}^2(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_{z,}\omega)}{(1 - V(q_z,R_1)\chi_L^{(1)}(q_z,\omega))\left[(1 - V(q_z,R_2)\chi_L^{(2)}(q_z,\omega))(1 - V(q_z,R_1)\chi_L^{(2)}(q_z,\omega)) - \right.}\cdots\right.$$

$$\left.\frac{}{\left.-V_{12}^2(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_{z,}\omega)\right]}\right] B_L^{(1)}(q_z,\omega_p) + \left[\frac{R_2 V_{12}(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega)}{R_1(1 - V(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega))}\cdots\right.$$

$$\cdots\frac{\left[V(q_z,R_2)\chi_L^{(2)}(q_z,\omega)-V(q_z,R_1)V(q_z,R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_z,\omega)\right]}{\left[(1-V_{12}(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega))(1-V(q_z,R_2)\chi_L^{(2)}(q_z,\omega))\right]}\cdots$$
$$\cdots\left.\frac{+V_{12}^2(q_z,R_1R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_z,\omega)}{-V_{12}^2(q_z,R_1R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_z,\omega)}\right]+\left.\frac{V(q_z,R_1R_2)R_2\chi_L^{(1)}(q_z,\omega)}{R_1(1-V(q_z,R_1)\chi_L^{(1)}(q_z,\omega))}\right]B_L^{(2)}(q_z,\omega_p)$$

(2.3.56)

and

$$A_L^{(2)}(q_z,\omega)=$$
$$\left[\frac{V_{12}(q_z,R_1,R_2)R_1\chi_L^{(2)}(q_{z,}\omega)}{R_2\left[(1-V(q_z,R_1)\chi_L^{(1)}(q_z,\omega))(1-V(q_z,R_2)\chi_L^{(2)}(q_z,\omega))\right]}\cdots\right.$$
$$\left.\cdots\frac{}{-V_{12}^2(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_z,\omega)\Big]}\right]B_L^{(1)}(q_z,\omega_p)+$$
$$+\left[\frac{V_{12}(q_z,R_1,R_2)R_1\chi_L^{(2)}(q_{z,}\omega)}{R_2\left[(1-V(q_z,R_1)\chi_L^{(1)}(q_z,\omega))(1-V(q_z,R_2)\chi_L^{(2)}(q_z,\omega))\right.}\cdots\right.$$
$$\left.\cdots\frac{}{-V_{12}^2(q_z,R_1,R_2)\chi_L^{(1)}(q_z,\omega)\chi_L^{(2)}(q_z,\omega)}\right]B_L^{(2)}(q_z,\omega_p)$$

(2.3.57)

Where the polarization function of the electron gas on the nanotube is defined by

$$\chi_L^{(j)}(q_z,\omega)\equiv 2\sum_{l,l'=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}\left[\frac{f_0(\varepsilon_{j,k_z,l})-f_0(\varepsilon_{j,k_z-q_z,l-L})}{\hbar\omega-\varepsilon_{j,k_z,l}+\varepsilon_{j,k_z-q_z,l-L}}\right]$$
$$=\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}2\sum_{l'=-\infty}^{\infty}\left[\frac{f_0(\varepsilon_{j,k_z,l})-f_0(\varepsilon_{j,k_z-q_z,l-L})}{\hbar\omega-\varepsilon_{j,k_z,l}+\varepsilon_{j,k_z-q_z,l-L}}\right]$$
$$=\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}\Pi_0^{(j)}(l,k_z;l-L,k_z-q_z)\qquad(2.3.58)$$

Additionally, we have defined the term,

$$B_L^{(j)}(q_z,\omega_p)\equiv\frac{e}{\pi\varepsilon_s R_j}\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}dk_z\Pi_0^{(j)}(l,k_z;l-L,k_z-q_z)\int d\vec{r}\Psi^*_{j,k_z,l}(\vec{r})\varphi_{ext}(\vec{r})\Psi_{j,k_z-q_z,l-L}(\vec{r})$$

(2.3.59)

where

$$V(q_z,R_1,R_2)\equiv\frac{e^2}{\pi\varepsilon_s}I_L(q_z,R_1)K_L(q_z,R_2) \tag{2.3.60}$$

The former of which arises due to the external electric field.

Equations (2.3.56) and (2.3.57) can be re-written more compactly if we made use the following replacements

$$\varepsilon_L^{(j)}(q_z,\omega)\equiv 1-\frac{e^2}{\pi\varepsilon_s}I_L(q_z,R_j)K_L(q_z,R_j)\chi_L^{(j)}(q_{z,}\omega) \tag{2.3.61}$$

$$D_L(q_z,\omega;R_1,R_2)=\varepsilon_L^{(1)}(q_z,\omega)\varepsilon_L^{(2)}(q_z,\omega)-V^2(q_z,R_1,R_2)\chi_L^{(1)}(q_{z,}\omega)\chi_L^{(2)}(q_{z,}\omega)$$

(2.3.62)

In the absence of the perturbing electric field, $B_L^{(j)}(q_z,\omega_p)=0$. Non-vanishing solutions for $A_L^{(j)}(q_z,\omega)$ are akin to setting $D_L(q_z,\omega;R_1,R_2)=0$.

For our model, energy was found to be absorbed when the electric field was parallel or perpendicular to the z-axis. If one should take the direction of the electric field to be parallel to the x-axis, which is simultaneously perpendicular to the z-axis. We obtain

$$\vec{r}_{j,\upsilon,\upsilon'}=\delta_{l',l}\delta_{k_z',k_z}\,\mathrm{R}_j\hat{\mathrm{e}}_x \tag{2.3.63}$$

$$V_{\alpha\alpha'}=\varphi_{l-l'}(R_j,k-k_z',\omega) \tag{2.3.64}$$

Wherein $\hat{\mathrm{e}}_x$ is a unit vector in the x-direction. 'Back-substituting' these results into Eqn. (2.3.30) yields

$$\alpha_L(\omega) = e^2 \sum_j (\chi_0^{(j)})_{L=0}(\omega) R_j \left\{ R_j - \frac{\varphi_{L=0}(R_j; k_z - k_z'; \omega)}{E_{ext}} \right\} \tag{2.3.65}$$

We can separate the contributions to the absorption coefficient from plasmons and single-particle excitations. Since we assumed that the electric field used to probe the structure is was uniform, only the long wavelength excitations contribute to the absorption coefficient via the Lorentz ratio in Eqn.(2.3.65). However, should the external potential be spatially dependent as in $\varphi_{ext}(\vec{r}, \omega) = \Omega e^{iL\varphi} e^{iq_z z}$ where Ω, **is a normalization constant,** then one may show that $\alpha_L = \alpha_L(\varphi_{L\neq 0}(R_j; q_z; \omega))$. The normal modes of oscillation for each tubule when the coupling, $V(q_z, R_1, R_2)$ between them is neglected are the zeros of the equation, $\varepsilon_L^{(j)}(q_z, \omega) = 0$. We derive below, explicit results for the induced potential for a single tubule of radius, R.

For a single tubule of radius, R, we write the Fourier components of the induced potential as

$$\varphi_L(r, q_z, \omega) \equiv \begin{cases} D_1 I_L(q_z, r), r < R \\ D_2 K_L(q_z, r), r > R \end{cases} \tag{2.3.66}$$

By applying the boundary conditions on the surface of the tubule, as well as the continuity of the potential and the discontinuity of its derivative as seen in Eqn. (2.3.45), we obtain

$$D_1 = -\left(A_L(q_z, \omega) + B_L(q_z, \omega_p)\right) K_L(q_z, R_2) R \tag{2.3.67}$$

$$D_2 = -\left(A_L(q_z, \omega) + B_L(q_z, \omega_p)\right) I_L(q_z, R) R \tag{2.3.68}$$

Where, $A_L(q_z, \omega)$ and $B_L(q_z, \omega_p)$ were previously defined for a tubule of radius, R . 'Back-substituting Eqns. (2.3.66), (2.3.67) and (2.3.68) into Eqn. (3.2.109), yields

$$\left(A_L(q_z, \omega) + B_L(q_z, \omega_p)\right) = \frac{B_L(q_z, \omega_p)}{\varepsilon_L(q_z, \omega_p)} \tag{2.3.69}$$

This result can now be used to determine the induced potential, $\varphi_L(r,q_z,\omega)$ in all regions *via* Eqns. (2.3.66), (2.3.67) and (2.3.68). In the above, $\varepsilon_L(q_z,\omega_p)$ is expressed by way of Eqn. (2.3.61) in which we made the replacement, $R_j \to R$.

In the absence of an external electric field, we must set $\varphi_{ext}(\vec{r})=0$ in Eqn. (2.3.59). This result yields $B_L(q_z,\omega_p)=0$ in Eqn. (2.3.69), which further reduces to $\varepsilon_L(q_z,\omega_p)A_L(q_z,\omega)=0$, where $\varepsilon_L(q_z,\omega)\equiv 1-\frac{e^2}{\pi\varepsilon_s}I_L(q_z,R)K_L(q_z,R)\chi_L(q_{z,}\omega)$ is the dielectric function for the nanotube. Note that non-trivial solutions for $A_L(q_z,\omega)$, lead to the plasma dispersion equation $\varepsilon_L(q_z,\omega)=0$ for the *self-sustaining plasma oscillations*. However, in the presence of an external electric field, the solution to Eqn.(2.3.69) for $A_L(q_z,\omega)$ in terms of $B_L(q_z,\omega)$ leads to the coefficients D_1 and D_1 in Eqn.(2.3.67) and (2.3.68) since $D_1=-\frac{K_L(q_z,R)B_L(q_z,\omega_p)R}{\varepsilon_L(q_z,\omega_p)}$ and $D_2=-\frac{I_L(q_z,R)B_L(q_z,\omega_p)R}{\varepsilon_L(q_z,\omega_p)}$. When these results are substituted into Eqn.(2.3.66), we obtain a closed-form analytic result for $\varphi_L(r,q_z,\omega)$ and consequently $\varphi_{ind}(r,\varphi,z;\omega)$ in Eqn.(2.3.44) *via* a Fourier series expansion. We may now use these results to obtain $V'_{\alpha\alpha'}(\omega)$ in Eqn.(2.3.41) which could be substituted in the Lorentz ratio in Eqn.(2.3.42) in calculating the absorption coefficient, $\beta_{abs}(\omega)$ in Eqn.(2.3.28).

We will now analyze contributions to the Lorentz ratio, $\alpha_L(\omega)$ in Eqn.(2.3.65). That is, we must examine when the factor $\Im m\left\{(\chi_0^{(j)})_L(\omega)\varphi_L(R_j;q_z;\omega)\right\}\neq 0$. Hence, we must determine $\Im m\left\{D_L^{-1}(R_j;q_z;\omega)\right\}=-D_{\Im m}\left\{D_{\Im m}^2+D_{\Re}^2\right\}^{-1}$ where $D_{\Re}$ and $D_{\Im m}$ are the real and imaginary parts of D_L. As a result, the only non-zero contributions to $\beta_{abs}(\omega)$ arise when either $D_{\Im m}$ is finite, i.e., form single particle excitations, or when $D_{\Re}$ *both* $D_{\Im m}$ and vanish simultaneously. The latter condition is due to Plasmon excitations which are not Landau damped by the particle-hole modes.

For finite q_z and L, *id est*, $(q_z, L \neq 0)$ the Lorentz ratio for n concentric nanotubes is

$$\alpha_{L,j}(q_z;\omega) = -e^2 \int d\vec{r} \int d\vec{r}' \sum_{j=1}^{n} \chi_{j,L}^{(0)}(\vec{r},\vec{r}';\omega) \left\{ \sum_{q_z \neq 0, L} e^{iq_z z} e^{iL\varphi} \Phi(q_z;L) + \varphi_{ind}(\vec{r};\omega) \right\}$$
$$\sum_{q_z \neq 0, L} \frac{1}{e^{i(L\varphi + q_z z)} \Phi(q_z;\omega) \left\{ \frac{L^2}{R^2} + q_z^2 \right\}}, R \neq 0 \tag{2.3.70}$$

Making the following substitution

$$\chi_{j,L}^{(0)}(\vec{r},\vec{r}';\omega) \to 2 \sum_{\alpha,\alpha'} \frac{f_0(\varepsilon_{\alpha'}) - f_0(\varepsilon_\alpha)}{\varepsilon_\alpha - \varepsilon_{\alpha'} + \hbar\omega} \psi_\alpha^\dagger(\vec{r}') \psi_{\alpha'}(\vec{r}') \psi_{\alpha'}^\dagger(\vec{r}) \psi_\alpha(\vec{r}) \tag{2.3.71}$$

with regard to the above equation for the Lorentz ratio, we obtain

$$\alpha_{L,j}(q_z;\omega) = -e^2 \sum_{\alpha,\alpha'} \Pi_{\alpha,\alpha'}^{(0)}(\omega) \left\{ \sum_{q_z \neq 0, L} \Phi(q_z;L) \aleph_{\alpha,\alpha'}(q_z;L) + V'_{\alpha,\alpha'}(\omega) \right\}$$
$$\times \sum_{q_z \neq 0, L} \frac{1}{e^{i(L\varphi + q_z z)} \Phi(q_z;\omega) \left\{ \frac{L^2}{R^2} + q_z^2 \right\}}, R \neq 0 \tag{2.3.72}$$

Wherein we defined

$$V'_{\alpha,\alpha'}(\omega) \equiv \int d\vec{r}' \psi_{\alpha'}^\dagger(\vec{r}') \varphi_{ind}(\vec{r}';\omega) \psi_\alpha(\vec{r}') \tag{2.3.73}$$

$$\aleph_{\alpha,\alpha'}(q_z;L) \equiv \int d\vec{r}' \psi_\alpha^\dagger(\vec{r}') e^{i(L\varphi + q_z z)} \psi_{\alpha'}(\vec{r}') \tag{2.3.74}$$

$$\Pi_{\alpha,\alpha'}^{(0)}(\omega) \equiv 2 \sum_{\alpha,\alpha'} \frac{f_0(\varepsilon_{\alpha'}) - f_0(\varepsilon_\alpha)}{\varepsilon_\alpha - \varepsilon_{\alpha'} + \hbar\omega} \tag{2.3.75}$$

Chapter 3

Dispersion Formula for a Single Cylindrical Nanotube.

3.1. Single-walled Nanotube

If an electron is confined to the surface of a right circular cylinder of radius, R in the absence of a uniform magnetic field, $\vec{B}$ the Eigen functions and Eigen energies are

$$\psi_\alpha(\rho,\varphi,z) = \frac{1}{\sqrt{L_z}} e^{ik_z z} P(\rho) \frac{1}{\sqrt{2\pi R}} e^{il\varphi}, P^2(\rho) = \delta(\rho - R) \tag{3.1.76}$$

$$\varepsilon_\alpha = \frac{\hbar^2 k_z^2}{2m^*} + \frac{m^* R^2}{8\hbar^2}\left[\frac{2l\hbar^2}{m^* R^2}\right]^2, \tag{3.1.77}$$

With, $\alpha = \{k_z, l\}, k_z = \dfrac{2\pi n}{L_z}$ and $n, l \in \mathbb{Z}, ...0,$ inclusive. In this notation $\omega_c = eB/cm^*$ is the cyclotron frequency. Plasmon excitations can be obtained by calculating the density matrix from its equation of motion, $i\hbar\dfrac{\partial\hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]$. For small perturbations, $\hat{\rho} = \hat{\rho}^0 + \hat{\rho}^1$ and $\hat{H} = \hat{H}^0 - e\varphi_{ext}(\rho,\varphi,z;t)$, where $\hat{\rho}^0$ is the equilibrium density matrix and $\hat{\rho}^1$ its perturbation, $\hat{H}^0$ is the unperturbed Hamiltonian and $\varphi_{ext}(\rho,\varphi,z;t)$ is the fluctuation in the electric potential corresponding to $\hat{\rho}^1$. In the basis set (1), we have

$$< \alpha | \hat{\rho}_0 | \alpha >= 2 f_0(\varepsilon_\alpha)\delta_{\alpha\alpha'}, < \alpha | \hat{H}_0 | \alpha >= \varepsilon_\alpha \delta_{\alpha\alpha'}, \tag{3.1.78}$$

where, $f_0(\varepsilon_\alpha)$ is the Fermi function. Substituting Eq. (3.1.78) into the equation of motion for the density matrix, and solving it in the lowest order, we obtain

$$<\alpha|\hat{\rho}^1|\alpha'> = 2e\frac{f_0(\varepsilon_\alpha)-f_0(\varepsilon_{\alpha'})}{\hbar\omega+\varepsilon_\alpha-\varepsilon_{\alpha'}}<\alpha|\varphi_{ext}|\alpha'>. \tag{3.1.79}$$

The electrostatic potential $\varphi_{ext}(\rho,\varphi,z;\omega)$ can be Fourier transformed with respect to the variables φ and z as

$$\varphi_{ext}(\rho,\varphi,z;\omega)=\sum_{q_z,m}\varphi_{ext}^{(m)}(\rho,q_z,\omega)e^{iq_z z}e^{im\varphi},\ \text{with}\ q_z=\frac{2n\,\pi}{L_z}\ \text{where}\ n,m\in\mathbb{Z},...0,$$

inclusive. (3.1.80)

From Eqns. (3.1.76) and (3.1.80), we obtain the following results for $<\alpha|\varphi_{ext}|\alpha'>$

$$<k_z l|\varphi_{ext}|k_z' l'> = \varphi_{ext}^{(l-l')}(R,k_z-k_z') \tag{3.1.81}$$

and from Eq. (3.1.79)

$$<k_z l|\hat{\rho}^1|k_z' l'> = 2e\frac{f_0(\varepsilon_{k_z l})-f_0(\varepsilon_{k_z' l'})}{\hbar\omega+\varepsilon_{k_z l}-\varepsilon_{k_z' l'}}\varphi_{ext}^{(l-l')}(R,k_z-k_z'). \tag{3.1.82}$$

We take account of the screening due to the background medium by assuming that the array is immersed in a material with effective dielectric constant ε_s. In order to proceed in our calculation of the plasmon excitations, we need to solve Poisson's equation

$$\nabla^2\varphi_{ext}(\rho,\varphi,z)=\frac{4\pi e}{\varepsilon_s}\sum_{\alpha\alpha'}|\alpha><\alpha|\hat{\rho}^1|\alpha'><\alpha'|. \tag{3.1.83}$$

Using the explicit form of the eigenfunctions in Eqn. (3.1.76) in the right-hand side of Eqn. (3.1.83) and expressing ∇^2 in cylindrical coordinates, we obtain

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\varphi_{ext}(\rho,\varphi,z)}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\varphi_{ext}(\rho,\varphi,z)}{\partial\varphi^2}+\frac{\partial^2\varphi_{ext}(\rho,\varphi,z)}{\partial z^2}$$

$$=\frac{4\pi e}{\varepsilon_s 2\pi L_z R}P^2(\rho)\sum_{k_z l;k_z' l'}<k_z l|\hat{\rho}_1|k_z' l'>e^{i(k_z-k_z')z}e^{i(l-l')\varphi}, \tag{3.1.84}$$

Or taking Fourier transforms over φ and z, we have

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\varphi_{ext}^{(m)}(\rho,q,\omega)}{\partial\rho}\right)-\frac{m}{\rho^2}\varphi_{ext}^{(m)}(\rho,q,\omega)-q^2\varphi_{ext}^{(m)}(\rho,q,\omega)=A_m(q)\delta(\rho-R),$$

(3.1.85)

Wherein

$$A_m(q)=\frac{e}{\varepsilon_s\pi R}\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}dk_z<k_zl\,|\,\hat{\rho}^1\,|\,k_z-q,l-m>. \tag{3.1.86}$$

Combining Eqns. (3.1.82) and (3.1.86), we have

$$A_m(q)=\frac{2e^2}{\varepsilon_s\pi R}\varphi_{ext}^{(m)}(R,q,\omega)\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}dk_z\frac{f_0(\varepsilon_{k_zl})-f_0(\varepsilon_{k_z-q,l-m})}{\hbar\omega+\varepsilon_{k_z-q,l-m}-\varepsilon_{k_zl}}. \tag{3.1.87}$$

The integral in Eqn. (3.1.87) can be easily carried out using the energy spectrum in Eq. (3.1.77). This gives

$$A_m(q)=\frac{2e^2}{\varepsilon_s\pi R}\varphi_{ext}^{(m)}(R,q,\omega)\chi(q,m,\omega), \tag{3.1.88}$$

With the response of the system to the external perturbation being

$$\chi(q,m;\omega)\equiv\frac{2m^*}{\hbar^2q}\sum_{l=-S_j}^{S_j}\ln\left|\frac{\hbar^2(\omega)^2-E_+^2(l,m;k_F(l,\omega),q)}{\hbar^2(\omega)^2-E_-^2(l,m;k_F(l,\omega),q)}\right| \tag{3.1.89}$$

Wherein

$$E_\pm^2(l,m;k_F(l,\omega)\ \ ,q)=\left\{\left[\frac{\hbar^2(q^2\pm2k_F(l;\omega)q)}{2m^*}\right]-\left[\frac{\hbar^2(2ml+m^2)}{2m^*R^2}\right]\right\}^2 \tag{3.1.90}$$

$$k_F(l;\omega)\equiv\left\{\frac{2m^*}{\hbar^2}\left[\varepsilon_F-\frac{m^*R^2}{8\hbar^2}\left[\frac{2l\hbar^2}{m^*R^2}\right]^2\right]\right\}^{\frac{1}{2}} \tag{3.1.91}$$

Where S_j is the maximum value of l for the levels occupied by electrons and $k_F(l;\omega_c)$ is the Fermi wave vector in the z direction for the level with given l. In the absence of an external magnetic field $\left(\omega_c = \frac{eB}{cm^*}\big|_{B=0} = 0\right)$, Eqns. (3.1.89) – (3.1.91) reduce to

$$\chi(q,m,\omega) = \frac{2m^*}{\hbar^2 q}\sum_{l=-S}^{S}\ln\left|\frac{\hbar^2\omega^2 - E_+^2(l,m;k_F(l),q)}{\hbar^2\omega^2 - E_-^2(l,m;k_F(l),q)}\right|, \tag{3.1.92}$$

Wherein

$$E_\pm^2(l,m;k_F(l),q) = \frac{\hbar^2(q^2 \pm 2k_F(l)q)}{2m^*} + \frac{\hbar^2(2ml+m^2)}{2m^*R^2} \tag{3.1.93}$$

Where,

$$k_F(l) = \sqrt{\frac{2m^*\varepsilon_F}{\hbar^2} - \frac{l^2}{R^2}} \tag{3.1.94}$$

It follows from Eqn. (3.1.85) that for $\rho \neq R$, the potential $\varphi_{ext}^{(m)}(\rho,q,\omega)$ satisfies the following equation

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\varphi_{ext}^{(m)}(\rho,q,\omega)}{\partial\rho}\right) - \frac{m}{\rho^2}\varphi_{ext}^{(m)}(\rho,q,\omega) - q^2\varphi_{ext}^{(m)}(\rho,q,\omega) = 0, \tag{3.1.95}$$

This is the standard equation for modified Bessel functions with general solution

$$\varphi_{ext}^{(m)}(\rho,q,\omega) = a_1 I_m(q\rho) + a_2 K_m(q\rho), \tag{3.1.96}$$

Wherein a_1 and a_2 are arbitrary constants, I_m and K_m are modified m^{th} -order Bessel functions of the first and second kind, respectively. Using the boundary conditions, $\varphi_{ext}^{(m)}(\rho = 0,q,\omega) < \infty$ and $\varphi_{ext}^{(m)}(\rho \to \infty,q,\omega) \to 0$, we obtain

$$\varphi_{ext}^{(m)}(\rho,q,\omega) = \begin{cases} C_1 I_m(q\rho) & \rho < R \\ C_2 K_m(q\rho) & \rho > R \end{cases}, \tag{3.1.97}$$

Wherein C_1 and C_2 are some constants to be determined from the continuity of $\varphi_{ext}^{(m)}(\rho,q,\omega)$ at $\rho = R$ and the step-like change of $\frac{\partial\varphi_{ext}^{(m)}(\rho,q,\omega)}{\partial\rho}$ at $\rho = R$, see Eqn. (3.1.85). We have

$$C_1 I_m(qR) - C_2 K_m(qR) = 0 \tag{3.1.98}$$

$$C_2 K_m^{'}(qR) - C_1 I_m^{'}(qR) = \frac{A_m(q)}{q}, \tag{3.1.99}$$

With solutions

$$C_1 = \frac{A_m(q) K_m(qR)}{q\left[I_m(qR)K_m^{'}(qR) - K_m(qR)I_m^{'}(qR)\right]}, \tag{3.1.100}$$

$$C_2 = \frac{A_m(q) I_m(qR)}{q\left[I_m(qR)K_m^{'}(qR) - K_m(qR)I_m^{'}(qR)\right]}. \tag{3.1.101}$$

Using the following identity for Bessel functions

$$I_m(qR)K_m^{'}(qR) - K_m(qR)I_m^{'}(qR) = \frac{1}{qR}, \tag{3.1.102}$$

Wherein a prime denotes taking a derivative with respect to the argument, we obtain

$$C_1 = -A_m(q) R K_m(qR), C_2 = -A_m(q) R I_m(qR). \tag{3.1.103}$$

It follows from Eqns. (3.1.97) and (3.1.103) that

$$\varphi_{ext}^{(m)}(R, q, \omega) = -A_m(q) R K_m(qR) I_m(qR). \tag{3.1.104}$$

Combining Eqns. (3.1.88) and (3.1.104), we have

$$\left[1 - \frac{e^2}{\pi \varepsilon_s} I_m(qR) K_m(qR) \chi(q, m, \omega)\right] A_m(q) = 0. \tag{3.1.105}$$

For a nontrivial solution of Eqn. (3.1.105), $A_m(q) \neq 0$ and we obtain the following plasmon dispersion equation

$$1 - V(q, R)\chi(q, m, \omega) = 0 \tag{3.1.106}$$

Wherein $V(q,R) = \frac{4\pi e^2}{\varepsilon_s} I_m(qR) K_m(qR)$. It turns out that Eqn. (3.1.106) agrees with the dispersion equation in Lin's paper, for zero magnetic field, i.e., $\varepsilon(q, m, \omega) = 0$ where $\varepsilon(q, m, \omega)$ is defined in Eqn. (4) of Ref. [4].

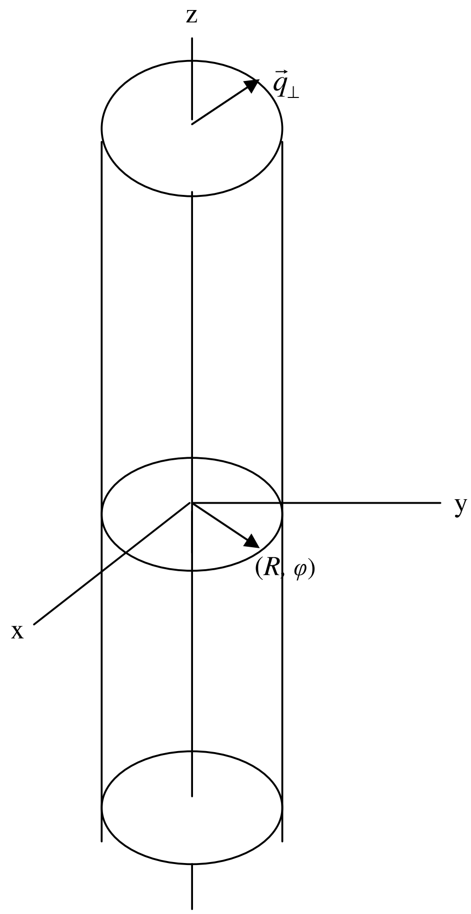


Fig. 2

In our idealized version of a carbon nanotube, the tube is perceived to be of infinite extent along the z-axis. We denote its radius by 'R' and the angle that it makes with respect to the x-axis (i.e. the azimuth angle) by φ. The lateral surface of this tube is then bedecked with electrons (which never leave its surface). The momentum $\vec{q}_\perp$ is fixed with respect to the z-axis as well as in the xy-plane for the nanotube. Excitations due to a small perturbation are observed.

3.2 The Double-Walled Nanotube

We now turn our attention to deriving the plasmon dispersion equation of two coaxial tubules, with inner radius R_1 and outer radius R_2. We will also label as (φ_3, R_3), any point in the xy-plane between the nanotubes. It must be emphasized that this point does not rest on either lateral surface of the nanotubes; it is simply a point in the plane twixt cylinders.

A straightforward generalization of the results in the preceding section shows that the density matrix is given by

$$< k_z l \,|\, \hat{\rho}_1 \,|\, k_z^{'} l^{'} >= 2e \sum_{i=1}^{2} \frac{f_0(\varepsilon_{k_z l}^{i}) - f_0(\varepsilon_{k_z^{'} l^{'}}^{i})}{\hbar\omega + \varepsilon_{k_z l}^{i} - \varepsilon_{k_z^{'} l^{'}}^{i}} \varphi_{ext}^{(l-l^{'})}(R_i, k_z - k_z^{'}) P_i^2(\rho), \qquad (3.2.107)$$

Where

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho \frac{\partial \varphi_{ext}^{(m)}(\rho,q,\omega)}{\partial r}\right) - \frac{L}{\rho^2}\varphi_{ext}^{(m)}(\rho,q,\omega) - q^2 \varphi_{ext}^{(m)}(\rho,q,\omega) = \sum_{i=1}^{2} A_m^{(i)}(q)\delta(\rho - R_i),$$

(3.2.108)

With

$$A_m^{(i)}(q) = \frac{2e^2}{\varepsilon_s \pi R_i} \varphi_{ext}^{(m)}(R_i,q,\omega) \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} dk_z \, \frac{f_0(\varepsilon_{k_z l}^{i}) - f_0(\varepsilon_{k_z - q, l-m}^{i})}{\hbar\omega + \varepsilon_{k_z - q, l-m}^{i} - \varepsilon_{k_z l}^{i}}$$

$$\equiv \frac{e^2}{\pi R_i \varepsilon_s} \varphi_{ext}^{(m)}(R_i,q,\omega) \chi_i(q,m;\omega), \qquad (3.2.109)$$

and the eigenenergies $\varepsilon_{k_z,l}^{i}$ are obtained from Eq. (3.1.77) by replacing R by R_i.

Now, $\varphi_{ext}^{(m)}(\rho,q,\omega)$ is given by

$$\varphi_{ext}^{(m)}(\rho,q,\omega)=\begin{cases}\overline{C}_1 I_m(q\rho), & \rho<R_1\\ \overline{C}_3 I_m(q\rho)+\overline{C}_4 K_m(q\rho), & R_1\le\rho\le R_2\\ \overline{C}_2 K_m(q\rho), & \rho>R_2\end{cases}, \tag{3.2.110}$$

Wherein $\overline{C}_1$, $\overline{C}_2$ and $\overline{C}_3$ are some constants to be determined from the continuity of $\varphi_{ext}^{(m)}(r,q,\omega)$ at $\rho=R_1,R_2$ and the step-like change of $\dfrac{\partial\varphi_{ext}^{(m)}(\rho,q,\omega)}{\partial\rho}$ at $\rho=R_1,R_2$, see Eqn. (3.2.108). We have

$$\begin{pmatrix} I_m(qR_1) & 0 & -I_m(qR_1) & -K_m(qR_1)\\ 0 & -K_m(qR_2) & I_m(qR_2) & K_m(qR_2)\\ -I_m'(qR_1) & 0 & I_m'(qR_1) & K_m'(qR_1)\\ 0 & K_m'(qR_2) & -I_m'(qR_2) & -K_m'(qR_2)\end{pmatrix}\begin{pmatrix}\overline{C}_1\\ \overline{C}_2\\ \overline{C}_3\\ \overline{C}_4\end{pmatrix}=\begin{pmatrix}0\\ 0\\ \dfrac{A_m^{(1)}(q)}{q}\\ \dfrac{A_m^{(2)}(q)}{q}\end{pmatrix}, \tag{3.2.111}$$

Which we have solved for $\overline{C}_1$, $\overline{C}_2$, $\overline{C}_3$ and $\overline{C}_4$ to obtain

$$\overline{C}_1=R_1K_m(qR_1)A_m^{(1)}(q)+R_2K_m(qR_2)A_m^{(2)}(q), \tag{3.2.112}$$

$$\overline{C}_2=R_1I_m(qR_1)A_m^{(1)}(q)+R_2I_m(qR_2)A_m^{(2)}(q), \tag{3.2.113}$$

$$\overline{C}_3=R_2K_m(qR_2)A_m^{(2)}(q), \tag{3.2.114}$$

$$\overline{C}_4=R_1I_m(qR_1)A_m^{(1)}(q). \tag{3.2.115}$$

Combining Eqns. (3.2.109) and (3.2.110) and making use of the results for $\overline{C}_1$, $\overline{C}_2$, $\overline{C}_3$ and $\overline{C}_4$ in Eqns. (3.2.112) through (3.2.115), we obtain the following system of equations

$$\begin{bmatrix} 1-V(q,R_1)\chi_1(q,m;\omega) & \dfrac{-R_2}{R_1}V(q,R_1,R_2)\chi_1(q,m;\omega) & 0\\ \dfrac{-R_1}{R_2}V(q,R_1,R_2)\chi_2(q,m;\omega) & 1-V(q,R_2)\chi_2(q,m;\omega) & 0\\ \dfrac{R_1}{R_3}V(q,R_1,R_3)\chi_3(q,m;\omega) & \dfrac{R_2}{R_3}V(q,R_2,R_3)\chi_3(q,m;\omega) & -1\end{bmatrix}\begin{bmatrix}A_m^{(1)}(q)\\ A_m^{(2)}(q)\\ A_m^{(3)}(q)\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}$$

(3.2.116)

Wherein $V(q,R_1,R_2)=\dfrac{e^2}{\pi\varepsilon_s}I_m(qR_1)K_m(qR_2)$, $V(q,R_1,R_3)=\dfrac{e^2}{\pi\varepsilon_s}I_m(qR_1)K_m(qR_3)$ and $V(q,R_2,R_3)=\dfrac{e^2}{\pi\varepsilon_s}I_m(qR_2)K_m(qR_3)$. Equation (3.2.116) has non-trivial solutions for $A_m^{(1)}(q)$, $A_m^{(2)}(q)$, $A_m^{(3)}(q)$ and $A_m^{(4)}(q)$ if only if the determinant of the coefficient matrix is zero, i.e.,

$$\begin{aligned}&1-\left[V(q,R_1)\chi_1(q,m;\omega)+V(q,R_2)\chi_2(q,m;\omega)\right]\\&\qquad+\left[V(q,R_1)V(q,R_2)-V^2(q,R_1,R_2)\right]\chi_1(q,m;\omega)\chi_2(q,m;\omega)=0,\end{aligned} \tag{3.2.117}$$

Which agrees with the dispersion equations (2.1.13) and (2.2.34) in Lin's and G. Gumbs'papers respectively.

Now, in the limit as $R_3\to R_2$, Eqn. (2.2.37) reduces to a two-dimensional matrix, thereby leading to results similar to G.Gumbs, *et al* as well as that of Lin, *et al*. Furthermore, in the limit as $R_2\to\infty$, and in light of the aforementioned limiting case, the cylinders decouple and the system reduces to that of a single nanotube.

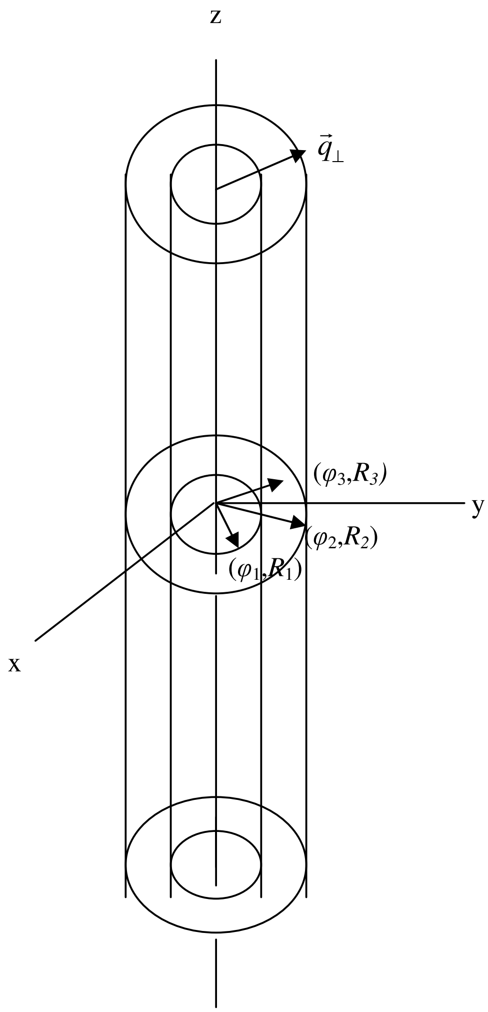


Fig. 3

The concentric nanotubules are perceived to be of infinite extent along the z-axis. We denote their radii by R_1 and R_2 and the angle each radius makes with respect to the x-axis by φ_1 and φ_2 respectively. Additionally, (φ_3,R_3) is a point between the nanotubes in the xy-plane. The momentum $\vec{q}_\perp$ is fixed with respect to the z-axis as well as in the xy-plane for the nanotubes.

3.3 Plasmons in a System of N Co-Axial Tubules

In a straightforward way, we can extend the aforementioned procedures to obtain the plasmon dispersion relation for a system of N co-axial tubules with radii $R_1, R_2, \cdots, R_N$.

The Eigen functions and eigenenergies are given by

$$\psi_\alpha(\rho,\varphi,z) = \frac{1}{\sqrt{L_z}} e^{ik_z z} P(\rho) \frac{1}{\sqrt{2\pi R_i}} e^{il\varphi}, P_i^2(\rho) = \delta(\rho - R_i) \tag{3.3.118}$$

Where

$$\varepsilon_\alpha = \frac{\hbar^2 k_z^2}{2m^*} + \frac{m^* R_i^2}{8\hbar^2}\left[\frac{2l\hbar^2}{m^* R_i^2}\right]^2, \tag{3.3.119}$$

Wherein, $\alpha = \{i, k_z, l\}$, $\forall i \in \mathbb{Z}_+ \le N$, and $-\infty < k_z < \infty$. Using the same procedure as was applied in deriving Eqns. (3.1.76)-(3.1.82), we obtain for the matrix element of the density matrix

$$< ik_z l \,|\, \hat{\rho}^1 \,|\, jk_z' l' >= 2e \frac{f_0(\varepsilon_{ik_z l}) - f_0(\varepsilon_{ik_z' l'})}{\hbar\omega + \varepsilon_{ik_z l} - \varepsilon_{ik_z' l'}} \varphi_{ext}^{(l-l')}(R_i, k_z - k_z')\delta_{ij}. \tag{3.3.120}$$

Wherein $\varphi_{ext}^{l-l'}(R_i, k_z - k_z')$ is defined in Eqn. (3.1.81). Poisson equation can be considered in the same way as in Eqns. (3.1.83)-(3.1.85)

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho \frac{\partial \varphi_{ext}^{(m)}(\rho,q,\omega)}{\partial\rho}\right) - \frac{m}{\rho^2}\varphi_{ext}^{(m)}(\rho,q,\omega) - q^2 \varphi_{ext}^{(m)}(\rho,q,\omega) = \sum_{i=1}^{N} A_{im}(q)\delta(\rho - R_i), \tag{3.3.121}$$

Wherein

$$A_{im}(q) = \frac{e}{\varepsilon_s \pi R_i} \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} dk_z < k_z l \,|\, \hat{\rho}^1 \,|\, k_z - q, l - m > . \tag{3.3.122}$$

Combining Eqns. (3.1.82) and (3.1.86), we have

$$A_{im}(q) = \frac{2e^2}{\varepsilon_s \pi R_i} \varphi_{ext}^{(m)}(R_i, q, \omega) \chi_i(q, m, \omega). \tag{3.3.123}$$

and $\chi_i(q, m, \omega)$ is given by (see Eqn. (3.1.92))

$$\chi_i(q, m; \omega) \equiv \frac{2m^*}{\hbar^2 q} \sum_{l=-S_j}^{S_j} \ln \left| \frac{\hbar^2 \omega^2 - E_+^2(l, m; k_F(l, \omega)_i, q)}{\hbar^2 \omega^2 - E_-^2(l, m; k_F(l, \omega)_i, q)} \right| \tag{3.3.124}$$

$$E_\pm^2(l, m; k_F(l, \omega)_i, q) = \left\{ \left[\frac{\hbar^2 (q^2 \pm 2k_F(l; \omega)_i q)}{2m^*} \right] - \left[\frac{\hbar^2 (2ml + m^2)}{2m^* R_i^2} \right] \right\}^2 \tag{3.3.125}$$

Where

$$k_F(l; \omega)_i \equiv \left\{ \frac{2m^*}{\hbar^2} \left[\varepsilon_F - \frac{m^* R_i^2}{8\hbar^2} \left[\frac{2l\hbar^2}{m^* R_i^2} \right]^2 \right] \right\}^{\frac{1}{2}} \tag{3.3.126}$$

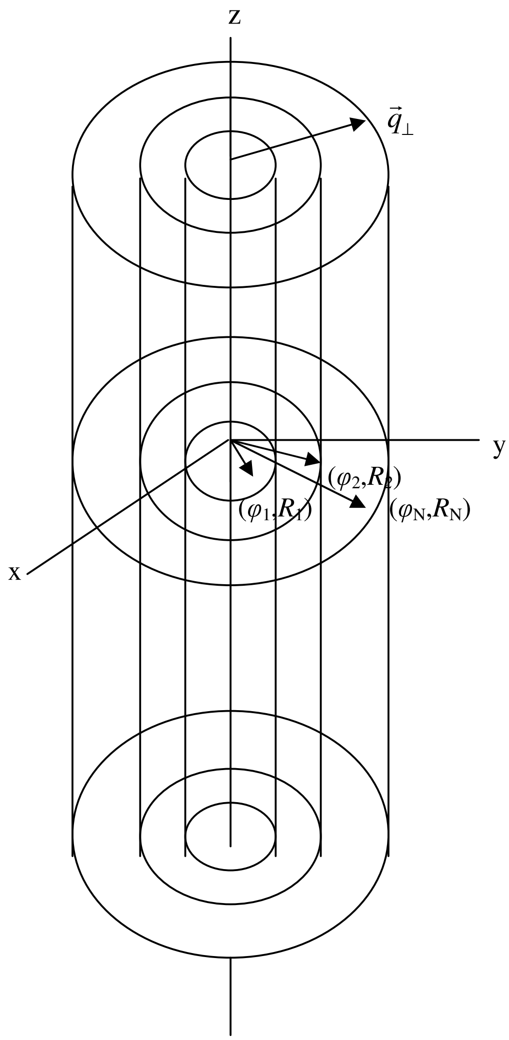


Fig. 4

System of N concentric nanotubules, the tubule is perceived to be of infinite extent along the z-axis. We denote their radii by R_1 and $R_2,\ldots,$ R_N and the angle each radius makes with respect to the xy-plane plane by φ_1, φ_2 …, φ_N respectively. The momentum $\vec{q}_\perp$ is fixed with respect to the z-axis as well as in the xy-plane for the nanotubes.

Chapter 4

One-Dimensional Array of Tubules in the Absence of a Magnetic Field.

4.1. Theoretical Formalism

In this chapter, we'll look at the 2D model, but first we must review the results of Gumbs-Ayzin. In their formalism as well as ours, we will exclude the **B**-Field. The reason for doing so is that in the tight binding approximation (TBA), there is translation symmetry throughout the lattice in the absence of a magnetic field. The symmetry is broken when the field is present. This is due to the variation in the origin with respect to each cylinder and its relationship to the vector potential. This poses a difficult problem, and as a consequence, we can not use the eigenfunction and eigenenergies for the zero field case in their usual form.

Let us consider a 1D array of nanotubes, shown schematically in Fig. 5, with their axes parallel to the z direction. For simplicity, we assume that each cylindrical tubule is infinitesimally thin. The axis of each nanotubule is at $x = n_x a_x$ $(n_x = 0, \pm 1, \pm 2, \cdots)$ on the x axis. Each nanotube consists of N concentric cylindrical tubules with radii $R_1 < R_2 < \cdots < R_N$, where $a > 2R_N$. We will construct the electron wave functions in the form of Bloch combinations as described by Huang and Gumbs for an array of rings [13]. In the absence of tunneling between the tubules, the single-particle Bloch wave functions for the nanotube array with the periodicity of the lattice are given by

$$|i\nu>= \tilde{\psi}_{i\nu}(\mathbf{r}) = \frac{e^{ik_z z}}{\sqrt{L_z}} \frac{1}{\sqrt{N_x}} \sum_{j=-\frac{N_x}{2}}^{\frac{N_x}{2}} e^{ik_x ja} \Psi_{il}(\vec{\rho} - ja_x \hat{x}), \Psi_{il}(\vec{\rho}) = \frac{1}{\sqrt{2\pi}} e^{il\phi} \frac{1}{\sqrt{\rho}} P_i(\rho),$$

(4.1.127)

Wherein $i=1,2,\cdots,N$ labels the tubules in the nanotube, $\nu=\{k_z,k_x,l\}$ is a composite index for the electron eigenstates, $\Psi_{il}(\vec{\rho})e^{ik_z z}$ is the wave function for an electron in the i^{th} tubule, with wave vector k_z in the axial direction and angular momentum quantum number $l=0,\pm1,\pm2,\cdots$, $P_i^2(\rho)=\delta(\rho-R_i)$ and $k_x=\frac{2\pi}{L_x}n$ with $n=0,\pm1,\pm2,\cdots,\pm\frac{N_x}{2}$. Here, $N_x=L_x/a_x$ is the number of nanotubes in the array with periodic boundary conditions. Electron motion in the azimuthal direction around the tubule is quantized and characterized by the angular momentum quantum number l, whereas motion in the axial z direction is free. Thus, the electron spectrum in each tubule will consist of 1D sub bands, with l serving as a sub-band index. The spectrum does not depend on k_x and hence has the form

$$\varepsilon_{i\nu}=\frac{\hbar^2k_z^2}{2m^*}+\frac{\hbar^2l^2}{2m^*R_i^2}. \tag{4.1.128}$$

Plasmons can be obtained from the solution of the density matrix equation $i\hbar\frac{\partial\hat{\rho}}{\partial t}=[\hat{H},\hat{\rho}]$ [14]. For $\hat{H}=\hat{H}^0-e\varphi_{ind}(\vec{r})$ and $\hat{\rho}=\hat{\rho}^0+\delta\hat{\rho}$, with $<i\nu|\hat{H}^0|i'\nu'>=\varepsilon_{i\nu}\delta_{\nu\nu'}\delta_{ii'}$, $<i\nu|\hat{\rho}^0|i'\nu'>=2f_0(\varepsilon_{i\nu})\delta_{\nu\nu'}\delta_{ii'}$, we obtain in the lowest order of perturbation theory

$$<i\nu|\delta\hat{\rho}|i'\nu'>=2e\frac{f_0(\varepsilon_{i\nu})-f_0(\varepsilon_{i'\nu'})}{\hbar\omega-\varepsilon_{i\nu}+\varepsilon_{i'\nu'}}<i\nu|\varphi_{ind}(\vec{r})|i'\nu'>, \tag{4.1.129}$$

Wherein the Fermi function is $f_0(\varepsilon)$ and $\varphi_{ind}(\vec{r})$ is the induced potential which analogously satisfies Poisson's equation

$$\nabla^2\varphi_{ind}(\vec{r})=\frac{4\pi e}{\varepsilon_s}\delta n_{ind}(\vec{r}), \tag{4.1.130}$$

Wherein, $\delta n_{ind}(\vec{r})$ is the fluctuation or change in the electron density.

Making use of the relation

$$\delta n_{ind}(\vec{r}) = \sum_{ii'} \sum_{\nu,\nu'} | i\nu >< i\nu | \delta\hat{\rho} | i'\nu' >< i'\nu' | \quad (4.1.131)$$

and Eqn. (4.1.129), we can write in Fourier representation

$$\delta n_{ind}(\vec{q}) = \frac{2e}{\Omega} \sum_{ii'} \sum_{\nu,\nu'} \frac{f_0(\varepsilon_{i\nu}) - f_0(\varepsilon_{i'\nu'})}{\hbar\omega - \varepsilon_{i\nu} + \varepsilon_{i'\nu'}} < i'\nu' | e^{-i\vec{q}\cdot\vec{r}} | i\nu > \sum_{\vec{q}'} \varphi_{ind}(\vec{q}') < i\nu | e^{i\vec{q}'\cdot\vec{r}} | i'\nu' >,$$

(4.1.132)

Wherein $\delta n_{ind}(\vec{q})$ and $\varphi_{ind}(\vec{q})$ are 3D Fourier transforms with respect to $\vec{q}$, of $\delta n_{ind}(\vec{r})$ and $\varphi_{ind}(\vec{q})$, respectively and $\vec{q} = (q_x, q_y, q_z)$. The matrix elements $< i\nu | e^{i\vec{q}\cdot\vec{r}} | i'\nu' >$ with wave functions $| i\nu >$ given in Eqn. (4.1.127) can be evaluated as follows

$$< i\nu | e^{i\vec{q}\cdot\vec{r}} | i'\nu' > = \delta_{ii'} \delta_{k_z - k_z', q_z} \delta_{k_x - k_x', q_x + G_{N_x}} e^{-im\vartheta} i^m J_m(q_\perp R_i), \quad (4.1.133)$$

wherein $G_{N_x} = \frac{2\pi N_x}{a_x}$ with $N_x, l' \in \mathbb{Z},...,0$, inclusive $m = (l - l') \in \mathbb{Z},...,0$, $\vec{q}_\perp = (q_x, q_y)$, ϑ is the angle between $\vec{q}_\perp$ and $\hat{x}$ ($0 \le \vartheta < 2\pi$) and $J_m(x)$ is a Bessel function of the first kind.

Substituting Eqn. (4.1.133) into Eqn. (4.1.132), we obtain

$$\delta n_{ind}(\vec{q}) = \frac{e}{\pi a_x L_z} \sum_{k_z} \sum_{i} \sum_{l,m} \frac{f_0(\varepsilon_{i,k_z,l}) - f_0(\varepsilon_{i,k_z - q_z, l-m})}{\hbar\omega + \varepsilon_{i,k_z - q_z, l-m} - \varepsilon_{i,k_z,l}} e^{im\vartheta} J_m(q_\perp R_i)$$

$$\times \sum_{N_x = -\infty}^{\infty} \int dq_y' \varphi^{app}\left(q_x + G_{N_x}, q_y', q_z\right) J_m\left(\sqrt{\left(q_x + G_{N_x}\right)^2 + q_y'^2} R_i\right) \left(\frac{q_x + G_{N_x} - iq_y'}{\sqrt{(q_x + G_{N_x})^2 + q_y'^2}}\right)^m .$$

(4.1.134)

The potential $\varphi_{ind}(\vec{q})$ can be written in terms of $\delta n_{ind}(\vec{q})$ as $\varphi_{ind}(\vec{q}) = -4\pi e \delta n_{ind}(\vec{q}) / \varepsilon_s q^2$. Using this relation in Eqn. (4.1.134), we obtain

$$\delta n_{ind}(\vec{q}) = -\frac{e^2}{\pi a_x \varepsilon_s}\sum_{i,m}\chi_{i,m}(q_z,\omega)e^{im\vartheta}J_m\left(q_\perp R_i\right)U_{i,m}(q_x,q_z), \tag{4.1.135}$$

where

$$\chi_{i,m}(q_z,\omega) = 2\sum_{l=-\infty}^{\infty}\int dk_z\,\frac{f_0(\varepsilon_{i,k_z,l}) - f_0(\varepsilon_{i,k_z-q_z,l-m})}{\hbar\omega+\varepsilon_{i,k_z-q_z,l-m}-\varepsilon_{i,k_z,l}} \tag{4.1.136}$$

is the polarization function in a single cylindrical tubule of radius R_i and

$$U_{i,m}(q_x,q_z) = \sum_{N=-\infty}^{\infty}\int dq_y\,\frac{\delta n(q_x+G_{N_x},q_y,q_z)}{\left(q_x+G_{N_x}\right)^2+q_y^2+q_z^2}J_m\left(\sqrt{\left(q_x+G_{N_x}\right)^2+q_y^2}\,R_i\right)$$

$$\times\left(\frac{q_x+G_{N_x}-iq_y}{\sqrt{(q_x+G_{N_x})^2+q_y^2}}\right)^m. \tag{4.1.137}$$

Substituting the expression for $\delta n_{ind}(\vec{q})$ given in Eqn. (4.1.135) into Eqn. (4.1.137), we obtain

$$U_{i,m}(q_x,q_z)+\frac{e^2}{\pi a_x\varepsilon_s}\sum_{i'}\sum_{m'}\chi_{i',m'}(q_z,\omega)$$

$$\times\sum_{N=-\infty}^{\infty}\int dq_y\,\frac{J_{m'}\left(\sqrt{\left(q_x+G_{N_x}\right)^2+q_y^2}\,R_{i'}\right)J_m\left(\sqrt{\left(q_x+G_{N_x}\right)^2+q_y^2}\,R_i\right)}{\left(q_x+G_{N_x}\right)^2+q_y^2+q_z^2}$$

$$\times\left(\frac{q_x+G_{N_x}+iq_y}{\sqrt{(q_x+G_{N_x})^2+q_y^2}}\right)^{m'-m}U_{i',m'}(q_x,q_z)=0. \tag{4.1.138}$$

This system of linear equations has nontrivial solutions provided the following determinant is zero,

$$\left\| \delta_{mm'}\delta_{ii'} + \frac{e^2}{\pi a_x \varepsilon_s}\chi_{i'm'}(q_z,\omega) \right.$$

$$\times \sum_{N=-\infty}^{\infty} \int_{-\infty}^{\infty} dq_y \, \frac{J_{m'}\left(\sqrt{\left(q_x+G_{N_x}\right)^2+q_y^2}\,R_{i'}\right) J_m\left(\sqrt{\left(q_x+G_{N_x}\right)^2+q_y^2}\,R_i\right)}{\left(q_x+G_{N_x}\right)^2+q_y^2+q_z^2}$$

$$\left. \left(\frac{q_x+G_{N_x}+iq_y}{\sqrt{(q_x+G_{N_x})^2+q_y^2}} \right)^{m'-m} \right\| = 0, \qquad (4.1.139)$$

with $m, m' \in \mathbb{Z},..,0,$ inclusive, and $i, i' \in \mathbb{N}, \leq N$ where $i \neq i'$

Equation (4.1.139) determines the dispersion equation for the plasmon collective excitations. At $T = 0$ K, it is a straightforward matter to evaluate the polarization function $\chi_{i,m}(q_z,\omega)$ in Eqn. (4.1.136) with the result

$$\chi_{i,m}(q_z,\omega) = \frac{2m^*}{\hbar^2 q_z}\sum_{l=-S_i}^{S_i} \ln\left| \frac{\hbar^2\omega^2 - E_+^2(l,m,q_z,k_F(l)_i)}{\hbar^2\omega^2 - E_-^2(l,m,q_z,k_F(l)_i)} \right|, \qquad (4.1.140)$$

where S_i is the maximum value of $|l|$ among the sub-bands occupied by electrons in the i^{th} cylindrical tubule, $k_F(l)_i = \sqrt{\dfrac{2m^* E_F}{\hbar^2} - \dfrac{l^2}{R_i^2}}$ is the Fermi wave vector in the z direction for the sub-band with given l and

$$E_\pm(l,m,q_z,k_F(l)_i) = \frac{\hbar^2(q_z^2 \pm 2k_F(l)_i q_z)}{2m^*} + \frac{\hbar^2(2ml+m^2)}{2m^* R_i^2}. \qquad (4.1.141)$$

Equation (4.1.139) shows that the symmetry of the lattice is maintained in the dispersion equation and that the plasmon excitations depend on the wave vector q_x in the x direction with period $G_{N_x} = 2\pi / a_x$ as well as the wave vector q_z.

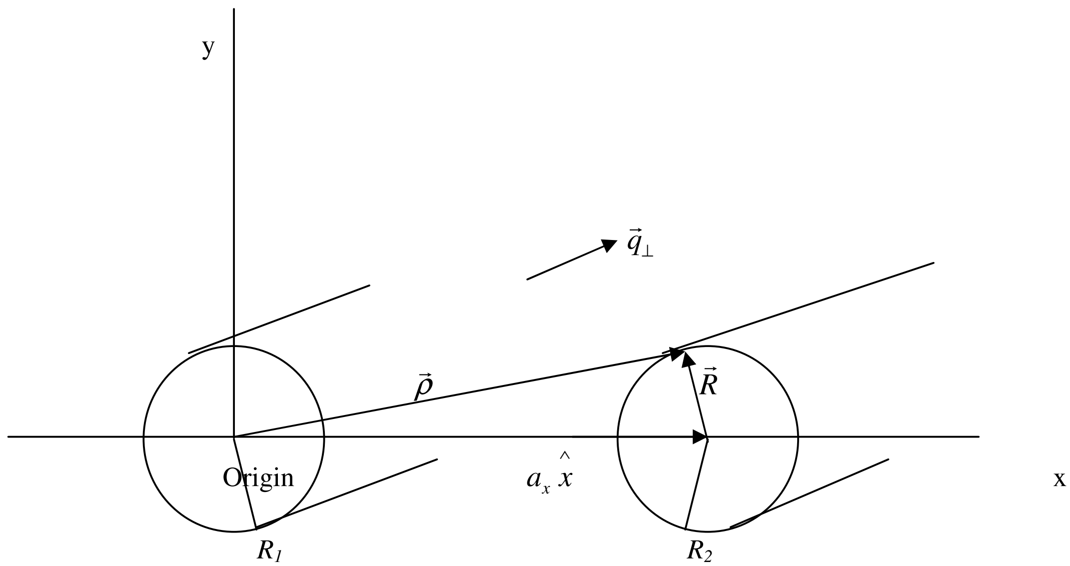


Fig. 5

The tubules are perceived to be of infinite extent along the z-axis and are equally infinite in number along the x-axis. We denote their radii by R_1 and R_2 , … R_N and the angle each radius makes with respect to the xy-plane plane by φ_1, φ_2 …, φ_N respectively. The momentum $\vec{q}_{\perp}$ is fixed with respect to the z-axis as well as in the xy-plane for the nanotubes.

In the limit $a_x \to \infty$, the sum over reciprocal lattice vectors in Eqn. (4.1.138) gets transformed into an integral, and the determinantal matrix in Eqn. (4.1.139) becomes diagonal in the indices m and $m^{'}$. Using [4]

$$\overline{V}_m\left(q_z, R_i, R_{i^{'}}\right) \equiv \int_0^{\infty} q_{\|} dq_{\|} \frac{J_m(q_{\|}R_i) J_m(q_{\|}R_{i^{'}})}{q_{\|}^2 + q_z^2} = \begin{cases} I_m(q_z R_i) K_m(q_z R_{i^{'}}) & R_i < R_{i^{'}}, \\ I_m(q_z R_{i^{'}}) K_m(q_z R_i) & R_{i^{'}} > R_i \end{cases} \tag{4.1.142}$$

we obtain the following dispersion equation

$$\prod_{m=0,\pm 1,\cdots} Det\left[\delta_{ii^{'}} + \frac{e^2}{\pi\varepsilon_s}\overline{V}_m\left(q_z, R_i, R_{i^{'}}\right)\chi_{i,m}(q_z,\omega)\right] = 0. \tag{4.1.143}$$

Equation (4.1.143) is the dispersion equation for plasmons in a single nanotube consisting of N coaxial cylindrical tubules and agrees with Ref. [4]. It follows from Eqn. (4.1.143) that the plasmon modes in a single coaxial nanotube can be labeled by the quantum numbers m and q_z where $m = l - l^{'}$ is an angular momentum transfer in the electron intersub-band transitions ($l \xleftrightarrow{\rightarrow} l^{'}$) contributing to the given plasmon mode. When a_x is finite, the non-diagonal in $m, m^{'}$ elements of the matrix in Eqn. (4.1.139) are not equal to zero and modes with different values of m are in general coupled to each other. It will be shown that this coupling modifies the plasmon spectrum. Subsequently, we will solve Eqn. (4.1.139) numerically for $N = 1$, and $m, m^{'} = 0, \pm 1$. For $\vec{B} = 0$ and $\vec{B} \neq 0$.

4.2. Infinite 2D Array of Nanotubes

Barring tunneling between the tubules, the single-particle eigenfunctions of the wave equations for the 2D periodic array are the product a plane wave $e^{i\vec{k}\cdot\vec{r}}$ and the function, $\psi_\alpha(r,\varphi,z)$ with the periodic array. Simply put, the Bloch functions for a 2D system of $j \in \mathbb{N}$ nanotubes with lattice vectors $n_x a_x \vec{x}$ and $n_y a_y \vec{y}$ are

$$\psi_{j\upsilon}(\rho,\varphi,z) = \frac{1}{\sqrt{L_z N_x N_y}} e^{ik_z z} \sum_{n_x=-\frac{N_x}{2}}^{\frac{N_x}{2}} \sum_{n_y=-\frac{Ny}{2}}^{\frac{Ny}{2}} e^{ik_x na_x} e^{ik_y na_y} \psi_{jl}(\vec{\rho} - (na_x\vec{x} + na_y\vec{y}))$$

(4.2.144)

With $n_x, n_y \in \mathbb{Z}; k_x = \frac{2\pi}{L_z} n_x, k_y = \frac{2\pi}{L_z} n_y; \upsilon = (k_z, k_x, k_y; l); N_x = \frac{L_x}{a_x}, N_y = \frac{L_y}{a_y}$

(4.2.145)

and where

$$\psi_{jl}(\rho) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{\rho}} e^{il\varphi} P_j(\rho) \tag{4.2.146}$$

By multiplying Eqn. (4.2.146) by $e^{ik_z z}/\sqrt{L_z}$, we obtain the eigenfunction for an electron in the j^{th} tubule having wave vector k_z and angular momentum $l \in \mathbb{Z}$, respectively. Thus

$$\frac{e^{il\varphi}}{\sqrt{2\pi}} \frac{P_j(\rho)}{\sqrt{\rho}} \frac{e^{ik_z z}}{\sqrt{L_z}} \tag{4.2.147}$$

The total Hamiltonian for our system is

$$\begin{aligned} \hat{H} &= \hat{H}^0 + \hat{H}^1 \\ &= \hat{H}^0 + (-e\sum_j \delta(\varphi_{ind}(\vec{q}\,'))) \end{aligned} \tag{4.2.148}$$

Now, $\varphi_{ind}(\vec{q}\,')$ is related to the change in electron density *via* the well known relation

$$\delta n(\vec{r}) = \iiint\limits_{allspace} \chi(\vec{r}-\vec{r}')\delta(\varphi_{ind}(\vec{q}'))d^3\vec{r}' \tag{4.2.149}$$

Where

$\delta(\varphi_{ind}(\vec{q}'))$) is the applied induced potential and $\chi(\vec{r}-\vec{r}')$ is the response.

Taking the Fourier transform with respect to $\vec{q}$, of both sides of Eqn. (4.2.149) and integrating over all space yields

$$\int\limits_{allspace} d^3\vec{r}\,\delta n_{ind}(\vec{r})e^{-i\vec{q}\cdot\vec{r}} = \int\limits_{allspace} d^3\vec{r} \iiint\limits_{allspace} \chi(\vec{r}-\vec{r}')\delta(\varphi_{ind}(\vec{q}'))e^{-i\vec{q}\cdot\vec{r}}d^3\vec{r}'$$

$$= \int\limits_{allspace} d^3\vec{r} \iiint\limits_{allspace} d^3\vec{r}'\chi(\vec{r}-\vec{r}')\delta(\varphi_{ind}(\vec{q}'))e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}e^{-i\vec{q}\cdot\vec{r}'}$$

(4.2.150)

However,

$$\int\limits_{allspace} d^3\vec{r}\,\delta n_{ind}(\vec{r})e^{-i\vec{q}\cdot\vec{r}} \equiv \delta n_{ind}(\vec{q}) \tag{4.2.151}$$

Via the transitive property, we may equate Eqns. (4.2.150) and (4.2.151) which gives us the following

$$\delta n_{ind}(\vec{q}) = \int\limits_{allspace} d^3\vec{r} \iiint\limits_{allspace} d^3\vec{r}'\chi(\vec{r}-\vec{r}')\delta(\varphi_{ind}(\vec{q}'))e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}e^{-i\vec{q}\cdot\vec{r}'} \tag{4.2.152}$$

In addition, if one integrates Eqn. (4.2.151) with respect to $(\vec{r}-\vec{r}')$, we obtain the more familiar form:

$$\delta n_{ind}(\vec{q}) = \int\limits_{allspace} d^3(\vec{r}-\vec{r}')\chi(\vec{r}-\vec{r}')e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} \iiint\limits_{allspace} d^3\vec{r}'\delta(\varphi_{ind}(\vec{q}'))e^{-i\vec{q}\cdot\vec{r}}$$

$$= \chi(\vec{q})\delta(\varphi_{ind}(\vec{q})) \tag{4.2.153}$$

This tells us that the response, $\chi(\vec{q})$ of the system is a ratio of the change in the density of electrons to the change in the applied induced potential.

Equation (4.2.153) is the fundamental equation upon which we will construct the mathematical formalism required to describe the physics of elementary excitations for a 2D periodic array of nanotubes.

4.3. The Induced Potential

How does one obtain $\varphi_{ind}(\vec{q})$? It is known that the total potential φ_{Total}, consists of the sum of an external potential φ_{ext}, and the induced screened potential φ_{ind}, which itself is further related to the induced change in electron density (electron density fluctuation)

$$\delta n_{ind}(\vec{r}) = \frac{1}{\Omega}\sum_{q} e^{-iq\cdot r}\sum_{j,\upsilon}\langle j\upsilon\left|\rho^{(1)}\right| j'\upsilon'\rangle \tag{4.3.154}$$

(Where, Ω is the volume of the sample)

Now by way of Poisson's Equation

$$\nabla^2\varphi_{ind}(\vec{r}) = -\frac{4\pi e^2}{\varepsilon_s}\delta n_{ind}(\vec{r}) \tag{4.3.155}$$

Whose solution via Fourier discrete transformation with respect to $\vec{q}$ is

$$\varphi_{ind}(\vec{q}) = -\frac{4\pi e^2}{q^2\varepsilon_s}\sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}}\delta n_{ind}(\vec{r}) \tag{4.3.156}$$

Equation (4.3.156) may be re-written in an alternate form if we back substitute Eqn. (4.3.154) into Eqn. (4.3.156), which yields

$$\varphi_{ind}(\vec{q}) = \frac{4\pi e^2}{q^2\Omega\varepsilon_s}\sum_{j,\upsilon}\langle j\upsilon\left|\rho^{(1)}\right| j'\upsilon'\rangle, \vec{r}' = \vec{r} \tag{4.3.157}$$

and

$$\varphi_{ind}(q) = \frac{4\pi e^2}{q^2\Omega\varepsilon_s}\sum_{\vec{r}} e^{-i\vec{q}\cdot\vec{r}}\sum_{\vec{q}'} e^{i\vec{q}'\cdot r}\sum_{j,\upsilon}\langle j\upsilon\left|\rho^{(1)}\right| j'\upsilon'\rangle\ ,\ \vec{r}' \neq \vec{r} \tag{4.3.158}$$

Where, $\rho^{(1)}$ arose from the solution to the single-particle density matrix Liouville equation (See comments between Equations (3.1.76) and (3.1.78).).

4.4 The Matrix Elements and Change in Electron Density

Next, we will evaluate the matrix element associated with the change in the operator,

$$\rho^{(1)} \equiv \delta(\hat{\rho}) \qquad (4.4.159)$$

represented by the single-particle density matrix.

It is known that alternatively, the change in the number density may be written as

$$\delta n_{ind}(\vec{r}) = \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \delta n_{ind}(\vec{q}) \qquad (4.4.160)$$

Which, by making use of the relation,

$$\delta n_{ind}(\vec{r}) = \sum_{k,k'} \left|k\right\rangle\left\langle k\right|\rho^{(1)}\left|k'\right\rangle\left\langle k'\right| \qquad (4.4.161)$$

may be re-written as

$$\delta n_{ind}(\vec{r}) = \sum_{j,j'} \sum_{\upsilon,\upsilon'} \left|j\upsilon\right\rangle\left\langle j\upsilon\right|\delta\hat{\rho}\left|j'\upsilon'\right\rangle\left\langle j'\upsilon'\right| \qquad (4.4.162)$$

As previously outlined, the self-consistent field approach is then used to calculate the matrix element of $\delta(\hat{\rho})$ to lowest order in perturbation theory *ibid*, Eqn. (4.1.129). Reproduced here for convenience

$$\delta n_{ind}(\vec{q}) = \frac{2e}{\Omega} \sum_{jj'} \sum_{\nu,\nu'} \frac{f_0(\varepsilon_{j\nu}) - f_0(\varepsilon_{j'\nu'})}{\hbar\omega - \varepsilon_{j\nu} + \varepsilon_{j'\nu'}} < j'\nu' \,|\, e^{-i\vec{q}\cdot\vec{r}} \,|\, j\nu > \sum_{\vec{q}'} \varphi_{ind}(\vec{q}') < j\nu \,|\, e^{i\vec{q}'\cdot\vec{r}} \,|\, j'\nu' >$$

The matrix elements $< j\nu \,|\, e^{i\vec{q}\cdot\vec{r}} \,|\, j'\nu' >$ with wave functions $|\, j\nu >$ given in Eqn. (4.2.144) can be evaluated as follows

$$< j\nu \,|\, e^{iq'_{\perp}\cdot\vec{r}} \,|\, j'\nu' > = \delta_{jj'} \delta_{k_z - k'_z, q'_z} \delta_{k_x - k'_x, q'_x + G_{N_x}} \delta_{k_y - k'_y, q'_y + G_{N_y}} e^{-im\vartheta} i^m J_m(q'_{\perp} R_j) \qquad (4.4.163)$$

where $G_{N_x} = \frac{2\pi N_x}{a_x}$ and $G_{N_y} = \frac{2\pi N_y}{a_y}$ with $N_{x,y} = 0, \pm 1, \pm 2, \cdots$, $m = l - l^{'}$, $\vec{q}_{\perp} = (q_x, q_y)$, ϑ is the angle between $\vec{q}_{\perp}$ and $\hat{x}$ ($0 \leq \vartheta < 2\pi$) and $J_m(x)$ is a Bessel function of the first kind.

Back-substituting Eqn. (4.4.163) into the Eqn. (4.1.129) for the change in electron density, we obtain

$$\delta n_{ind}(\vec{q}) = \frac{e}{\pi a_x a_y L_z} \sum_j \sum_m 2 \sum_l \sum_{k_z} \frac{f_0(\varepsilon_{j,k_z,l}) - f_0(\varepsilon_{j,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{j,k_z-q_z,l-m} - \varepsilon_{j,k_z,l}} e^{im\vartheta} J_m\left(R_j\sqrt{q_x^2+q_y^2}\right)$$

$$\sum_{N_x=-\infty}^{\infty} \sum_{N_y=-\infty}^{\infty} \varphi^{app}\left(q_x + \tfrac{2\pi N_x}{a_x}, q_y + \tfrac{2\pi N_y}{a_y}, q_z\right) J_m\left(R_j\sqrt{\left(q_x + \tfrac{2\pi N_x}{a_x}\right)^2 + \left(q_y + \tfrac{2\pi N_y}{a_y}\right)^2}\right) \times$$

$$\times\left(\frac{q_x + \frac{2\pi N_x}{a_x} - i\left(q_y + \frac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x + \frac{2\pi N_x}{a_x}\right)^2 + \left(q_y + \frac{2\pi N_y}{a_y}\right)^2}}\right)^m \tag{4.4.164}$$

However, recall that the induced potential is also expressible as

$$\varphi_{ind}(\vec{q}) = \frac{-4\pi e}{q^2 \varepsilon_s} \delta n_{ind}(\vec{q}) \tag{4.4.165}$$

Back-substituting Eqn. (4.4.165) into Eqn. (4.4.164) we obtain

$$\delta n_{ind}(\vec{q}) = \frac{-e}{a_x a_y L_z} \sum_j \sum_m 2 \sum_l \sum_{k_z} \frac{f_0(\varepsilon_{j,k_z,l}) - f_0(\varepsilon_{j,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{j,k_z-q_z,l-m} - \varepsilon_{j,k_z,l}} e^{im\vartheta} J_m\left(R_j\sqrt{q_x^2+q_y^2}\right) \times$$

$$\times \sum_{N_x=-\infty}^{\infty} \sum_{N_y=-\infty}^{\infty} \frac{4\pi e}{\varepsilon_s} \frac{\delta n_{ind}\left(q_x + \frac{2\pi N_x}{a_x}, q_y + \frac{2\pi N_y}{a_y}, q_z\right)}{\left(q_x + \frac{2\pi N_x}{a_x}\right)^2 + \left(q_y + \frac{2\pi N_y}{a_y}\right)^2 + q_z^{\,2}} J_m\left(R_j\sqrt{\left(q_x + \tfrac{2\pi N_x}{a_x}\right)^2 + \left(q_y + \tfrac{2\pi N_y}{a_y}\right)^2}\right) \times$$

$$\times\left(\frac{q_x + \frac{2\pi N_x}{a_x} - i\left(q_y + \frac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x + \frac{2\pi N_x}{a_x}\right)^2 + \left(q_y + \frac{2\pi N_y}{a_y}\right)^2}}\right)^m \tag{4.4.166}$$

Now, in the limit as $\lim_{L_z \to \infty} \sum_{k_z} \to \frac{L_z}{2\pi} \int dk_z$ and we obtain via back-substitution into Eqn. (4.4.166), the following:

$$\delta n_{ind}(\vec{q}) = \frac{-2e^2}{a_x a_y \varepsilon_s}\sum_j \sum_m 2\sum_l \int dk_z \; \frac{f_0(\varepsilon_{j,k_z,l}) - f_0(\varepsilon_{j,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{j,k_z-q_z,l-m} - \varepsilon_{j,k_z,l}} e^{im\vartheta} J_m\left(R_j\sqrt{q_x^2+q_y^2}\right)\times$$

$$\times\sum_{N_x=-\infty}^{\infty}\sum_{N_y=-\infty}^{\infty}\frac{\delta n_{ind}\left(q_x+\frac{2\pi N_x}{a_x}, q_y+\frac{2\pi N_y}{a_y}, q_z\right)}{\left(q_x+\frac{2\pi N_x}{a_x}\right)^2+\left(q_y+\frac{2\pi N_y}{a_y}\right)^2+q_z{}^2} J_m\left(R_j\sqrt{\left(q_x+\frac{2\pi N_x}{a_x}\right)^2+\left(q_y+\frac{2\pi N_y}{a_y}\right)^2}\right)\times$$

$$\times\left(\frac{q_x+\frac{2\pi N_x}{a_x}-i\left(q_y+\frac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x+\frac{2\pi N_x}{a_x}\right)^2+\left(q_y+\frac{2\pi N_y}{a_y}\right)^2}}\right)^m \tag{4.4.167}$$

Let us define

$$\chi_{j,m}(q_z,\omega,\varepsilon_F) \equiv 2\sum_l \int dk_z \; \frac{f_0(\varepsilon_{j,k_z,l}) - f_0(\varepsilon_{j,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{j,k_z-q_z,l-m} - \varepsilon_{j,k_z,l}} \tag{4.4.168}$$

as the polarization response function.

$$U_{j,m}(q_x,q_y,q_z) \equiv \sum_{N_x=-\infty}^{\infty}\sum_{N_y=-\infty}^{\infty}\frac{\delta n_{ind}\left(q_x+\frac{2\pi N_x}{a_x}, q_y+\frac{2\pi N_y}{a_y}, q_z\right)}{\left(q_x+\frac{2\pi N_x}{a_x}\right)^2+\left(q_y+\frac{2\pi N_y}{a_y}\right)^2+q_z{}^2}$$

$$\times J_m\left(R_j\sqrt{\left(q_x+\frac{2\pi N_x}{a_x}\right)^2+\left(q_y+\frac{2\pi N_y}{a_y}\right)^2}\right)\left(\frac{q_x+\frac{2\pi N_x}{a_x}-i\left(q_y+\frac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x+\frac{2\pi N_x}{a_x}\right)^2+\left(q_y+\frac{2\pi N_y}{a_y}\right)^2}}\right)^m$$

(4.4.169)

and

$$\delta n_{ind}(q_x,q_y,q_z) \equiv \frac{-2e^2}{a_x a_y \varepsilon_s}\sum_j\sum_m \chi_{j,m}(q_z,\omega,\varepsilon_F)\left(\frac{q_x+iq_y}{\sqrt{q_x^2+q_y^2}}\right)^m$$

$$\times J_m\left(R_j\sqrt{q_x^2+q_y^2}\right)U_{j,m}(q_x,q_y,q_z)$$

(4.4.170)

Or with the replacement by translated arguments of $q_x \to q_x + \frac{2\pi N_x}{a_x}$ and of $q_y \to q_y + \frac{2\pi N_y}{a_y}$ in Eqn. (4.4.170), we obtain

$$\delta n_{ind}\left(q_x+\tfrac{2\pi N_x}{a_x},q_y+\tfrac{2\pi N_y}{a_y},q_z\right)\equiv\frac{-2e^2}{a_x a_y \varepsilon_s}\sum_{j'}\sum_{m'}\chi_{j',m'}\left(q_z,\omega,\varepsilon_F\right)$$
$$\times\left(\frac{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)+i\left(q_y+\tfrac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}}\right)^m J_m\left(R_j\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}\right)U_{j',m'}\left(q_x,q_y,q_z\right)$$

(4.4.171)

Back-substituting Eqn. (4.4.171) into the numerator of Eqn. (4.4.169) gives us

$$\Bigg[1 \quad \frac{2e^2}{a_x a_y \varepsilon_s}\sum_{j'}\sum_{m'}\sum_{N_x=-\infty}^{\infty}\sum_{N_y=-\infty}^{\infty}\chi_{j',m'}\left(q_z,\omega,\varepsilon_F\right)J_{m'}\left(R_{j'}\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}\right)$$
$$\times\frac{J_m\left(R_j\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}\right)}{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2+q_z^{\,2}}\left(\frac{q_x+\tfrac{2\pi N_x}{a_x}+i\left(q_y+\tfrac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}}\right)^{m'-m}\Bigg]$$
$$\times\begin{bmatrix}U_{j,m}\left(q_x,q_y,q_z\right)\\ U_{j',m'}\left(q_x,q_y,q_z\right)\end{bmatrix}=0 \qquad (4.4.172)$$

For non-vanishing solutions of Eqn. (4.4.172) to exist, the determinant of the succeeding equation must vanish.

$$\Bigg\|\delta_{j,j'}\delta_{m,m'}+\frac{2e^2}{a_x a_y \varepsilon_s}\sum_{N_x=-\infty}^{\infty}\sum_{N_y=-\infty}^{\infty}\chi_{j',m'}\left(q_z,\omega,\varepsilon_F\right)J_{m'}\left(R_{j'}\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}\right)\times$$
$$\times\frac{J_m\left(R_j\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}\right)}{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2+q_z^{\,2}}\left(\frac{q_x+\tfrac{2\pi N_x}{a_x}+i\left(q_y+\tfrac{2\pi N_y}{a_y}\right)}{\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+\left(q_y+\tfrac{2\pi N_y}{a_y}\right)^2}}\right)^{m'-m}\Bigg\|=0$$

(4.4.173)

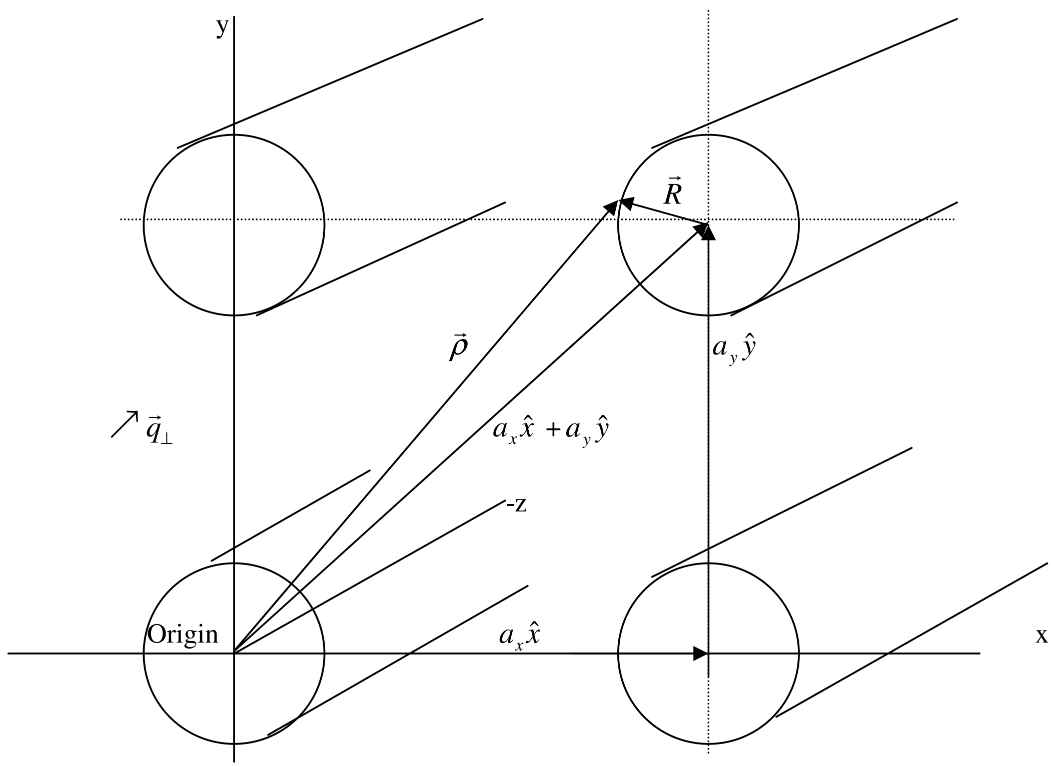


Fig. 6

Above is a sector from a two-dimensional infinite array of nanotubules. The tubules are perceived to be of infinite extent along the z-axis. We denote their radii by R_1 and R_2 , … R_N and the angle each radius makes with respect to the xy-plane plane by φ_1 , φ_2 …, φ_N respectively. The momentum $\vec{q}_\perp$ is fixed with respect to the z-axis as well as in the xy-plane for the nanotubes.

4.5 The Gumbs-Aizn Dispersion Relation as a Special Case

It is interesting to note that by keeping q_x fixed and in taking the limit as $a_y \to \infty$, we find that $\frac{2\pi N_y}{a_y} \to 0$ and $\sum_{N_y} \to \frac{a_y}{2\pi}\int dq_y$ in Eqn. (4.4.173). Thus Eqn. (4.4.173) reduces to

$$\left\| \delta_{j,j'}\delta_{m,m'} + \frac{e^2}{\pi a_x \varepsilon_s}\chi_{j',m'}(q_z,\omega,\varepsilon_F)\sum_{N_x=-\infty}^{\infty}\int dq_y J_{m'}\left(R_{j'}\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+q_y^2}\right) \right.$$
$$\left. \times\frac{J_m\left(R_j\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+q_y^2}\right)}{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+q_y^2+q_z^2}\left(\frac{q_x+\tfrac{2\pi N_x}{a_x}+iq_y}{\sqrt{\left(q_x+\tfrac{2\pi N_x}{a_x}\right)^2+q_y^2}}\right)^{m'-m} \right\| = 0$$

(4.5.174a)

This corresponds to the result obtained by Gumbs, *et al* for an infinite linear array of aligned carbon nanotubules in the absence of a **B**-field (Phys.Rev. **B** 65, 195407)

The Single Nanotubule Limit

It turns out that in the limit as $(a_x,a_y)\to\infty$, we find that $\left(\frac{2\pi N_x}{a_x},\frac{2\pi N_y}{a_y}\right)\to 0$ and $\left(\sum_{N_x=-\infty}^{\infty},\sum_{N_y=-\infty}^{\infty}\right)\to\left(\frac{a_x}{2\pi}\int dq_x,\frac{a_y}{2\pi}\int dq_y\right)$ in Eqn. (4.4.173)

$$\left\| \delta_{j,j'} + \frac{e^2}{\pi\varepsilon_s}\chi_{j',m'}(q_z,\omega,\varepsilon_F)\int_0^{\infty} q_{\|}dq_{\|}\frac{J_m\left(R_{j'}q_{\|}\right)J_m\left(R_j q_{\|}\right)}{q_{\|}^2+q_z^{\,2}} \right\| = 0 \qquad (4.5.174b)$$

which is the dispersion result for a single nanotubule obtained by Gumbs, et al (see above), in addition to that obtained by Lin, et al.

Chapter 5

Finite 2D Lower Triangular Array of Nanotubules

5.1 Example of a Bundle.

Let us consider a coupled triad of infinitesimally thin nanotubules, with their axes aligned in the z-direction. The axes of one of the tubules of radius R_1 is located at the origin at $x=0$ and the remaining two tubules each of radius R_2 and R_3 are located at a distance of $x=a_x$ and $y=a_y$ from zero on the x and y-axes respectively. We shall impose the condition that $a_x > R_1+R_2$ and $a_y > R_1+R_3$. Barring tunneling between the tubules, the eigenfunctions for an electron on the j$^{\text{th}}$ nanotube $(j=1,2)$, with axial wave vector k_z and angular momentum quantum number $l=0,\pm1,\pm2,\pm3,...$ are given by

$$|i\nu>_x=\frac{e^{ik_z z}}{\sqrt{L_z}}\Psi_{jl}(\vec{\rho}-(j-1)a_x\hat{x}) \tag{5.1.175}$$

$$|i\nu>_y=\frac{e^{ik_z z}}{\sqrt{L_z}}\Psi_{jl}(\vec{\rho}-(j-1)a_y\hat{y}) \tag{5.1.176}$$

with

$$\Psi_{jl}(\vec{\rho})=\frac{1}{\sqrt{2\pi}}e^{il\phi}\frac{1}{\sqrt{\rho}}P_j(\rho) \tag{5.1.177}$$

Wherein $j=1,2$ labels the tubules in the nanotube, $\nu=\{k_z,k_x,l\}$ is a composite index for the electron eigenstates, $\Psi_{il}(\vec{\rho})e^{ik_z z}$ is the wave function for an electron in the j-th tubule, with wave vector k_z in the axial direction and angular momentum quantum number $l = 0, \pm 1, \pm 2, \cdots$, $P_i^2(\rho) = \delta(\rho - R_i)$. Thus, the electron spectrum in each tubule consists of a sequence of 1D sub-bands with l serving as a sub-band index. The energy spectrum does not depend on k_x and has the form

$$\varepsilon_{i\nu} = \frac{\hbar^2 k_z^2}{2m^*} + \frac{\hbar^2 l^2}{2m^* R_i^2}. \tag{5.1.178}$$

Plasmons can be obtained from the solution of the density matrix equation $i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]$ [14]. For $\hat{H} = \hat{H}^0 - e\varphi_{ind}$ and $\hat{\rho} = \hat{\rho}^0 + \delta\hat{\rho}$, with $< i\nu \,|\, \hat{H}^0 \,|\, i'\nu' >= \varepsilon_{i\nu} \delta_{\nu\nu'} \delta_{ii'}$, $< i\nu \,|\, \hat{\rho}^0 \,|\, i'\nu' >= 2 f_0(\varepsilon_{i\nu}) \delta_{\nu\nu'} \delta_{ii'}$, we obtain in the lowest order of perturbation theory

$$< i\nu \,|\, \delta\hat{\rho} \,|\, i'\nu' >= 2e \frac{f_0(\varepsilon_{i\nu}) - f_0(\varepsilon_{i'\nu'})}{\hbar\omega - \varepsilon_{i\nu} + \varepsilon_{i'\nu'}} < i\nu \,|\, \varphi_{ind}(\vec{r}) \,|\, i'\nu' >, \tag{5.1.179}$$

Wherein $f_0(\varepsilon)$ is the Fermi function and $\varphi_{ind}(\vec{r})$ is the induced potential. The potential $\varphi_{ind}(\vec{r})$ satisfies Poisson's equation

$$\nabla^2 \varphi_{ind}(\vec{r}) = \frac{4\pi e}{\varepsilon_s} \delta n_{ind}(\vec{r}), \tag{5.1.180}$$

See preceding discussions for further details.

Now, the matrix elements with respect to the 1st, 2nd and 3rd tubules are

$$\left\langle 1\upsilon \middle| e^{i\vec{q}_\perp \cdot \vec{r}} \middle| 1\upsilon' \right\rangle = \delta_{k_z - q_z, k_z'} e^{-im\vartheta_1} i^m J_m(q_\perp R_1) \tag{5.1.181}$$

$$\left\langle 2\upsilon \middle| e^{i\vec{q}_\perp \cdot \vec{r}} \middle| 2\upsilon' \right\rangle = \delta_{k_z - q_z, k_z'} e^{iq_x a_x} e^{-im\vartheta_2} J_m(q_\perp R_2) \tag{5.1.182}$$

$$\left\langle 3\upsilon \middle| e^{i\vec{q}_\perp \cdot \vec{r}} \middle| 3\upsilon' \right\rangle = \delta_{k_z - q_z, k_z'} e^{iq_y a_y} e^{-im\vartheta_3} J_m(q_\perp R_3) \tag{5.1.183}$$

Back-substituting the explicit forms of Eqns. (5.1.181) - (5.1.183) into Eqn. (4.1.132)

$$\delta n_{ind}(\vec{q}) = \frac{2e}{\Omega}\sum_{ii'}\sum_{\nu,\nu'}\frac{f_0(\varepsilon_{i\nu}) - f_0(\varepsilon_{i'\nu'})}{\hbar\omega - \varepsilon_{i\nu} + \varepsilon_{i'\nu'}} < i'\nu' \mid e^{-i\vec{q}\cdot\vec{r}} \mid i\nu > \sum_{\vec{q}'}\varphi_{ind}(\vec{q}') < i\nu \mid e^{i\vec{q}'\cdot\vec{r}} \mid i'\nu' > ,$$

yields

$$\delta n_{ind}(\vec{q}) = \frac{2e}{\Omega}\sum_{k_z}\frac{f_0(\varepsilon_{1,k_z,l}) - f_0(\varepsilon_{1,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{1,k_z-q_z,l-m} - \varepsilon_{1,k_z,l}} e^{-im\vartheta_1} J_m(q_\perp R_1)$$

$$\times\sum_{q_x',q_y'}\varphi_{ind}(q_x', q_y', q_z) J_m(q_\perp' R_1)\left(\frac{q_x' - iq_y'}{q_\perp'}\right)^m +$$

$$+\frac{2e}{\Omega}\sum_{k_z}\frac{f_0(\varepsilon_{2,k_z,l}) - f_0(\varepsilon_{2,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{2,k_z-q_z,l-m} - \varepsilon_{2,k_z,l}} F_1^*(m, q_\perp, \vartheta_2; R_2)\sum_{q_x',q_y'}\varphi_{ind}(q_x', q_y', q_z)$$
$$\times e^{-iq_x' a_x} F_1(m, q_\perp', \vartheta_2; R_2)$$

$$+\frac{2e}{\Omega}\sum_{k_z}\frac{f_0(\varepsilon_{3,k_z,l}) - f_0(\varepsilon_{3,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{3,k_z-q_z,l-m} - \varepsilon_{3,k_z,l}} e^{-iq_y a_y} F_2^*(m, q_\perp, \vartheta_3; R_3)$$

$$\times\sum_{q_x',q_y'}\varphi^{app}(q_x', q_y', q_z) e^{iq_y' a_y} F_2(m, q_\perp', \vartheta_3; R_3) \tag{5.1.184}$$

where,

$$F_1(m, q_\perp', \vartheta_2; R_2) = e^{-im\vartheta_2} J_m(q_\perp R_2) \tag{5.1.185}$$

$$F_2(m, q_\perp', \vartheta_3; R_3) = e^{-im\vartheta_3} J_m(q_\perp R_3) \tag{5.1.186}$$

The potential $\varphi_{ind}(\vec{q})$ in Eqn. (5.1.184) can be re-expressed in terms of $\delta n_{ind}(\vec{q})$ *via* Eqn. (4.4.165). Thus upon back-substitution Eqn. (5.1.184) becomes

$$\delta n_{ind}(\vec{q}) = \frac{-2e^2}{\varepsilon_s}\chi_{1,m}(q_z,\omega) J_m(q_\perp R_1) U_{1,m}(q_z)\left(\frac{q_x + iq_y}{q_\perp}\right)^m -$$

$$-\frac{2e^2}{\varepsilon_s}\chi_{2,m}(q_z,\omega) e^{-iq_x a_x} F_1^*(m, q_\perp, \vartheta_2; R_2) U_{2,m}(q_z) -$$

$$-\frac{2e^2}{\varepsilon_s}\chi_{3,m}(q_z,\omega) e^{-iq_y a_y} F_2^*(m, q_\perp, \vartheta_3; R_3) U_{3,m}(q_z) \tag{5.1.187}$$

where

$$q_\perp = |\vec{q}_\perp| \equiv \left[q_x^2 + q_y{}^2 \right]^{\frac{1}{2}} \tag{5.1.188}$$

and

$$U_{1,m}(q_z) \equiv \frac{1}{L_x L_y} \sum_{q'_x, q'_y} \frac{\delta n_{ind}\left(q'_x, q'_y, q_z\right)}{q'^2_x + q'^2_y + q_z{}^2} J_m(q'_\perp R_1) \left(\frac{q'_x - i q'_y}{q'_\perp} \right)^m \tag{5.1.189}$$

$$U_{2,m}(q_z) \equiv \frac{1}{L_x L_y} \sum_{q'_x, q'_y} \frac{\delta n_{ind}\left(q'_x, q'_y, q_z\right)}{q'^2_x + q'^2_y + q_z{}^2} e^{i q'_x a_x} F_1(m, q'_\perp, \vartheta_2; R_2) \tag{5.1.190}$$

$$U_{3,m}(q_z) \equiv \frac{1}{L_x L_y} \sum_{q'_x, q'_y} \frac{\delta n_{ind}\left(q'_x, q'_y, q_z\right)}{q'^2_x + q'^2_y + q_z{}^2} e^{i q'_y a_y} F_2(m, q'_\perp, \vartheta_3; R_3) \tag{5.1.191}$$

and

$$\chi_{j,m}(q_z, \omega) \equiv 2 \sum_{l=-\infty}^{\infty} \int dk_z \frac{f_0(\varepsilon_{j,k_z,l}) - f_0(\varepsilon_{j,k_z-q_z,l-m})}{\hbar\omega + \varepsilon_{j,k_z-q_z,l-m} - \varepsilon_{j,k_z,l}} \tag{5.1.192}$$

Back-substituting Eqn. (5.1.187) into Eqns. (5.1.189), (5.1.190) and (5.1.191) gives us

$$U_{1,m}(q_z) \equiv \frac{-2e^2}{\varepsilon_s} \chi_{1,m'}(q_z, \omega) U_{1,m'}(q_z) \frac{1}{L_x L_y} \sum_{q'_x, q'_y} \frac{J_{m'}(q'_\perp R_1) J_m(q'_\perp R_1)}{q'^2_x + q'^2_y + q_z{}^2} \left(\frac{q'_x + i q'_y}{q'_\perp} \right)^{m'-m}$$

$$\frac{-2e^2}{\varepsilon_s} \chi_{2,m'}(q_z, \omega) U_{2,m'}(q_z) \frac{1}{L_x L_y} \sum_{q'_x, q'_y} e^{-i q'_x a_x} \frac{F_1^*(m', q'_\perp, \vartheta_2; R_2) J_m(q'_\perp R_1)}{q'^2_x + q_z{}^2} \left(\frac{q'_x + i q'_y}{q'_\perp} \right)^{-m}$$

$$\frac{-2e^2}{\varepsilon_s} \chi_{3,m'}(q_z, \omega) U_{3,m'}(q_z) \frac{1}{L_x L_y} \sum_{q'_x, q'_y} e^{-i q'_y a_y} \frac{F_2^*(m', q'_\perp, \vartheta_3; R_3) J_m(q'_\perp R_1)}{q'^2_x + q_z{}^2} \left(\frac{q'_x + i q'_y}{q'_\perp} \right)^{-m}$$

(5.1.193)

$$U_{2,m}(q_z) \equiv \frac{-2e^2}{\varepsilon_s} \chi_{1,m'}(q_z, \omega) U_{1,m'}(q_z) \frac{1}{L_x L_y} \sum_{q'_x, q'_y} e^{i q'_x a_x} \frac{F_1(m, q'_\perp, \vartheta_2; R_2) J_{m'}(q'_\perp R_1)}{q'^2_\perp + q_z{}^2}$$

$$\times \left(\frac{q'_x + i q'_y}{q'_\perp} \right)^{m'} \frac{-2e^2}{\varepsilon_s} \chi_{2,m'}(q_z, \omega) U_{2,m'}(q_z) \frac{1}{L_x L_y} \sum_{q'_x, q'_y} \frac{F_1^*(m', q'_\perp, \vartheta_2; R_2) F_1(m, q'_\perp, \vartheta_2; R_2)}{q'^2_\perp + q_z{}^2}$$

$$\times e^{-i q_x a_x} e^{i q'_x a_x}$$

$$\frac{-2e^2}{\varepsilon_s} \chi_{3,m'}(q_z, \omega) U_{3,m'}(q_z) \frac{1}{L_x L_y} \sum_{q'_x, q'_y} \frac{F_2^*(m', q'_\perp, \vartheta_3; R_3) F_1(m, q'_\perp, \vartheta_2; R_2)}{q'^2_\perp + q_z{}^2} e^{-i q_y a_y} e^{i q'_x a_x}$$

(5.1.194)

$$U_{3,m}(q_z) \equiv \frac{-2e^2}{\varepsilon_s}\chi_{1,m'}(q_z,\omega)U_{1,m'}(q_z)\frac{1}{L_xL_y}\sum_{q_x',q_y'} e^{iq_y'a_y}\frac{F_2(m,q_\perp',\vartheta_3;R_3)J_{m'}(q_\perp'R_1)}{{q_\perp'}^2+{q_z}^2}$$
$$\times\left(\frac{q_x'+iq_y'}{q_\perp'}\right)^{m'}\frac{-2e^2}{\varepsilon_s}\chi_{2,m'}(q_z,\omega)U_{2,m'}(q_z)\frac{1}{L_xL_y}\sum_{q_x',q_y'}\frac{F_1^*(m',q_\perp',\vartheta_2;R_2)F_2(m,q_\perp',\vartheta_3;R_3)}{{q_\perp'}^2+{q_z}^2}$$
$$\times e^{-iq_xa_x}e^{iq_y'a_y}\frac{-2e^2}{\varepsilon_s}\chi_{3,m'}(q_z,\omega)U_{3,m'}(q_z)\frac{1}{L_xL_y}\sum_{q_x',q_y'}\frac{F_2^*(m',q_\perp',\vartheta_3;R_3)F_2(m,q_\perp',\vartheta_3;R_3)}{{q_\perp'}^2+{q_z}^2}$$
$$\times e^{-iq_ya_y}e^{iq_y'a_y}$$

(5.1.195)

We will at once notice that Eqns. (5.1.193) – (5.1.195) form a system of equations. Indeed, if we set

$$-A_{mm'} = \frac{-2e^2}{\varepsilon_s}\chi_{1,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q_x',q_y'}\frac{J_{m'}(q_\perp'R_1)J_m(q_\perp'R_1)}{{q_x'}^2+{q_y'}^2+{q_z}^2}\left(\frac{q_x'+iq_y'}{q_\perp'}\right)^{m'-m} \quad (5.1.196)$$

$$-B_{mm'} = \frac{-2e^2}{\varepsilon_s}\sum_{m'=\infty}^{\infty}\chi_{2,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q_x',q_y'} e^{-iq_x'a_x}\frac{F_1^*(m',q_\perp',\vartheta_2;R_2)J_m(q_\perp'R_1)}{{q_\perp'}^2+{q_z}^2}\left(\frac{q_x'+iq_y'}{q_\perp'}\right)^{-m}$$

(5.1.197)

$$-C_{mm'} = \frac{-2e^2}{\varepsilon_s}\chi_{3,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q_x',q_y'}\frac{e^{-iq_y'a_y}F_2^*(m',q_\perp',\vartheta_3;R_3)}{{q_\perp'}^2+{q_z}^2}J_m(q_\perp'R_1)\left(\frac{q_x'+iq_y'}{q_\perp'}\right)^{-m}$$

(5.1.198)

$$-D_{mm'} = \frac{-2e^2}{\varepsilon_s}\chi_{1,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q_x',q_y'} e^{iq_x'a_x}\frac{F_1(m,q_\perp',\vartheta_2;R_2)J_{m'}(q_\perp'R_1)}{{q_\perp'}^2+{q_z}^2}\left(\frac{q_x'+iq_y'}{q_\perp'}\right)^{m'}$$

(5.1.199)

$$-E_{mm'}=\frac{-2e^2}{\varepsilon_s}\chi_{2,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q'_x,q'_y}\frac{F_1^*(m',q'_\perp,\vartheta_2;R_2)F_1(m,q'_\perp,\vartheta_2;R_2)}{q'^{\,2}_\perp+q_z^{\,2}}e^{-iq_xa_x}e^{iq'_xa_x}$$

(5.1.200)

$$-F_{mm'}=\frac{-2e^2}{\varepsilon_s}\chi_{3,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q'_x,q'_y}\frac{F_2^*(m',q'_\perp,\vartheta_3;R_3)F_1(m,q'_\perp,\vartheta_2;R_2)}{q'^{\,2}_\perp+q_z^{\,2}}e^{-iq_ya_y}e^{iq'_xa_x}$$

(5.1.201)

$$-G_{mm'}=\frac{-2e^2}{\varepsilon_s}\chi_{1,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q'_x,q'_y}e^{iq'_ya_y}\frac{F_2(m,q'_\perp,\vartheta_3;R_3)J_{m'}(q'_\perp R_1)}{q'^{\,2}_\perp+q_z^{\,2}}\left(\frac{q'_x+iq'_y}{q'_\perp}\right)^{m'}$$

(5.1.202)

$$-H_{mm'}=\frac{-2e^2}{\varepsilon_s}\chi_{2,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q'_x,q'_y}\frac{F_1^*(m',q'_\perp,\vartheta_2;R_2)F_2(m,q'_\perp,\vartheta_3;R_3)}{q'^{\,2}_\perp+q_z^{\,2}}e^{-iq_xa_x}e^{iq'_ya_y}$$

(5.1.203)

$$-I_{mm'}=\frac{-2e^2}{\varepsilon_s}\chi_{3,m'}(q_z,\omega)\frac{1}{L_xL_y}\sum_{q'_x,q'_y}\frac{F_2^*(m',q'_\perp,\vartheta_3;R_3)F_2(m,q'_\perp,\vartheta_3;R_3)}{q'^{\,2}_\perp+q_z^{\,2}}e^{-iq_ya_y}e^{iq'_ya_y}$$

(5.1.04)

Back-substituting Eqns. (5.1.196)-(5.1.204) into Eqns. (5.1.193), (5.1.194) and (5.1.195), respectively, yields the following compact system of equations

$$U_{1,m}+\sum_{m'}A_{mm'}U_{1,m'}+\sum_{m'}B_{mm'}U_{2,m'}+\sum_{m'}C_{mm'}U_{3,m'}=0 \qquad (5.1.205)$$

$$U_{2,m}+\sum_{m'}D_{mm'}U_{1,m'}+\sum_{m'}E_{mm'}U_{2,m'}+\sum_{m'}F_{mm'}U_{3,m'}=0 \qquad (5.1.206)$$

$$U_{3,m} + \sum_{m'} G_{mm'} U_{1,m'} + \sum_{m'} H_{mm'} U_{2,m'} + \sum_{m'} I_{mm'} U_{3,m'} = 0 \tag{5.1.207}$$

The dimension of the associated coefficient matrix above is dependent on the type of transitions being investigated. So, as to obtain a matrix of modest dimensions, let us for the sake of argument pick only the intra-band transitions (i.e., $m = m' = 0$). For such transitions, we have

$$U_{1,0} + A_{00} U_{1,0} + B_{00} U_{2,0} + C_{00} U_{3,0} = 0 \tag{5.1.208}$$

$$U_{2,0} + D_{00} U_{1,0} + E_{00} U_{2,0} + F_{00} U_{3,0} = 0 \tag{5.1.209}$$

$$U_{3,0} + G_{00} U_{1,0} + H_{00} U_{2,0} + I_{00} U_{3,0} = 0 \tag{5.1.210}$$

Whose coefficient matrix assumes the following form

$$\begin{bmatrix} (1+A_{00}) & B_{00} & C_{00} \\ D_{00} & (1+E_{00}) & F_{00} \\ G_{00} & H_{00} & (1+I_{00}) \end{bmatrix} \begin{bmatrix} U_{1,0}(q_z) \\ U_{2,0}(q_z) \\ U_{3,0}(q_z) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{5.1.211}$$

Now for non trivial solutions of Eqn. (5.1.211) to exist, one requires that the determinant of the coefficient matrix vanish. That is

$$\begin{aligned} &(1+A_{00})((1+E_{00})-(1+I_{00})) + B_{00}(F_{00}G_{00} - D_{00}(1+I_{00})) + \\ &+C_{00}(D_{00}H_{00} - G_{00}(1+E_{00})) = 0 \end{aligned} \tag{5.1.212}$$

This is the dispersion formula for the plasmons and particle-hole modes intra-band transition only.

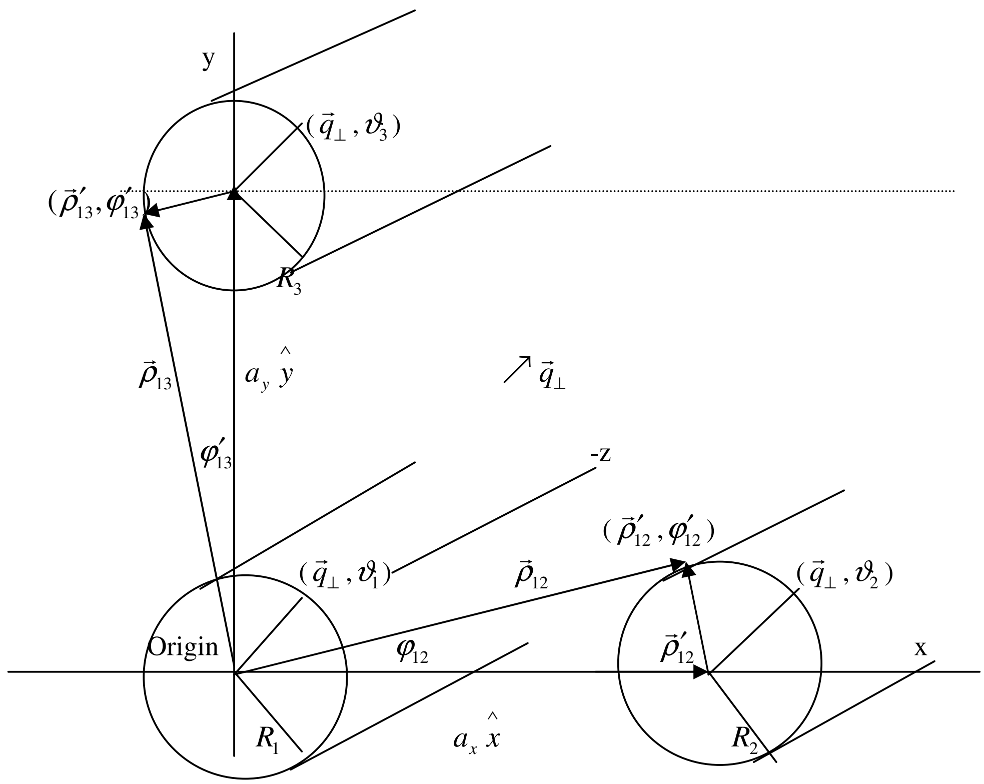


Fig. 7

Pictured is a finite-dimensional system of three nanotubules. The tubules are perceived to be of infinite extent along the z-axis. We denote their radii by R_1 , R_2 and R_3. The momentum $\vec{q}_\perp$ is fixed with respect to the z-axis as well as in the xy-plane for the nanotubes.

5.2. Limiting Cases

Let us again consider the intra-band case wherein we allow $a_x, a_y \to \infty$, respectively. Without regard to imposing these limiting criteria, the matrix Eqn. (5.1.211) remains invariant. However, as regards to the former criterion, $a_x \to \infty$ all elements in the first row of the matrix as well as elements in the first column's second and third rows vanish. Also, with respect to the latter criterion, $a_y \to \infty$, elements in the 3rd column, namely, $C_{mm'}$ and $F_{mm'}$ and the 2nd addend, $I_{mm'}$ within the matrix vanish, as does the elements in columns 1 and 2 in the 3rd row. If we now let $a_y \to \infty$ and $a_x \to \infty$, and set all off-diagonal elements equal to zero, it is now a simple matter to determine the determinant of the coefficient matrix; as it is now a product of the diagonal elements. In general, an explicit determination of the elements of the matrix yields for $m = m'$:

$$-A_{mm} = \frac{-e^2}{\pi \varepsilon_s} \chi_{1,m}(q_z;\omega) I_m(q_z;R_1) K_m(q_z,R_1), \tag{5.2.213}$$

$$-B_{mm} = \frac{e^2}{\pi \varepsilon_s} \chi_{2,m}(q_z;\omega) \int_0^\infty q_\perp dq_\perp \frac{J_0(q_\perp a_x) J_m(q_\perp R_1) J_m(q_\perp R_2)}{q_\perp^2 + q_z^2}$$

$$\equiv \frac{e^2}{\pi \varepsilon_s} \chi_{2,m}(q_z;\omega) V_{mm}^*(q_z;R_1,R_2,a_x) \tag{5.2.214}$$

$$-C_{mm} = \frac{e^2}{\pi \varepsilon_s} \chi_{3,m}(q_z;\omega) \int_0^\infty q_\perp dq_\perp \frac{J_0(q_\perp a_y) J_m(q_\perp R_1) J_m(q_\perp R_3)}{q_\perp^2 + q_z^2}$$

$$\equiv \frac{e^2}{\pi \varepsilon_s} \chi_{3,m}(q_z;\omega) V_{mm}^*(q_z;R_1,R_3,a_y) \tag{5.2.215}$$

$$-D_{mm} = \frac{-e^2}{\pi\varepsilon_s}\chi_{1,m}(q_z;\omega)\int_0^\infty q_\perp dq_\perp \frac{J_0(q_\perp a_x)J_{m'}(q_\perp R_1)J_m(q_\perp R_2)}{q_\perp^2+q_z^2}$$

$$\equiv \frac{e^2}{\pi\varepsilon_s}\chi_{1,m}(q_z;\omega)V_{mm}(q_z;R_1,R_2,a_x) \qquad (5.2.216)$$

$$-E_{mm} = \frac{-e^2}{\pi\varepsilon_s} I_m(q_z;R_2)K_m(q_z,R_2)\chi_{2,m}(q_z;\omega) \qquad (5.2.217)$$

$$-F = -\frac{e^2}{\pi\varepsilon_s}\chi_{3,m}(q_z;\omega)\int_0^\infty q_\perp dq_\perp \sum_{k,k'=-\infty}^{\infty} \frac{i^k J_k(q_\perp a_x)J_{k'}(q_\perp a_y)J_m(q_\perp R_2)J_m(q_\perp R_3)}{q_\perp^2+q_z^2}$$

$$\equiv \frac{-e^2}{\pi\varepsilon_s}\chi_{3,m}(q_z;\omega)V_{mm}(q_z;R_2,R_3,a_x,a_y) \qquad (5.2.218)$$

Similarly, if we make the replacements $-a_x \to a_x$ and $a_y \to -a_y$ in the elemental equation for $-F_{mm'}$, and using the Jacobi-Anger Formule [26]

$$e^{\pm iz\sin\vartheta} = \sum_{j=-\infty}^{+\infty} J_j(z)e^{\pm ij\vartheta} \qquad (5.2.219)$$

as well as the identity

$$J_j(-z) = (-1)^j J_j(z) \qquad (5.2.220)$$

the elemental equation for $-H_{mm'}$ would be

$$-H_{mm} = -\frac{e^2}{\pi\varepsilon_s}\chi_{1,m}(q_z;\omega)\int_0^\infty q_\perp dq_\perp \sum_{k,k'=-\infty}^{\infty} \frac{i^k(-1)^k J_k(q_\perp a_x)J_{k'}(q_\perp a_y)J_m(q_\perp R_2)J_m(q_\perp R_3)}{q_\perp^2+q_z^2}$$

$$\equiv \frac{-e^2}{\pi\varepsilon_s}\chi_{1,m}(q_z;\omega)V^*_{mm}(q_z;R_2,R_3,a_x,a_y) \qquad (5.2.221)$$

$$-G_{mm} = \frac{-e^2}{\pi\varepsilon_s}\chi_{1,m}(q_z;\omega)\int_0^\infty q_\perp dq_\perp \frac{J_0(q_\perp a_y)J_m(q_\perp R_1)J_m(q_\perp R_3)}{q_\perp^2+q_z^2}$$

$$\equiv \frac{-e^2}{\pi\varepsilon_s}\chi_{1,m}(q_z;\omega)V_{mm}(q_z;R_1,R_3,a_y) \qquad (5.2.222)$$

$$-I_{mm} = \frac{-e^2}{\pi\varepsilon_s}\chi_{3,m}(q_z;\omega)I_m(q_z;R_1)K_m(q_z,R_1) \qquad (5.2.223)$$

For $m = m' = 0$, the system of equations (5.1.208) – (5.1.210) in light of equations (5.2.213) – (5.2.223) reduce to

$$\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_1)K_0(q_zR_1)\chi_{1,0}(q_z,\omega)\right]U_{1,0}(q_z)+\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_1,R_2,a_x)U_{2,0}(q_z)$$
$$+\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)V_{00}^*(q_z;R_1,R_3,a_y)U_{3,0}(q_z)=0 \qquad (5.2.224)$$

$$\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}^*(q_z;R_1,R_2,a_x)U_{1,0}(q_z)+\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_2)K_0(q_zR_2)\chi_{2,0}(q_z,\omega)\right]U_{2,0}(q_z)$$
$$+\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)V_{00}(q_z;R_2,R_3,a_x,a_y)U_{3,0}(q_z)=0 \qquad (5.2.225)$$

$$\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}(q_z;R_1,R_3,a_y)U_{1,0}(q_z)+\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_2,R_3,a_x,a_y)U_{2,0}(q_z)$$

$$+\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_3)K_0(q_zR_3)\chi_{3,0}(q_z,\omega)\right]U_{3,0}(q_z)=0 \qquad (5.2.226)$$

Whose secular determinantal equation is

$$\left\|\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_1)K_0(q_zR_1)\chi_{1,0}(q_z,\omega)\right]\left(\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_2)K_0(q_zR_2)\chi_{2,0}(q_z,\omega)\right]\right.\right.$$

$$\times\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_3)K_0(q_zR_3)\chi_{3,0}(q_z,\omega)\right]-\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)V_{00}(q_z;R_2,R_3,a_x,a_y)$$

$$\left.\times\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_2,R_3,a_x,a_y)\right)+\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_1,R_2,a_x)$$

$$\times\left(\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)V_{00}(q_z;R_2,R_3,a_x,a_y)\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}(q_z;R_1,R_3,a_y)-\right.$$

$$\left.-\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}(q_z;R_1,R_2,a_x)\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_3)K_0(q_zR_3)\chi_{3,0}(q_z,\omega)\right]\right)$$

$$\times\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_2,R_3,a_x,a_y)-\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}(q_z;R_1,R_3,a_y)\times$$

$$\left.\left.\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_2)K_0(q_zR_2)\chi_{2,0}(q_z,\omega)\right]\right)\right\|=0 \qquad (5.2.227)$$

Now in the limit as $a_y\to\infty$ (That is, when the nanotube on the y-axis is infinitely far away.) the following terms in Eqn. (5.2.227) go to zero:

$V_{00}(q_z;R_2,R_3,a_x,a_y)$,

$V_{00}^*(q_z;R_2,R_3,a_x,a_y)$,

$V_{00}(q_z;R_1,R_3,a_y)$,

and $V_{00}^*(q_z;R_1,R_3,a_y)$.

Thus reducing Eqn. (5.2.227) to

$$\left[1+\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)I_0(q_zR_3)K_0(q_zR_3)\right]\left(\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_1)K_0(q_zR_1)\chi_{1,0}(q_z,\omega)\right]\right.$$

$$\times\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_2)K_0(q_zR_2)\chi_{2,0}(q_z,\omega)\right]-\left[\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_1,R_2,a_x)\right.$$

$$\left.\left.\times\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}(q_z;R_1,R_2,a_x)\right]\right)=0 \tag{5.2.228}$$

The solution is trivial for

$$\left[1+\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)I_0(q_zR_3)K_0(q_zR_3)\right]=0 \tag{5.2.229}$$

Or for plasmon frequencies, ω such that

$$\frac{e^2}{\pi\varepsilon_s}\chi_{3,0}(q_z,\omega)I_0(q_zR_3)K_0(q_zR_3)=-1 \tag{5.2.230}$$

However, it is not a trivial matter to find the zeros corresponding to the plasmon frequencies for the remaining post factor in Eqn. (5.2.228)

$$\left(\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_1)K_0(q_zR_1)\chi_{1,0}(q_z,\omega)\right]\left[1+\frac{e^2}{\pi\varepsilon_s}I_0(q_zR_2)K_0(q_zR_2)\chi_{2,0}(q_z,\omega)\right]\right.$$

$$\left.-\left[\frac{e^2}{\pi\varepsilon_s}\chi_{2,0}(q_z,\omega)V_{00}^*(q_z;R_1,R_2,a_x)\frac{e^2}{\pi\varepsilon_s}\chi_{1,0}(q_z,\omega)V_{00}(q_z;R_1,R_2,a_x)\right]\right)=0$$

(5.2.231)

One can simplify the subtrahend in Eqn. (5.2.231). Indeed, if we again consider intra-band transitions wherein $m = m'$, we find via the integral representations of $V_{mm'}(q_z; R_1, R_2, a_x)$ and $V^*_{mm'}(q_z; R_1, R_2, a_x)$ respectively, that

$$(V^*_{mm'})_{m=m'} = (V_{mm'})_{m=m'} \tag{5.2.232}$$

Hence in Eqn. (5.2.231) where $m = m' = 0$ we have

$$V^*_{00} = V_{00} \tag{5.2.233}$$

and so *via* Eqn. (5.2.233) , Eqn. (5.2.231) reduces to

$$\left[1 + \frac{e^2}{\pi\varepsilon_s} I_0(q_z R_1) K_0(q_z R_1) \chi_{1,0}(q_z, \omega)\right]\left[1 + \frac{e^2}{\pi\varepsilon_s} I_0(q_z R_2) K_0(q_z R_2) \chi_{2,0}(q_z, \omega)\right]$$

$$-\left[\frac{e^2}{\pi\varepsilon_s} V_{00}(q_z; R_1, R_2, a_x)\right]^2 \chi_{2,0}(q_z, \omega) \chi_{1,0}(q_z, \omega) = 0 \tag{5.2.234}$$

It is interesting to note that Eqn. (5.2.234) is similar to the dispersion relation for the two nanotube system as obtained by G.Gumbs, *et al,* (Phys. Rev. B **68** 075405-1). Furthermore, if we separate the nanotubes to the extent that the distance between them is effectively infinite (Which is akin to letting $a_x \to \infty$), one finds that

$$V^*_{00}(q_z; R_1, R_2, a_x) \underset{(a_x \to \infty)}{\longrightarrow} 0 \tag{5.2.235}$$

&

$$V_{00}(q_z; R_1, R_2, a_x) \underset{(a_x \to \infty)}{\longrightarrow} 0 \tag{5.2.236}$$

Consequently, the system of cylinders become decoupled and may be viewed as three distinct systems, each consisting of a single nanotube with its associated elementary excitations. The single nanotube theory compares well with results obtained by M. Lin, *et al,* (Phys. Rev B **47** 6617).

Chapter 6

Plasma Excitations and Oscillator Strengths

6.1. Theoretical Formalism

It is well known that, when an electron gas is subject to an external perturbation, the electrons begin, depending on the magnitude of the perturbation, to oscillate. Taken as a collective, the electron oscillations are called plasma excitations. However, how does one determine the extent to which the plasma is excited at some instant in time, say? What are the frequencies of such a collective? We must look to the strength of the oscillations or oscillator strengths of the plasma for answers.

Fortunately, there exists a set of frequency-momentum sum rules, which are integrals over frequency, ω. These allow us to determine exactly, critical oscillator frequencies for complex longitudinal dielectric functions, $\varepsilon_j(q,m,\omega)$ as well as their reciprocals or 'inverses', $\varepsilon_j^{-1}(q,m,\omega)$. In fact, one can obtain various sum rules by integrating the imaginary parts of the longitudinal dielectric function with respect to ω. It is from the sum rule that we are able to determine the oscillator strengths of the plasmon and particle-hole modes respectively. Next, we will derive the *longitudinal f-sum rule*.

6.2. General derivation of the longitudinal f-sum rule

We will start by taking the mean with respect to the double commutator

$$C = \left\langle \left[\left[\hat{H}, \hat{\rho}(q) \right], \hat{\rho}(-q) \right] \right\rangle \Big|_{T \neq 0} \tag{6.2.237}$$

Wherein, the average is taken at finite temperatures, $T \neq 0$ over the thermodynamic states of the system. The Hamiltonian $\hat{H}$ is for the full homogeneous electron gas. Additionally, the density operator, $\hat{\rho}(\vec{q}) = \sum_{\vec{k}s} c_{\vec{k}+qs} c_{\vec{k}s}$ commutes with all terms in this Hamiltonian except the kinetic energy part. Hence the first commutator gives us

$$\left[\hat{H}, \hat{\rho}(q)\right] = \sum_{\vec{p}\vec{k}'} \xi_{\vec{p}} \left[c^{\dagger}{}_{\vec{p}s} c_{\vec{p}s}, c_{\vec{p}+\vec{q}\sigma} c_{\vec{p}\sigma}\right] = \sum_{\vec{p}s} \xi_{\vec{p}} (c^{\dagger}{}_{\vec{p}s} c_{\vec{p}-\vec{q}s} - c^{\dagger}{}_{\vec{p}+\vec{q}s} c_{\vec{p}s})$$

$$= \sum_{\vec{p}s} c^{\dagger}{}_{\vec{p}+\vec{q}s} c_{\vec{p}s} (\varepsilon_{\vec{p}+\vec{q}} - \varepsilon_{\vec{p}})$$

$$= \frac{\hbar^2 q^2}{2m} \rho(q) + \frac{\hbar^2}{m} \sum_{\vec{p}s} \vec{q} \cdot \vec{p} c^{\dagger}{}_{\vec{p}+\vec{q}s} c_{\vec{p}s} \tag{6.2.238}$$

The term that is proportional to $\hat{\rho}(\vec{q})$ will commute with $\hat{\rho}(-\vec{q})$. So only the other terms need to be evaluated,

$$C = \left\langle \left[\left[\hat{H}, \hat{\rho}(q)\right], \hat{\rho}(-q)\right] \right\rangle \Big|_{T \neq 0}$$

$$= \left\langle \left[\frac{\hbar^2}{m} \sum \vec{q} \cdot \vec{p} c^{\dagger}{}_{\vec{p}+\vec{q}s} c_{\vec{p}s}, \hat{\rho}(-q)\right] \right\rangle$$

$$= \frac{\hbar^2}{m} \sum_{\vec{p}\vec{q}'} \vec{q} \cdot \vec{p} \left\langle (c^{\dagger}{}_{\vec{p}+\vec{q}s} c_{\vec{p}+qs} - c^{\dagger}{}_{\vec{p}s} c_{\vec{p}s}) \right\rangle$$

$$= \frac{\hbar^2}{m} \sum_{\vec{p}\vec{q}} \left\langle c^{\dagger}{}_{\vec{p}s} c_{\vec{p}s} \right\rangle [(\vec{p} - \vec{q}) \cdot \vec{q} - \vec{q} \cdot \vec{p}]$$

$$= \frac{-\hbar^2 q^2}{m} \sum_{\vec{p}s} n_{\vec{p}}$$

$$= \frac{-\hbar^2 q^2 N}{m} \tag{6.2.239}$$

Let us now evaluate this double commutator by inserting the complete set of states $|n\rangle$ and $|m\rangle$, which are eigenfunctions of the Hamiltonian, inserting appropriately the unit operator $\sum |n\rangle\langle n| = 1$ (and as such we assume that the Hamiltonian is invariant under time reversal symmetry), and then collecting like terms:

$$-C = \left\langle \left[\left[\hat{H}, \hat{\rho}(q) \right], \hat{\rho}(-q) \right] \right\rangle \Big|_{T\neq 0}$$

$$= \sum_{n,m} \left(e^{-\beta E_n} \langle n | \left[\hat{H}, \hat{\rho}(q) \right] | m \rangle \langle m | \hat{\rho}(-q) | n \rangle - e^{-\beta E_m} \langle m | \hat{\rho}(-q) | n \rangle \langle n | \left[\hat{H}, \hat{\rho}(q) \right] | m \rangle \right) \Big|_{T\neq 0}$$

$$= \sum_{n,m} \left| \langle n | \hat{\rho}(\vec{q}) | m \rangle \right|^2 \left(e^{-\beta E_n} - e^{-\beta E_m} \right) (E_m - E_n) \Big|_{T\neq 0}$$

(6.2.240)

However, the imaginary part of the inverse longitudinal dielectric function is given by [16]

$$\Im m \left[\frac{1}{\varepsilon(q,m,\omega)} \right] = -\pi (1 - e^{-\beta\omega}) \frac{4\pi e^2}{q^2 \upsilon} \sum_{n,m} e^{-\beta E_n} \left| \langle n | \hat{\rho}(\vec{q}) | m \rangle \right|^2 \delta(\omega + E_n - E_m) \Big|_{T\neq 0}$$

(6.2.241)

Which we integrate with respect to ω and obtain the sum rule

$$-\frac{q^2 \upsilon}{4\pi\pi e^2} \int_{-\infty}^{\infty} d\omega \left[\omega \Im m \left[\frac{1}{\varepsilon(q,m,\omega)} \right] \right] = \sum_{n,m} \left| \langle n | \hat{\rho}(\vec{q}) | m \rangle \right|^2 (E_m - E_n) \left(e^{-\beta E_n} - e^{-\beta E_m} \right) \Big|_{T\neq 0}$$

(6.2.242)

Via the transitive property, we may now equate Eqns. (6.2.242) and (6.2.240) and obtain

$$-\frac{q^2 \upsilon}{4\pi^2 e^2} \int_{-\infty}^{\infty} d\omega \left[\omega \Im m \left[\frac{1}{\varepsilon(q,m,\omega)} \right] \right] = -C \qquad (6.2.243)$$

Which we solve for the integral obtaining the sum rule

$$\int_{-\infty}^{\infty} d\omega \left[\omega \Im m \left[\frac{1}{\varepsilon(q,m,\omega)} \right] \right] = -\pi \omega_p^2 \qquad (6.2.244)$$

Wherein we define $\omega_p \equiv \dfrac{4\pi e^2 n_0}{m}$, as the plasma frequency.

When one looks in part at the integrand, the product $\omega\varepsilon^{-1}(q,m,\omega)$ forms an even function. Indeed, for $\varepsilon^{-1}(q,m,\omega)$ is an odd function in the argument, ω and so is the pre-factor, ω. Hence their product is an even function. Now it is well known from elementary calculus that the integral of an even function of x say, over a symmetric interval, $-l < f_{even}(x) < +l$ is just $2f_{even}(x)$ integrated over the interval $0 < f_{even}(x) < +l$. Hence we may integrate Eqn. (6.2.244) over the domain of definition, $0 \le f_{even}(\omega) < +\infty$ and then double the resulting answer

$$2\int_0^\infty d\omega\left[\omega\Im m\left[\frac{1}{\varepsilon(q,m,\omega)}\right]\right] = -\pi\omega_p^2 \tag{6.2.245}$$

Or

$$\int_0^\infty d\omega\left[\omega\Im m\left[\frac{1}{\varepsilon(q,m,\omega)}\right]\right] = \frac{-\pi\omega_p^2}{2} \tag{6.2.246}$$

Or

$$\int_0^\infty d\omega\left[\omega\Im m\left[\frac{-1}{\varepsilon(q,m,\omega)}\right]\right] = \frac{\pi\omega_0^2(q,m)}{2\varepsilon_0} \tag{6.2.247}$$

Both Eqns. (6.2.246) and (6.2.247) are in accord with Mahan and Lin's results respectively, i.e., as regards to the general form of the sum rule, to which $\varepsilon(q,m,\omega)$ must conform. It is up to us to determine the actual analytic expression for, ω_0 in terms of our nanotube geometry. This will be further developed in the dissertation as its form is critical in determining the plasmons and particle-hole modes strengths with regard to nanotubes.

6.3. Plasmon oscillator strengths

As was previously mentioned in section 6.1, the longitudinal dielectric constant is complex. Namely,

$$\varepsilon(q,m,\omega) \equiv \varepsilon_1(q,m,\omega) + i\varepsilon_2(q,m,\omega) \tag{6.3.248}$$

Wherein, $\varepsilon_1(q,m,\omega)$ and $\varepsilon_2(q,m,\omega)$ are its real and imaginary parts, respectively. The rationalized reciprocal or inverse (not in the strict mathematical sense of the word) of $\varepsilon(q,m,\omega)$ is

$$\frac{1}{\varepsilon(\vec{q},m,\omega)} \equiv \frac{\varepsilon_1(\vec{q},m,\omega)}{\varepsilon_1^2(\vec{q},m,\omega)+\varepsilon_2^2(\vec{q},m,\omega)} + i\frac{\varepsilon_2(\vec{q},m,\omega)}{\varepsilon_1^2(\vec{q},m,\omega)+\varepsilon_2^2(\vec{q},m,\omega)} \tag{6.3.249}$$

Wherein we find that

$$\Re e\left[\frac{1}{\varepsilon(\vec{q},m,\omega)}\right] \equiv \frac{\varepsilon_1(\vec{q},m,\omega)}{\varepsilon_1^2(\vec{q},m,\omega)+\varepsilon_2^2(\vec{q},m,\omega)} \tag{6.3.250}$$

and

$$\Im m\left[\frac{1}{\varepsilon(\vec{q},m,\omega)}\right] \equiv \frac{\varepsilon_2(\vec{q},m,\omega)}{\varepsilon_1^2(\vec{q},m,\omega)+\varepsilon_2^2(\vec{q},m,\omega)} \tag{6.3.251}$$

are the real and imaginary parts of the inverse longitudinal dielectric function respectively.

The oscillator strength of the plasmons arises from a careful physical analysis of Eqn. (6.3.251). Indeed one notices that the plasmons and particle-hole modes occur at frequencies for which $\varepsilon_2(\vec{q},m,\omega)$ vanishes and respectively, at frequencies for which it does not. In short, when $\varepsilon_2(\vec{q},m,\omega)=0$, there is evidence of plasmons, whereas when $\varepsilon_2(\vec{q},m,\omega)\neq 0$ we see particle-hole modes. However, when both $\varepsilon_1(\vec{q},m,\omega)$ and $\varepsilon_2(\vec{q},m,\omega)$ go to zero, we may replace the right hand side of Eqn. (6.3.251) by a delta function.

$$\frac{\varepsilon_2(\vec{q},m,\omega)}{\varepsilon_1^2(\vec{q},m,\omega)+\varepsilon_2^2(\vec{q},m,\omega)} \to \delta(\varepsilon_1(\vec{q},m,\omega)) \tag{6.3.252}$$

As a further consequence of the aforementioned replacement, we may now replace the argument of the delta function by a first-order Taylor series expansion

$$\delta(\varepsilon_1(\vec{q},m,\omega)) = \delta\left\{(\omega-\omega_j)\frac{\partial}{\partial\omega}\varepsilon_1(\vec{q},m,\omega)\bigg|_{\omega=\omega_j}\right\} \tag{6.3.253}$$

Hence Eqn. (6.3.251) becomes

$$\Im m\left[\frac{1}{\varepsilon(\vec{q},m,\omega)}\right] \equiv \frac{\varepsilon_2(\vec{q},m,\omega)}{\varepsilon_1^2(\vec{q},m,\omega)+\varepsilon_2^2(\vec{q},m,\omega)} \to \delta(\varepsilon_1(\vec{q},m,\omega))$$

$$\to \delta\left\{(\omega-\omega_j)\frac{\partial}{\partial\omega}\varepsilon_1(\vec{q},m,\omega)\bigg|_{\omega=\omega_j}\right\} \tag{6.3.254}$$

However, from Eqn. (6.2.247) we obtain

$$\frac{2\varepsilon_0}{\pi\omega_0^2(q,m)}\int_0^\infty d\omega\left[\omega\Im m\left[\frac{-1}{\varepsilon(q,m,\omega)}\right]\right]=1 \tag{6.3.255}$$

Back-substituting Eqn. (6.3.254) into Eqn. (6.3.255) yields

$$\frac{2\varepsilon_0}{\pi\omega_0^2(q,m)}\int_0^\infty d\omega\left[\omega\delta\left\{(\omega-\omega_j)\frac{\partial}{\partial\omega}\varepsilon_1(\vec{q},m,\omega)\bigg|_{\omega=\omega_j}\right\}\right]=1 \tag{6.3.256}$$

but,

$$\frac{\partial}{\partial\omega}\varepsilon_1(\vec{q},m,\omega)=\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right) \tag{6.3.257}$$

Back-substituting Eqn. (6.3.257) into Eqn. (6.3.256) gives us

$$\frac{2\varepsilon_0}{\pi\omega_0^2(q,m)}\int_0^\infty d\omega\left[\omega\delta\left\{(\omega-\omega_j)\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right)\bigg|_{\omega=\omega_j}\right\}\right]=1 \tag{6.3.258}$$

There exists a property of the delta function [17] which states that

$$\delta(ax) = \frac{1}{|a|}\delta(x), a \neq 0 \tag{6.3.259}$$

Making use of this property, Eqn. (6.3.258) becomes

$$\frac{2\varepsilon_0}{\pi\omega_0^2(q,m)}\int_0^\infty d\omega\left[\frac{\omega\delta(\omega-\omega_j)}{\left|\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right)\Big|_{\omega=\omega_j}\right|}\right] = 1 \tag{6.3.260}$$

$$\frac{\varepsilon_0}{\pi\omega_0^2(q,m)}\int_{-\infty}^\infty d\omega\left[\frac{\omega\delta(\omega-\omega_j)}{\left|\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right)\Big|_{\omega=\omega_j}\right|}\right] = 1 \tag{6.3.261}$$

$$\frac{\varepsilon_0}{\pi\omega_0^2(q,m)\left|\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right)\Big|_{\omega=\omega_j}\right|}\int_{-\infty}^\infty d\omega\left[\omega\delta(\omega-\omega_j)\right] = 1 \tag{6.3.262}$$

Using yet another property of the delta function [17],

$$\int_{-\infty}^\infty dx\left[f(x)\delta(x-a)\right] \equiv f(a) \tag{6.3.263}$$

we may re-write the integral in Eqn. (6.3.262) as

$$\int_{-\infty}^\infty d\omega\left[\omega\delta(\omega-\omega_j)\right] = \omega_j \text{ (As in this instance, } f(\omega_j) = \omega_j\text{)} \tag{6.3.264}$$

Back-substituting Eqn. (6.3.264) into Eqn. (6.3.262) we obtain

$$\frac{\varepsilon_0\omega_j}{\pi\omega_0^2(q,m)\left|\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right)\Big|_{\omega=\omega_j}\right|} = 1 \tag{6.3.265}$$

This, upon solving for the oscillator strength of the plasmons, ω_j^{-1} yields

$$\omega_j^{-1} = f_j(q,m) = \frac{\varepsilon_0}{\pi} \frac{1}{\omega_0^2(q,m)\left|\frac{\partial}{\partial\omega}\Re e\left(\varepsilon(q,m,\omega)\right)\Big|_{\omega=\omega_j}\right|} \tag{6.3.266}$$

which stands in accord with Lin's result, to within a factor of $\frac{\varepsilon_0}{\pi}$.

6.4. Particle-hole modes

For the particle-hole modes we have

$$\int_0^\infty d\omega\left[\omega\Im m\left[\frac{-1}{\varepsilon(q,m,\omega)}\right]\right] = \frac{\pi\omega_0^2(q,m)}{2\varepsilon_0} \tag{6.4.267}$$

Equation (6.4.267) becomes upon normalization

$$\frac{2\varepsilon_0}{\pi}\int_0^\infty d\omega\left[\frac{\omega}{\omega_0^2(q,m)}\Im m\left[\frac{-1}{\varepsilon(q,m,\omega)}\right]\right] = 1 \tag{6.4.268}$$

with the condition (see the argument below the integral symbol)

$$\frac{2\varepsilon_0}{\pi}\int_{\mathrm{Im}[\varepsilon(q,m,\omega)\neq 0]} d\omega\left[\frac{\omega}{\omega_0^2(q,m)}\Im m\left[\frac{-1}{\varepsilon(q,m,\omega)}\right]\right] = 1 \tag{6.4.269}$$

Therefore, the oscillator strength of the particle-hole modes, is given by

$$f_{e-h}(q,m) = \frac{2\varepsilon_0}{\pi}\int_{\Im m[\varepsilon(q,m,\omega)\neq 0]} d\omega\left[\frac{\omega}{\omega_0^2(q,m)}\Im m\left[\frac{-1}{\varepsilon(q,m,\omega)}\right]\right] \tag{6.4.270}$$

The above implies that the particle-hole modes occur at or below a cut-off of unity and that the sum of all oscillator strengths is unity. The characteristics plots of both the Eqns. (6.4.268) and (6.3.266) as applied to nanotubes appears in our discussions towards the end of this dissertation.

Chapter 7

The Rashba Effect and 2D Confinement

7.1 The Origin of Spin-Orbit Coupling and its Effect Due to Cylindrical Confinement.

The magnetic field seen by the intrinsic magnetic moment of the electron includes not only externally applied fields, but also any fields internal to the electron system. The principal source of internal magnetic fields is the internal currents in the system. As these internal currents are due to the orbital motion of the charged particles, the interaction between the resulting magnetic fields and the intrinsic magnetic moments is called the spin-orbit interaction.

Indeed, the reference electron does not see its own magnetic field no more than it sees its own electric field. However, should the electron move, any external charge distribution moves relative to the electron, and giving rise to a magnetic field in the frame of reference of the electron itself. This magnetic field is seen by the intrinsic magnetic moment of the electron and as such, is related to the electric field in the laboratory frame via a Lorentz transformation [26].

The effects due to spin orbit coupling in semiconductor heterostructures have recently attracted much interest. The attention is in part due to the fact that these effects provide a useful tool in controlling the electron's orbital motion by coupling it to its spin degree of freedom, and the other way around. In light of this fact, spin-orbit coupling has become one of the key ingredients for phase-coherent spintronics applications [23]. In this chapter, we focus on the spin-orbit coupling induced by structural inversion asymmetry, i.e. the Rashba effect [21] on the band structure and absorption properties of nanotubes [47] in a number of configurations.

The Rashba effect, named after one of its discoverers, is an energy splitting, of what would otherwise be degenerate quantum states, caused by a spin-orbit interaction in conjunction with a structural-inversion asymmetry in the presence of interfacial electric fields in a semiconductor heterostructure. The magnitude of the energy split is proportional to the electron wave number.

In the non-relativistic limit (to lowest order in *v/c*) of the Dirac equation, one obtains the following Hamiltonian for a charged spin ½ particle in the presence of nuclei and an external electromagnetic field:

$$\hat{H}_T = \frac{\hat{\vec{p}}^2}{2m^*} - \frac{\hat{\vec{p}}^4}{8m^{*3}c^2} - \frac{\hbar^2}{\left(2m^*c\right)^2}\left(\nabla V \cdot \nabla\right) + \frac{\hbar}{\left(2m^*c\right)^2}\hat{\vec{\sigma}} \cdot \left(\nabla V \times \hat{\vec{p}}\right) - g_s\hat{\mu}_s \cdot \vec{B} - g_N\hat{\mu}_N \cdot \vec{B} \tag{7.1.271}$$

If we use the triple scalar product formula $\hat{\vec{\sigma}} \cdot \left(\nabla V \times \hat{\vec{p}}\right) = k \Rightarrow \nabla V \cdot \left(\hat{\vec{\sigma}} \times \hat{\vec{p}}\right) = -k$, where *k* is some positive scalar constant, the above Hamiltonian becomes

$$\hat{H}_T = \frac{\hat{\vec{p}}^2}{2m^*} - \frac{\hat{\vec{p}}^4}{8m^{*3}c^2} - \frac{\hbar^2}{\left(2m^*c\right)^2}\left(\nabla V \cdot \nabla\right) - \frac{\hbar}{\left(2m^*c\right)^2}\left(\nabla V\right) \cdot \left(\hat{\vec{\sigma}} \times \hat{\vec{p}}\right) - g_s\hat{\mu}_s \cdot \vec{B} - g_N\hat{\mu}_N \cdot \vec{B}$$

$$= \hat{H}^0 + \hat{H}^1 + \hat{H}^2 + \hat{H}^3 + \hat{H}^4 + \hat{H}^5 \tag{7.1.272}$$

The fifth and sixth terms are due to the electron-nucleon spin interactions with the external magnetic field. We are concerned with the first, fourth and fifth terms. The fourth being the spin-orbit interaction term which may be re-written as

$$\hat{H}^3_{SO} = \frac{\hbar}{\left(2m^*c\right)^2}\nabla V \cdot \left(\hat{\vec{\sigma}} \times \hat{\vec{p}}\right) = \vec{\alpha} \cdot \left(\hat{\vec{\sigma}} \times \hat{\vec{p}}\right) \tag{7.1.273}$$

Where the Rashba parameter, $\vec{\alpha}$ which depends on the system under consideration, is defined as

$$\vec{\alpha} \equiv \beta \langle \nabla V \rangle, \text{with } \beta = \frac{\hbar}{\left(2m^{*}c\right)^{2}} \tag{7.1.274}$$

and $(\hat{\vec{\sigma}} \times \hat{\vec{p}})$ forms the vector product of the spin operator, $\hat{\vec{\sigma}}$ and the momentum, $\hat{\vec{p}}$ of the electron. It should be noted that $\vec{\alpha} \cdot \left(\hat{\vec{\sigma}} \times \hat{\vec{p}}\right)_z$ represents in 2D, an average electric field at the hetero-surface.

In our problem, there are no nuclei (we just have a surface bound 2DEG). Consequently, the sixth term in Eqn. (7.1.272) vanishes. In addition, for the case of a weak external magnetic field (this is our case) there is no Zeeman splitting which is normally associated with the fifth term in Eqn. (7.1.272). However it still makes a small contribution in the weak external magnetic field limit and so will not be excluded from our formalism.

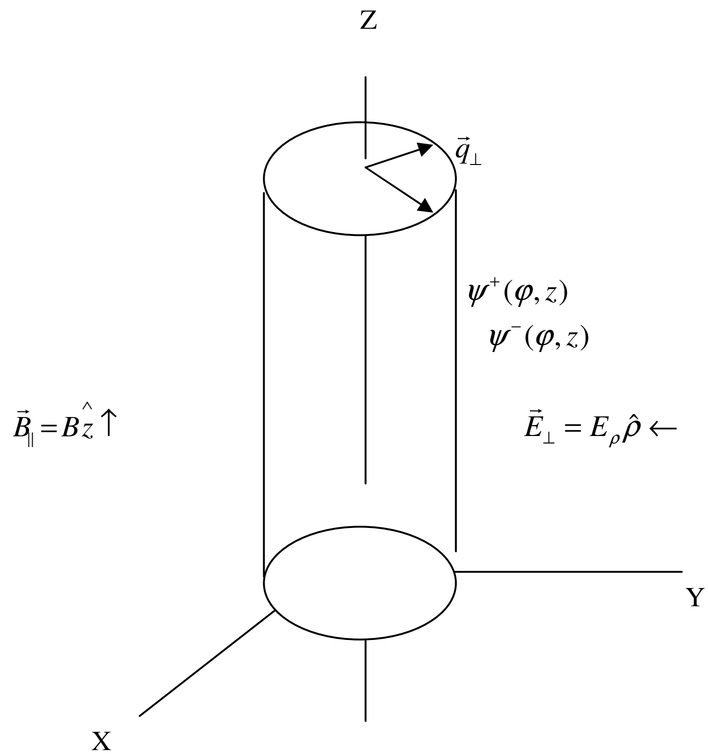


Fig. 8

Above is an oblique view of a portion of our nanotube showing the two-spinor surface states, $\psi^\pm$ which arise when we consider the Rashba effect with a surface confining potential in the $-\hat{\rho}$ direction. (Note that with regard to the above figure, $-\hat{\rho}$ is a radial unit vector in the xy-plane and points inward to the z-axis)

Now it is well known that in the xy- plane, the normalized Eigen functions in the presence of Rashba spin-orbit coupling will assume the form of a two-component spinor

$$\Psi_{2D} = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2A}}\begin{pmatrix} 1 \\ i\dfrac{\left(k_x - ik_y\right)}{k} \end{pmatrix}, \text{ where, } A \equiv \text{Area.} \tag{7.1.275}$$

Similarly, for a nanotube we can reasonably expect the general form of the normalized Eigen functions to be

$$\Psi = \frac{e^{ik_z z}e^{il\varphi}}{\sqrt{2\pi L_z R}} P\left(\rho\right)\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} \tag{7.1.276}$$

Where the spinors, $\psi^{\pm}$ are to be determined and then used to calculate the surface response function. The radial part $P\left(\rho\right)$ is defined as in Eqn. 3.1.76.

The unperturbed generalized Hamiltonian, $\hat{H}^0$ for an electron in cylindrical coordinates in the presence of an external magnetic field which is parallel to the z-axis [24] is

$$\hat{H}^0 = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] - \frac{ei\hbar B_z}{2m^*c}\frac{\partial}{\partial\varphi} + \frac{e^2B_z^2\rho^2}{8m^*c^2} + eV \tag{7.1.277}$$

For our purposes, the general 3D Hamiltonian for an electron in the presence of Rashba spin-orbit interaction in an external magnetic field is given by

$$\begin{aligned} \hat{H}_T &= \hat{H}^0 + \hat{H}^3_{SO} + \hat{H}^4 \\ &= \frac{1}{2m^*}\left(\hat{\vec{p}} + \frac{e}{c}\vec{A}\right)^2 + \beta\vec{E}\cdot\hat{\vec{\sigma}}\times\left(\hat{\vec{p}} + \frac{e}{c}\vec{A}\right) - g_s\hat{\mu}_s\cdot\vec{B} \end{aligned} \tag{7.1.278}$$

Back-substituting Eqn. (7.1.277) in which we employed the symmetric gauge,

$$\vec{A} = \left(0, \frac{1}{2}B\rho, 0\right) = \left(A_\rho, A_\varphi, A_z\right) \tag{7.1.279}$$

and noting that

$$\vec{E} = -\nabla V \tag{7.1.280}$$

Equation (7.1.278) becomes

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{ei\hbar B_z}{2m^*c}\frac{\partial}{\partial\varphi}+\frac{e^2B_z^2\rho^2}{8m^*c^2}+eV+$$

$$+\beta\vec{E}\cdot\hat{\vec{\sigma}}\times\left(-i\hbar\left\{\hat{\rho}\frac{\partial}{\partial\rho}+\hat{\varphi}\frac{1}{\rho}\frac{\partial}{\partial\varphi}+\hat{z}\frac{\partial}{\partial z}\right\}+\frac{e}{c}\frac{1}{2}B_z\rho\hat{\varphi}\right)-g_s\hat{\mu}_s\cdot\vec{B}$$

(7.1.281)

Recall that $\hat{\mu}_s = \frac{e\hbar}{2m^*c}\hat{\vec{\sigma}}$ and $\vec{B} = \hat{z}B_z$. So, upon back-substitution we get

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{ei\hbar B_z}{2m^*c}\frac{\partial}{\partial\varphi}+\frac{e^2B_z^2\rho^2}{8m^*c^2}+eV+$$

$$+\beta\vec{E}\cdot\hat{\vec{\sigma}}\times\left(-i\hbar\left\{\hat{\rho}\frac{\partial}{\partial\rho}+\hat{\varphi}\frac{1}{\rho}\frac{\partial}{\partial\varphi}+\hat{z}\frac{\partial}{\partial z}\right\}+\frac{m^*e}{m^*c}\frac{1}{2}B_z\rho\hat{\varphi}\right)-g_s\frac{e\hbar}{2m^*c}\sigma_zB_z$$

(7.1.282)

The particular form of this Hamiltonian for our geometry will emerge within the next few pages.

Let us define the cyclotron frequency as

$$\omega_c \equiv \frac{eB_z}{m^*c}, \Rightarrow -g_s\frac{e\hbar}{2m^*c}\sigma_zB_z = -\frac{\hbar}{2}\sigma_zg_s\frac{eB_z}{m^*c} = -\frac{\sigma_zg_s}{2}\hbar\omega_c \tag{7.1.283}$$

Back-substituting Eqn. (7.1.283) into Eqn. (7.1.282) yields

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i\hbar}{2}\omega_c\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8}\omega_c^2+eV+$$

$$+\beta\vec{E}\cdot\hat{\vec{\sigma}}\times\left(-i\hbar\left\{\hat{\rho}\frac{\partial}{\partial\rho}+\hat{\varphi}\frac{1}{\rho}\frac{\partial}{\partial\varphi}+\hat{z}\frac{\partial}{\partial z}\right\}+\frac{m^*\rho}{2}\omega_c\hat{\varphi}\right)-\frac{\sigma_zg_s}{2}\hbar\omega_c$$

(7.1.284)

If we further define

$$E(\omega_c) \equiv \hbar\omega_c, \Rightarrow -\frac{\sigma_z g_s}{2}\hbar\omega_c = -\frac{\sigma_z g_s}{2}E(\omega_c) \tag{7.1.285}$$

as the energy associated with the cyclotron frequency, then Eqn. (7.1.284) becomes

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+eV+$$

$$+\beta\hat{\vec{\sigma}}\cdot\left\{\hat{\rho}\left(E_\varphi i\hbar\frac{\partial}{\partial z}-E_z\frac{1}{\rho}i\hbar\frac{\partial}{\partial\varphi}+E_z\frac{m^*\rho}{2\hbar}E(\omega_c)\right)+\hat{\varphi}\left(E_z i\hbar\frac{\partial}{\partial\rho}-E_\rho i\hbar\frac{\partial}{\partial z}\right)+\right.$$

$$\left.+\hat{z}\left(E_\rho\frac{1}{\rho}i\hbar\frac{\partial}{\partial\varphi}-E_\varphi i\hbar\frac{\partial}{\partial\rho}-E_\rho\frac{m^*\rho}{2\hbar}E(\omega_c)\right)\right\}-\frac{\sigma_z g_s}{2}E(\omega_c) \tag{7.1.286}$$

Where

$$\hat{\vec{\sigma}} = \hat{\rho}\sigma_\rho+\hat{\varphi}\sigma_\varphi+\hat{z}\sigma_z \tag{7.1.287}$$

Let us make the following equivalent replacements of plane polar unit vectors

$$\hat{\varphi} \to -\hat{x}\sin\varphi+\hat{y}\cos\varphi \tag{7.1.288}$$

$$\hat{\rho} \to \hat{x}\cos\varphi+\hat{y}\sin\varphi \tag{7.1.289}$$

into Eqn. (7.1.286):

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+eV+$$

$$+\beta\hat{\vec{\sigma}}\cdot\left\{\hat{x}\left(\left(E_\varphi i\hbar\frac{\partial}{\partial z}-E_z\frac{1}{\rho}i\hbar\frac{\partial}{\partial\varphi}+E_z\frac{m^*\rho}{2\hbar}E(\omega_c)\right)\cos\varphi-\left(E_z i\hbar\frac{\partial}{\partial\rho}-E_\rho i\hbar\frac{\partial}{\partial z}\right)\sin\varphi\right)+\right.$$

$$+\hat{y}\left(\left(E_\varphi i\hbar\frac{\partial}{\partial z}-E_z\frac{1}{\rho}i\hbar\frac{\partial}{\partial\varphi}+E_z\frac{m^*\rho}{2\hbar}E(\omega_c)\right)\sin\varphi+\left(E_z i\hbar\frac{\partial}{\partial\rho}-E_\rho i\hbar\frac{\partial}{\partial z}\right)\cos\varphi\right)+$$

$$\left.+\hat{z}\left(E_\rho\frac{1}{\rho}i\hbar\frac{\partial}{\partial\varphi}-E_\varphi i\hbar\frac{\partial}{\partial\rho}-E_\rho\frac{m^*\rho}{2\hbar}E(\omega_c)\right)\right\}-\frac{\sigma_z g_s}{2}E(\omega_c) \tag{7.1.290}$$

Let us now redefine

$$\hat{\vec{\sigma}} \equiv \hat{x}\sigma_x + \hat{y}\sigma_y + \hat{z}\sigma_z \tag{7.1.291}$$

Back-substituting and dotting Eqn. (7.1.291) into Eqn. (7.1.290) gives us

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+eV+$$

$$+\beta i\hbar\left\{E_\rho\left[(\sigma_x\sin\varphi-\sigma_y\cos\varphi)\frac{\partial}{\partial z}+\left(\frac{1}{\rho}\frac{\partial}{\partial\varphi}-\frac{m^*\rho}{2i\hbar^2}E(\omega_c)\right)\sigma_z\right]+\right.$$

$$+E_\varphi\left[(\sigma_x\cos\varphi+\sigma_y\sin\varphi)\frac{\partial}{\partial z}-\sigma_z\frac{\partial}{\partial\rho}\right]+E_z\left[(\sigma_y\cos\varphi-\sigma_x\sin\varphi)\frac{\partial}{\partial\rho}-\right.$$

$$\left.\left.-\left(\sigma_x\frac{1}{\rho}\cos\varphi+\sigma_y\frac{1}{\rho}\sin\varphi\right)\frac{\partial}{\partial\varphi}+\frac{m^*\rho}{2i\hbar^2}E(\omega_c)(\sigma_x\cos\varphi+\sigma_y\sin\varphi)\right]\right\}-\frac{\sigma_z g_s}{2}E(\omega_c)$$

(7.1.292)

Equation (7.1.292) is the explicit general Rashba Hamiltonian in cylindrical coordinates, for an electron in a magnetic field.

Of course, the above form of the equation will be altered when we impose boundary conditions, which arise from the physical nature of the problem under investigation. In our problem, the electrons are confined to the lateral surface of the cylinder in the presence of a uniform magnetic field in the z-direction. This allows us to effectively set ρ = *constant.* Hence, differentials and derivatives of functions with respect to this parameter will vanish. There is also a confining potential in the radial direction, $-\hat{\rho}$ and so $\vec{E} = (E_\rho, E_\varphi, E_z) = (E_\rho, 0, 0)$. As a result, Eqn. (7.1.292) reduces to

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+eV+$$

$$+\beta i\hbar E_\rho\left[(\sigma_x\sin\varphi-\sigma_y\cos\varphi)\frac{\partial}{\partial z}+\left(\frac{1}{\rho}\frac{\partial}{\partial\varphi}-\frac{m^*\rho}{2i\hbar^2}E(\omega_c)\right)\sigma_z\right]-\frac{\sigma_z g_s}{2}E(\omega_c)$$

(7.1.293)

Using Eqns. (7.1.274) and (7.1.280) to redefine the Rashba parameter,

$$\alpha' = \beta\hbar\left\langle E_\rho \right\rangle \tag{7.1.294}$$

equation (7.1.293) becomes

$$\hat{H}_T = \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] - \frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi} + \frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c) + eV +$$

$$+i\alpha'\left[\left(\sigma_x \sin\varphi - \sigma_y \cos\varphi\right)\frac{\partial}{\partial z} + \left(\frac{1}{\rho}\frac{\partial}{\partial\varphi} - \frac{m^*\rho}{2i\hbar^2}E(\omega_c)\right)\sigma_z\right] - \frac{\sigma_z g_s}{2}E(\omega_c) \tag{7.1.295}$$

Where

$$\left(\sigma_x, \sigma_y, \sigma_z\right) \equiv \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right) \tag{7.1.296}$$

are the familiar Pauli matrices.

Back-substituting Eqn. (7.1.296) into Eqn. (7.1.295) and multiplying the left hand side of Eqn. (7.1.295) as well as the first, second, third and forth terms on the right hand side of the same equation by an identity matrix of dimension two(I_2), we obtain the matrix Hamiltonian operator equation

$$\begin{pmatrix} \hat{H}_T & 0 \\ 0 & \hat{H}_T \end{pmatrix} =$$

$$\begin{pmatrix} \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] & 0 \\ 0 & \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] \end{pmatrix} - \begin{pmatrix} \frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi} & 0 \\ 0 & \frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi} \end{pmatrix} +$$

$$\begin{pmatrix} \frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c) & 0 \\ 0 & \frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c) \end{pmatrix} + \begin{pmatrix} 0 & i\alpha'\sin\varphi\frac{\partial}{\partial z} \\ i\alpha'\sin\varphi\frac{\partial}{\partial z} & 0 \end{pmatrix} -$$

$$\begin{pmatrix} 0 & \alpha'\cos\varphi\frac{\partial}{\partial z} \\ -\alpha'\cos\varphi\frac{\partial}{\partial z} & 0 \end{pmatrix} +$$

$$+\begin{pmatrix} \frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi} - \frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c) & 0 \\ 0 & -\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi} + \frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c) \end{pmatrix} \tag{7.1.297}$$

As was previously mentioned, the normalized Eigen functions are expected to assume the following general form

$$\Psi = \frac{e^{ik_z z}e^{il\varphi}}{\sqrt{2\pi L_z R}}P(\rho)\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} \tag{7.1.298}$$

When the Hamiltonian operates on the column vector in Ψ we obtain

$$\begin{pmatrix} \hat{H}_T & 0 \\ 0 & \hat{H}_T \end{pmatrix}\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} = \begin{pmatrix} E^+ \\ E^- \end{pmatrix}\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} \tag{7.1.299}$$

$$\left[\begin{pmatrix} \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] & 0 \\ 0 & \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] \end{pmatrix} - \begin{pmatrix} \frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi} & 0 \\ 0 & \frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi} \end{pmatrix} +\right.$$

$$\begin{pmatrix} \frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c) & 0 \\ 0 & \frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c) \end{pmatrix} +$$

$$+\begin{pmatrix} 0 & i\alpha'\sin\varphi\frac{\partial}{\partial z} \\ i\alpha'\sin\varphi\frac{\partial}{\partial z} & 0 \end{pmatrix}-\begin{pmatrix} 0 & \alpha'\cos\varphi\frac{\partial}{\partial z} \\ -\alpha'\cos\varphi\frac{\partial}{\partial z} & 0 \end{pmatrix}+$$

$$+\begin{pmatrix} \frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}-\frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c) & 0 \\ 0 & -\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+\frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c) \end{pmatrix}+$$

$$\left.\begin{pmatrix} -\frac{g_s}{2}E(\omega_c) & 0 \\ 0 & \frac{g_s}{2}E(\omega_c) \end{pmatrix}+\begin{pmatrix} eV & 0 \\ 0 & eV \end{pmatrix}\right]$$

$$\cdot\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix}=\begin{pmatrix} E^+ & \\ & E^- \end{pmatrix}\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} \tag{7.1.300}$$

This gives rise to the following system of simultaneous partial differential equations

$$\left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}\right.$$

$$\left.-\frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c)-\frac{g_s}{2}E(\omega_c)+eV\right)\psi^+ +(i\alpha'\sin\varphi-\alpha'\cos\varphi)\frac{\partial}{\partial z}\psi^- = E\psi^+ \tag{7.1.301}$$

$$(i\alpha'\sin\varphi+\alpha'\cos\varphi)\frac{\partial}{\partial z}\psi^+ + \left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}+\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)\right.$$

$$\left.-\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+\frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c)+\frac{g_s}{2}E(\omega_c)+eV\right)\psi^- = E\psi^- \tag{7.1.302}$$

We know that in our problem, the electrons are free to move on the surface parallel to the z-axis as well as in the angular directions, $\pm\hat{\varphi}$ (where the signs denotes the sense of clockwise and counterclockwise revolutions) while on the nanotube, so we can in part assume general spinor solutions of the form

$$\psi^+ = \frac{A(\varphi)e^{ik_z z}}{\sqrt{L_z}} \tag{7.1.303}$$

$$\psi^- = \frac{B(\varphi)e^{ik_z z}}{\sqrt{L_z}} \tag{7.1.304}$$

It is interesting to note that for the zero-field case, $(\omega_c = 0)$ Eqns. (7.1.301) and (7.1.302) reduce to

$$\left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]+\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+eV\right)\psi^+ + (i\alpha'\sin\varphi-\alpha'\cos\varphi)\frac{\partial}{\partial z}\psi^- = E\psi^+ \tag{7.1.305}$$

$$(i\alpha'\sin\varphi+\alpha'\cos\varphi)\frac{\partial}{\partial z}\psi^+ + \left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+eV\right)\psi^- = E\psi^- \tag{7.1.306}$$

Whose spinor solutions can also assume the form given in Eqns. (7.1.303) and (7.1.304) respectively and should be less mathematically involved than the quest for solutions to Eqns. (7.1.301) and (7.1.302). Indeed, if we back-substitute Eqns. (7.1.303) and (7.1.304) into Eqns. (7.1.305) and (7.1.306) respectively, we obtain the following system of ordinary differential equations

$$\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{d^2A(\varphi)}{d\varphi^2}+k_z^2A(\varphi)\right]+\frac{i\alpha'}{\rho}\frac{dA(\varphi)}{d\varphi}+eVA(\varphi)-(\alpha'\sin\varphi+i\alpha'\cos\varphi)k_zB(\varphi)$$
$$= EA(\varphi)$$

$$\Leftrightarrow \frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{d^2A(\varphi)}{d\varphi^2}+k_z^2A(\varphi)\right]+\frac{i\alpha'}{\rho}\frac{dA(\varphi)}{d\varphi}+eVA(\varphi)-i\alpha'k_ze^{-i\varphi}B(\varphi)=EA(\varphi) \tag{7.1.307}$$

$$(-\alpha'\sin\varphi+i\alpha'\cos\varphi)A(\varphi)k_z+\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{d^2B(\varphi)}{d\varphi^2}+k_z^2B(\varphi)\right]-\frac{i\alpha'}{\rho}\frac{dB(\varphi)}{d\varphi}+eVB(\varphi)$$
$$= EB(\varphi)$$

$$\Leftrightarrow -i\alpha'k_ze^{i\varphi}A(\varphi)+\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{d^2B(\varphi)}{d\varphi^2}+k_z^2B(\varphi)\right]-\frac{i\alpha'}{\rho}\frac{dB(\varphi)}{d\varphi}+eVB(\varphi)=EB(\varphi)$$

(7.1.308)

Explicit forms of the variable spinor coefficients, $A(\varphi)$ and $B(\varphi)$ for both finite and zero magnetic fields will now be determined.

In the case of zero external magnetic fields, the respective spinor coefficients can assume the form of a pair of series solutions for zero and integral values of the index, *k* (or *l*). Thus

$$A(\varphi) = \frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} a_k e^{ik\varphi} \tag{7.1.309}$$

$$B(\varphi) = \frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} b_k e^{ik\varphi} \tag{7.1.310}$$

Back-substituting Eqns. (7.1.309) and (7.1.310) into Eqns. (7.1.307) and (7.1.308), yields

$$\frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} \left\{ \left[\frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left(\frac{k}{\rho} \right)^2 - \frac{k}{\rho} \alpha' - E_- \right] a_k - i\alpha' k_z b_{k+1} \right\} e^{ik\varphi} = 0 \tag{7.1.311}$$

$$\frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} \left\{ \left[\frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left(\frac{k}{\rho} \right)^2 + \frac{k}{\rho} \alpha' - E_+ \right] b_k + i\alpha' k_z a_{k-1} \right\} e^{ik\varphi} = 0 \tag{7.1.312}$$

It is worthy of note that in Eqns. (7.1.307), (7.1.308), (7.1.311) and (7.1.312) respectively, the confinement of electrons to the surface of the nanotube is due entirely to the presence of an inwardly radial electric field, $\vec{E}_\rho$. Also apparent is the link between the spin angular momentum of the electron, $\pm\frac{\hbar\hat{\sigma}}{2}$ and its quantum mechanical orbital angular momentum, $\hat{\vec{p}}$. This coupling of *momenta* persists regardless of the presence or absence of a magnetic field. This fact therefore bears witness as to the utility of the Rashba average $\vec{E}_\rho$-field approximation

It is obvious that the above system of equations is infinite dimensional and does not appear to lend themselves to solutions in closed form and so ought to be solved numerically. To further resolve this problem we can look to the strength of the Rashba parameter, α'. For if we consider the case of a weak potential, this would lessen the effect of the coupling parameter, α' in the above system of equations. The now uncoupled equations would become finite dimensional. However, we may use yet another approach which exploits the orthonormality of the Euler Eigen functions, $e^{ik\varphi}, e^{ik'\varphi}$. We shall choose the latter method.

Let us multiply the above system of equations by $e^{-ik'\varphi}$ and integrate over the variable, $-\pi \le \varphi \le \pi$.

With respect to the first of these equations we obtain

$$\int_{-\pi}^{\pi} d\varphi \frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} \left\{ \left[\frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left(\frac{k}{\rho} \right)^2 - \frac{k}{\rho} \alpha' - E_- \right] a_k - i\alpha' k_z b_{k+1} \right\} e^{ik\varphi} e^{-ik'\varphi} = 0$$

$$\frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} \left\{ \left[\frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left(\frac{k}{\rho} \right)^2 - \frac{k}{\rho} \alpha' - E_- \right] a_k - i\alpha' k_z b_{k+1} \right\} \int_{-\pi}^{\pi} d\varphi e^{ik\varphi} e^{-ik'\varphi} = 0$$

$$\frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} \left\{ \left[\frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left(\frac{k}{\rho} \right)^2 - \frac{k}{\rho} \alpha' - E_- \right] a_k - i\alpha' k_z b_{k+1} \right\} \int_{-\pi}^{\pi} d\varphi e^{i(k-k')\varphi} = 0$$

(7.1.313)

The integral is either zero or non-zero, in that it is equivalent to the Kroneker delta for certain values of the exponentiated parameters k and k'. That is

$$\int_{-\pi}^{\pi} d\varphi e^{i(k-k')\varphi} = 2\pi \delta_{kk'} . \tag{7.1.314}$$

For the non-trivial case $(k \neq k')$, Eqn.(7.1.313) reduces to

$$\frac{1}{\sqrt{2\pi}}\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-E_-\right]a_k-i\alpha' k_z b_{k+1}\right\}2\pi=0 \qquad (7.1.315)$$

We will now multiply both sides of Eqn. (7.1.315) by $\frac{\sqrt{2\pi}}{2\pi}$ which yields

$$\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-E_-\right]a_k-i\alpha' k_z b_{k+1}\right\}=0 \qquad (7.1.316)$$

Via similar arguments, Eqn. (7.1.312) subsequently reduces to the following form

$$\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2+\frac{k}{\rho}\alpha'-E_+\right]b_k+i\alpha' k_z a_{k-1}\right\}=0 \qquad (7.1.317)$$

The actual values of the expansion coefficients, a_k, a_{k-1}; b_k and b_{k+1} will be determined shortly.

For finite magnetic fields $\vec{B}\neq 0$:

For cases involving a finite magnetic field $(\omega_c \neq 0)$ we will 'back-substitute' a composite of the spinor-solutions from Eqns.(7.1.303), (7.1.304), (7.1.309) and (7.1.310) along with the replacement $l \to k$

$$\psi^+=\frac{1}{\sqrt{2\pi L_z}}\sum_{k=-\infty}^{\infty}a_k e^{ik_z z}e^{ik\varphi}=\frac{e^{ik_z z}}{\sqrt{2\pi L_z}}\sum_{k=-\infty}^{\infty}a_k e^{ik\varphi} \qquad (7.1.318)$$

$$\psi^-=\frac{e^{ik_z z}}{\sqrt{2\pi L_z}}\sum_{k=-\infty}^{\infty}b_k e^{ik\varphi} \qquad (7.1.319)$$

into Eqns. (7.1.301) and (7.1.302) respectively.

Better yet, for ease of computation, let us re-write Eqns. (7.1.301) and (7.1.302) as

$$\left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]+\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+eV\right)\psi^+ +\alpha'\left(i\sin\varphi-\cos\varphi\right)\frac{\partial}{\partial z}\psi^- +$$

$$+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)-\frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c)-\frac{g_s}{2}E(\omega_c)-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}\right)\psi^+=E_-\psi^+$$

(7.1.320)

$$\alpha'(i\sin\varphi+\cos\varphi)\frac{\partial}{\partial z}\psi^+ +\left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+eV\right)\psi^- +$$

$$+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+\frac{\alpha' m^*\rho}{2\hbar^2}E(\omega_c)+\frac{g_s}{2}E(\omega_c)-\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}\right)\psi^-=E_+\psi^-$$

(7.1.321)

With respect to the former equation, we obtain

$$\left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]+\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+eV\right)\psi^+-E_-\psi^++\alpha'(i\sin\varphi-\cos\varphi)\frac{\partial}{\partial z}\psi^-$$

$$=\left(-\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s\right)\frac{E(\omega_c)}{2}+\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}\right)\psi^+ \qquad (7.1.322)$$

Similarly, for latter Eqn. (7.1.321), we obtain

$$\left(\frac{-\hbar^2}{2m^*}\left[\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{i\alpha'}{\rho}\frac{\partial}{\partial\varphi}+eV\right)\psi^--E_+\psi^-+\alpha'(i\sin\varphi+\cos\varphi)\frac{\partial}{\partial z}\psi^+$$

$$=\left(-\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)-\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s\right)\frac{E(\omega_c)}{2}+\frac{i}{2}E(\omega_c)\frac{\partial}{\partial\varphi}\right)\psi^- \qquad (7.1.323)$$

We shall now 'back-substitute' equations (7.1.318) and (7.1.319), into equations (7.1.322) and (7.1.323), respectively.

One will notice upon substitution, that the first three terms on the left hand sides of equations (7.1.322) and (7.1.323) yield results that are congruent to those found in equations (7.1.311) and (7.1.312); when one includes the explicit form of the *Eigen functions*. Hence, equation (7.1.322) may be re-written in the following form

$$\sum_{k=-\infty}^{+\infty}\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-\left(-\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s\right)\frac{E(\omega_c)}{2}\right)-\right.\right.$$

$$-\frac{k}{2}E(\omega_c)-E_-\Bigg]a_k - i\alpha' k_z b_{k+1}\Bigg\}\frac{e^{ik\varphi}}{\sqrt{2\pi}}=0 \qquad (7.1.324)$$

Or

$$\sum_{k=-\infty}^{+\infty}\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-E_-+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)-\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s\right)\frac{E(\omega_c)}{2}\right)-\right.\right.$$

$$\left.\left.-\frac{k}{2}E(\omega_c)\right]a_k - i\alpha' k_z b_{k+1}\right\}\frac{e^{ik\varphi}}{\sqrt{2\pi}}=0$$

Or

$$\sum_{k=-\infty}^{+\infty}\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-E_-+\right.\right.$$

$$\left.\left.+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)-\frac{E(\omega_c)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\right]a_k - i\alpha' k_z b_{k+1}\right\}\frac{e^{ik\varphi}}{\sqrt{2\pi}}=0 \qquad (7.1.325)$$

By likened reasoning, equation (7.1.323) reduces to

$$\sum_{k=-\infty}^{+\infty}\left\{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2+\frac{k}{\rho}\alpha'-E_++\right.\right.$$

$$\left.\left.+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)+\frac{E(\omega_c)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\right]b_k + i\alpha' k_z a_{k-1}\right\}\frac{e^{ik\varphi}}{\sqrt{2\pi}}=0$$

(7.1.326)

Finally, we may combine equations (7.1.325) and (7.1.326) more compactly. Indeed, if in addition we multiply both equations by $e^{-ik'\varphi}$, integrate over the variable, $-\pi\le\varphi\le\pi$ and employ orthogonal arguments we obtain

$$\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2\mp\frac{k}{\rho}\alpha'-E_\mp+\right.$$

$$+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)\mp\frac{E(\omega_c)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\Bigg]\begin{pmatrix}a_k\\ b_k\end{pmatrix}\mp i\alpha' k_z\begin{pmatrix}b_{k+1}\\ a_{k-1}\end{pmatrix}=0$$

(7.1.327)

Where $\begin{pmatrix}a_k\\ b_k\end{pmatrix}$ and $\begin{pmatrix}b_{k+1}\\ a_{k-1}\end{pmatrix}$ are column matrices of the expansion coefficients.

Limiting Cases

In the limit as $\vec{B}=B\hat{z}\to 0,\omega_c\to 0$ and Eqn. (7.1.327) reduces to the results obtained for the zero $\vec{B}$-field case, *ibid* page 67 Eqns. (7.1.316) and (7.1.317). The spin-moment gyro magnetic ratio g_s is lost owing to the fact that it is being multiplied by the energy associated with the cyclotron frequency, $E(\omega_c)$ which is now zero. Remember, $E(\omega_c)\big|_{B_z=0}=0$.

The Expansion Coefficients

In taking the upper signs of Eqn. (7.1.327) we have the following

$$\Bigg[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-E_-+$$

$$+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)-\frac{E(\omega_c)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\Bigg]a_k-i\alpha' k_z b_{k+1}=0 \qquad (7.1.328)$$

Which, upon solving for a_k yields

$$a_k=\frac{i\alpha' k_z b_{k+1}}{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2-\frac{k}{\rho}\alpha'-E_-+\left(\frac{m^*\rho^2}{8\hbar^2}E^2(\omega_c)-\frac{E(\omega_c)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\right]}$$

$$=\mathrm{A} \qquad (7.1.329)$$

Likewise, the lower signs of Eqn. (7.1.327) give us

$$\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2+\frac{k}{\rho}\alpha'-E_+ + \right.$$

$$\left. +\left(\frac{m^*\rho^2}{8\hbar^2}E^2\left(\omega_c\right)+\frac{E\left(\omega_c\right)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\right]b_k+i\alpha' k_z a_{k-1}=0 \qquad (7.1.330)$$

Which we solve for b_k to obtain

$$b_k=\frac{-i\alpha' k_z a_{k-1}}{\left[\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2+\frac{k}{\rho}\alpha'-E_+ +\left(\frac{m^*\rho^2}{8\hbar^2}E^2\left(\omega_c\right)-\frac{E\left(\omega_c\right)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right)\right]}$$

$$=\mathrm{B} \qquad (7.1.331)$$

One can combine both Eqns. (7.1.329) and (7.1.331) into simple matrix form

$$\begin{pmatrix}\mathrm{A} & 0\\ 0 & \mathrm{B}\end{pmatrix}\begin{pmatrix}b_{k+1}\\ a_{k-1}\end{pmatrix}=\begin{pmatrix}a_k\\ b_k\end{pmatrix} \qquad (7.1.332)$$

From Eqn. (7.1.329) we have with the replacements,

$$E(k_z,k)\rightarrow\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{k}{\rho}\right)^2 \qquad (7.1.333)$$

and

$$\Delta\rightarrow\left(\frac{m^*\rho^2}{8\hbar^2}E^2\left(\omega_c\right)-\frac{E\left(\omega_c\right)}{2}\left(\frac{\alpha' m^*\rho}{\hbar^2}+g_s+k\right)\right) \qquad (7.1.334)$$

the following

$$a_k=\frac{i\alpha' k_z b_{k+1}}{\left[E(k_z,k)-E_- +\Delta-\frac{k}{\rho}\alpha'\right]} \qquad (7.1.335)$$

Let us shift the index, k in the above equation by (-1), i.e., replace $k\rightarrow k-1$. By so doing, Eqn.(7.1.335) becomes

$$a_{k-1} = \frac{i\alpha' k_z b_k}{\left[E(k_z, k-1) - E_- + \Delta - \frac{(k-1)}{\rho}\alpha' \right]} \tag{7.1.336}$$

Now, from Eqn.(7.1.331) we have with replacements *ibid,* Eqn. (7.1.333) and

$$\Delta' \rightarrow \left(\frac{m^* \rho^2}{8\hbar^2} E^2(\omega_c) + \frac{E(\omega_c)}{2}\left(\frac{\alpha' m^* \rho}{\hbar^2} + g_s + k \right) \right) \tag{7.1.337}$$

respectively, the following result

$$b_k = \frac{-i\alpha' k_z a_{k-1}}{\left[E(k_z, k) - E_+ + \Delta' + \frac{k}{\rho}\alpha' \right]} \tag{7.1.338}$$

Solving this equation for a_{k-1} we obtain

$$a_{k-1} = \frac{\left[E(k_z, k) - E_+ + \Delta' + \frac{k}{\rho}\alpha' \right] b_k}{-i\alpha' k_z} \tag{7.1.339}$$

Via the transitive property form algebra we may equate Eqns. (7.1.336) and (7.1.339) yielding

$$\frac{i\alpha' k_z b_k}{\left[E(k_z, k-1) - E_- + \Delta - \frac{(k-1)}{\rho}\alpha' \right]} = \frac{\left[E(k_z, k) - E_+ + \Delta' + \frac{k}{\rho}\alpha' \right] b_k}{-i\alpha' k_z} \tag{7.1.340}$$

$$\left[\frac{i\alpha' k_z}{\left[E(k_z, k-1) - E_- + \Delta - \frac{(k-1)}{\rho}\alpha' \right]} + \frac{\left[E(k_z, k) - E_+ + \Delta' + \frac{k}{\rho}\alpha' \right]}{i\alpha' k_z} \right] b_k = 0 \tag{7.1.341}$$

Since $b_k \neq 0$, it follows that

$$\left[\frac{i\alpha' k_z}{\left[E(k_z,k-1)-E_-+\Delta-\frac{(k-1)}{\rho}\alpha'\right]}+\frac{\left[E(k_z,k)-E_++\Delta'+\frac{k}{\rho}\alpha'\right]}{i\alpha' k_z}\right]=0$$

(7.1.342)

Equating the addends and cross-multiplying we obtain

$$\alpha'^2 k_z^2=\left[E(k_z,k-1)-E_-+\Delta-\frac{(k-1)}{\rho}\alpha'\right]\left[E(k_z,k)-E_++\Delta'+\frac{k}{\rho}\alpha'\right]$$

(7.1.343)

Or

$$\frac{\alpha'^2 k_z^2}{\left[E(k_z,k-1)-E_-+\Delta-\frac{(k-1)}{\rho}\alpha'\right]\left[E(k_z,k)-E_++\Delta'+\frac{k}{\rho}\alpha'\right]}=1$$

(7.1.344)

Or with the replacement, $l\to k$

$$\left[E(k_z,l-1)-E_-+\Delta-\frac{(l-1)}{\rho}\alpha'\right]\left[E(k_z,l)-E_++\Delta'+\frac{l}{\rho}\alpha'\right]-\alpha'^2 k_z^2=0$$

(7.1.345)

Let us re-write this equation with the interpretation that

$$E(k_z,l-1)\equiv E^{(0)}(k_z,l-1) \tag{7.1.346}$$

and

$$E(k_z,l)\equiv E^{(0)}(k_z,l) \tag{7.1.347}$$

in the following form

$$\left[E^{(2)}(k_z,l-1)-E\right]\left[E^{(1)}(k_z,l)-E\right]-\alpha'^2 k_z^2=0 \tag{7.1.348}$$

where

$$E^{(2)}(k_z, l-1) \equiv E(k_z, l-1) + \Delta - \frac{(l-1)}{\rho}\alpha' \tag{7.1.349}$$

$$E^{(1)}(k_z, l) \equiv E(k_z, l) + \Delta' + \frac{l}{\rho}\alpha' \tag{7.1.350}$$

and

$$E = E_{\pm} \tag{7.1.351}$$

An expansion of the minuend in Eqn.(7.1.348) leads to

$$E^{(1)}(k_z, l)E^{(2)}(k_z, l-1) - E^{(2)}(k_z, l-1)E - E^{(1)}(k_z, l)E + E^{(2)} \tag{7.1.352}$$

Which we then 'back-substitute' into the left hand side of Eqn.(7.1.348) yielding

$$E^{(2)} - \left(E^{(2)}(k_z, l-1) + E^{(1)}(k_z, l)\right)E^1 + \left(E^{(1)}(k_z, l)E^{(2)}(k_z, l-1) - \alpha'^2 k_z^2\right)E^0 = 0 \tag{7.1.353}$$

Please note that in the preceding and succeeding derivations,

$$E^{(2)} \neq E^2, E^{(1)} \neq E^1 \text{ and } E^{(0)} \neq E^0 = 1 \tag{7.1.354}$$

Provided that the energy eigenvalue, E is variable and that coefficients are constants, Eqn. (7.1.353) may be interpreted as a quadratic equation in E. Namely,

$$aE^2 + bE^1 + cE^0 = 0 \tag{7.1.355}$$

The zeros of which are

$$E_{\pm} = -\frac{b}{2a} \pm \frac{\left(b^2 - 4ac\right)^{\frac{1}{2}}}{2a}, a \neq 0 \tag{7.1.356}$$

By equating descending powers of E in Eqn. (7.1.355) with those of Eqn. (7.1.353), we find that for

$$E^2 \Big| a = 1 \tag{7.1.357}$$

$$E^1 \Big| b = -\left(E^{(1)}(k_z, l) + E^{(2)}(k_z, l-1)\right) \tag{7.1.358}$$

$$E^0\Big|c = \left(E^{(1)}(k_z,l)E^{(2)}(k_z,l-1) - \alpha'^2 k_z^2\right) \tag{7.1.359}$$

'Back-substituting' Eqns. (7.1.357) - (71.359) into Eqn. (7.1.356) yields the energy Eigen values associated with the spinor-Eigen functions

$$E_\pm = \frac{E^{(1)}(k_z,l) + E^{(2)}(k_z,l-1)}{2} \pm$$

$$\pm \frac{\left(\left(E^{(1)}(k_z,l) - E^{(2)}(k_z,l-1)\right)^2 + 4\alpha'^2 k_z^2\right)^{\frac{1}{2}}}{2} \tag{7.1.360}$$

The Spinor-Eigenfunctions or 'Eigenspinors', $\psi^\pm$

Recall from Eqn. (7.1.245) that

$$\begin{pmatrix} \hat{H}_T & 0 \\ 0 & \hat{H}_T \end{pmatrix}\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} = \begin{pmatrix} E_+ \\ E_- \end{pmatrix}\begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} \tag{7.1.361}$$

Wherein, $E_- \equiv E^{(1)}$ and $E_+ \equiv E^{(2)}$. In addition, $\psi^\pm$ are defined as in Eqns. (7.1.303), (7.1.304), (7.1.309) and (7.1.310), respectively. Firstly, we shall take an explicit look at the angular parts (φ-parts), of $\psi^\pm$. Secondly, we shall combine the former results with the linear parts (z -parts), of the spinor-Eigen functions.

As to the former, we commence for the sake of convenience, with the replacement $l \to k$ in Eqns. (7.1.309(310)) whereupon we obtain

$$\begin{pmatrix} \psi^+(\varphi) \\ \psi^-(\varphi) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2\pi}} \sum_{l=-\infty}^{\infty} a_l e^{il\varphi} \\ \frac{1}{\sqrt{2\pi}} \sum_{l=-\infty}^{\infty} b_l e^{il\varphi} \end{pmatrix} \tag{7.1.362}$$

Furthermore, we may express b_l in terms of a_l *via* Eqn. (7.1.338). The task is further accomplished by way of back-substitution and an appropriate shift in the index of $a_{l-1} \to a_{(l+1)-1} \to a_l$ in the same equation. Having done so, Eqn. (7.1.362) becomes

$$\begin{pmatrix}\psi^{+}(\varphi)\\ \psi^{-}(\varphi)\end{pmatrix}=\frac{1}{\sqrt{2\pi}}\sum_{l=-\infty}^{\infty}e^{il\varphi}\begin{pmatrix}a_l\\ \dfrac{-i\alpha' k_z a_l e^{i\varphi}}{\left[E^{(0)}\left(k_z,k+1\right)-E_{\pm}+\Delta'+\dfrac{\alpha'\left(k+1\right)}{\rho}\right]}\end{pmatrix}$$

$$=\frac{1}{\sqrt{2\pi}}\sum_{l=-\infty}^{\infty}a_l e^{il\varphi}\begin{pmatrix}1\\ \dfrac{-i\alpha' k_z e^{i\varphi}}{\left[E^{(0)}\left(k_z,k+1\right)-E_{\pm}+\Delta'+\dfrac{\alpha'\left(k+1\right)}{\rho}\right]}\end{pmatrix} \tag{7.1.363}$$

Which are the radial parts of the spinor-Eigen functions. The complete forms of the spin or-Eigen-functions are

$$\Psi(\varphi,z)=\begin{pmatrix}\psi^{+}(\varphi,z)\\ \psi^{-}(\varphi,z)\end{pmatrix}=\frac{k_z e^{ik_z z}}{\sqrt{2\pi L_z}}\sum_{l=-\infty}^{\infty}a_l e^{il\varphi}\begin{pmatrix}k_z^{-1}\\ \dfrac{-i\alpha' e^{i\varphi}}{\left[E^{(0)}\left(k_z,k+1\right)-E_{\pm}+\Delta'+\dfrac{\alpha'\left(k+1\right)}{\rho}\right]}\end{pmatrix}$$

(7.1.364)

Now from Eqn. (7.1.345) we have with the replacement, $k\to l$:

$$\left[E(k_z,l-1)-E_{-}+\Delta-\frac{(l-1)}{\rho}\alpha'\right]\left[E\left(k_z,l\right)-E_{+}+\Delta'+\frac{l}{\rho}\alpha'\right]=-\alpha'^2k_z^2 \tag{7.1.365}$$

The condition in Eqn. (7.1.365) is valid provided that l is fixed for some finite value L, say. In light of this sufficiency condition, all summations over $-\infty<l<+\infty$ are obviated and the set of equations, (7.1.363) and (7.1.364), reduce to

$$\begin{pmatrix}\psi^{+}(\varphi)\\ \psi^{-}(\varphi)\end{pmatrix}=\frac{a_L k_z e^{iL\varphi}}{\sqrt{2\pi}}\begin{pmatrix}k_z^{-1}\\ \dfrac{-i\alpha' e^{i\varphi}}{\left[E^{(0)}\left(k_z,L\right)-E_{\pm}+\Delta'+\dfrac{\alpha' L}{\rho}\right]}\end{pmatrix},\left(\rho,L_z\right)\neq 0 \tag{7.1.366}$$

$$\Psi(\varphi,z)=\begin{pmatrix}\psi^{+}(\varphi,z)\\ \psi^{-}(\varphi,z)\end{pmatrix}=\frac{a_L k_z e^{ik_z z}e^{iL\varphi}}{\sqrt{2\pi L_z}}\begin{pmatrix} k_z^{-1} \\ \dfrac{-i\alpha' e^{i\varphi}}{\left[E^{(0)}(k_z,L)-E_{\pm}+\Delta'+\dfrac{\alpha' L}{\rho}\right]}\end{pmatrix}$$

$$=\frac{a_L k_z e^{i(k_z z+L\varphi)}}{\sqrt{2\pi L_z}}\begin{pmatrix} k_z^{-1} \\ \dfrac{-i\alpha' e^{i\varphi}}{\left[E^{(0)}(k_z,L)-E_{\pm}+\Delta'+\dfrac{\alpha' L}{\rho}\right]}\end{pmatrix},(\rho,L_z)\neq 0 \qquad (7.1.367)$$

We can further express the denominators of the second elements,

$$E^{(0)}(k_z,k+1)-E_{\pm}+\Delta'+\frac{\alpha'(k+1)}{\rho} \qquad (7.1.368)$$

in the column matrices from Eqns. (7.1.363) and (7.1.364) in terms of $E^{(1)}$. Indeed, if in Eqn. (7.1.368) we set $l \rightarrow l+1$, we may define

$$E^{(1)}(k_z,l)\equiv E^{(0)}(k_z,k+1)+\frac{\alpha'(k+1)}{\rho}+\Delta' \qquad (7.1.369)$$

Which we then solve for $E^{(0)}(k_z,k+1)$:

$$E^{(0)}(k_z,k+1)=E^{(1)}(k_z,l)-\frac{\alpha'(k+1)}{\rho}-\Delta' \qquad (7.1.370)$$

Back-substituting Eqn. (7.1.369) into expression (7.1.368) yields

$$E^{(1)}(k_z,l)-E_{\pm} \qquad (7.1.371)$$

One may now make the replacement

$$\left(E^{(0)}(k_z,k+1)-E_{\pm}+\Delta'+\frac{\alpha'(k+1)}{\rho}\right)\rightarrow E^{(1)}(k_z,l)-E_{\pm} \qquad (7.1.372)$$

in Eqns. (7.1.363) and (7.1.364). The resulting equations are then subsequently ‘back-substituted’ into Eqns. (7.1.366) and (7.1.367) respectively. Hence

$$\begin{pmatrix} \psi^+(\varphi) \\ \psi^-(\varphi) \end{pmatrix} = \frac{k_z}{\sqrt{2\pi}} \sum_{l=-\infty}^{\infty} a_l e^{il\varphi} \begin{pmatrix} k_z^{-1} \\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}(k_z, l) - E_\pm} \end{pmatrix} \tag{7.1.373}$$

$$\Psi(\varphi, z) = \begin{pmatrix} \psi^+(\varphi, z) \\ \psi^-(\varphi, z) \end{pmatrix} = \frac{k_z e^{ik_z z}}{\sqrt{2\pi L_z}} \sum_{l=-\infty}^{\infty} a_l e^{il\varphi} \begin{pmatrix} k_z^{-1} \\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}(k_z, l) - E_\pm} \end{pmatrix} \tag{7.1.374}$$

Or for finite L:

$$\begin{pmatrix} \psi^+(\varphi) \\ \psi^-(\varphi) \end{pmatrix} = \frac{k_z a_L e^{iL\varphi}}{\sqrt{2\pi}} \begin{pmatrix} k_z^{-1} \\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}(k_z, L) - E_\pm} \end{pmatrix} \tag{7.1.375}$$

$$\Psi(\varphi, z) = \begin{pmatrix} \psi^+(\varphi, z) \\ \psi^-(\varphi, z) \end{pmatrix} = \frac{k_z a_L e^{i(k_z z + L\varphi)}}{\sqrt{2\pi L_z}} \begin{pmatrix} k_z^{-1} \\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}(k_z, l) - E_\pm} \end{pmatrix} \tag{7.1.376}$$

What of the magnetic field? One will notice that in the derivation of Eqn. (7.1.371), terms containing Δ' cancel each other! On one hand, this is expedient as it reinforces the fact that one does not need the presence of magnetic field in order to facilitate electron confinement to the surface of the nanotube. On the other hand, further analysis tells us that when there is a magnetic field, $\vec{B} \neq 0$, the terms containing it vanish depending on the manner in which $E^{(1)}(k_z, l-1)$ and $E^{(2)}(k_z, l-1)$ are defined. Setting the magnetic field equal to zero is a trivial matter for experimentalists and fellow theorists alike. However, having it disappear when finite, and as a consequence of algebra, is intriguing and warrants some clarification. To that end, let us redefine Eqns.(7.1.49) and (7.1.250) as

$$E^{(2)}(k_z, l-1) \equiv E^{(0)}(k_z, l-1) - \frac{(l-1)}{\rho}\alpha' \tag{7.1.377}$$

$$E^{(1)}(k_z, l-1) \equiv E^{(0)}(k_z, l) - \frac{l}{\rho}\alpha' \tag{7.1.378}$$

These two equations are then back-substituted into Eqn.(7.1.348) yielding

$$\left[E^{(2)}(k_z,l-1)-E+\Delta\right]\left[E^{(1)}\left(k_z,l\right)-E+\Delta'\right]-\alpha'^2k_z^2=0 \tag{7.1.379}$$

Now, we once more re-express Eqn. (7.1.368) in terms of Eqn. (7.1.378) but this time with the shifted index, $l \to l+1$:

$$E^{(1)}(k_z,l)\equiv E^{(0)}(k_z,l+1)+\frac{(l+1)}{\rho}\alpha' \tag{7.1.380}$$

Which, when solved for the first summand gives

$$E^{(0)}(k_z,l+1)=E^{(1)}(k_z,l)-\frac{(l+1)}{\rho}\alpha' \tag{7.1.381}$$

'Back-substituting' Eqn. (7.1.381) into expression (7.1.368) one finds that

$$E^{(1)}(k_z,l)-E\pm\Delta' \tag{7.1.382}$$

Take note that Δ' is now preserved.

Thus, in terms of the contribution from the magnetic field, the radial and complete Eigen functions for electrons confined to the lateral surface of a nanotube in the presence of Rashba Spin-Orbit coupling are for

Finite $l=L$:

$$\begin{pmatrix}\psi^+(\varphi)\\ \psi^-(\varphi)\end{pmatrix}=\frac{k_z a_L e^{iL\varphi}}{\sqrt{2\pi}}\begin{pmatrix}k_z^{-1}\\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}\left(k_z,L\right)-E_\pm+\Delta'}\end{pmatrix} \tag{7.1.383}$$

$$\Psi(\varphi,z)=\begin{pmatrix}\psi^+(\varphi,z)\\ \psi^-(\varphi,z)\end{pmatrix}=\frac{k_z a_L e^{i\left(k_z z+L\varphi\right)}}{\sqrt{2\pi L_z}}\begin{pmatrix}k_z^{-1}\\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}\left(k_z,l\right)-E_\pm+\Delta'}\end{pmatrix} \tag{7.1.384}$$

and for $-\infty<l<\infty$:

$$\begin{pmatrix}\psi^+(\varphi)\\ \psi^-(\varphi)\end{pmatrix}=\frac{k_z}{\sqrt{2\pi}}\sum_{l=-\infty}^{\infty}a_l e^{il\varphi}\begin{pmatrix}k_z^{-1}\\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}\left(k_z,l\right)-E_\pm+\Delta'}\end{pmatrix} \tag{7.1.385}$$

$$\Psi(\varphi,z)=\begin{pmatrix}\psi^{+}(\varphi,z)\\ \psi^{-}(\varphi,z)\end{pmatrix}=\frac{k_z e^{ik_z z}}{\sqrt{2\pi L_z}}\sum_{l=-\infty}^{\infty}a_l e^{il\varphi}\begin{pmatrix}k_z^{-1}\\ \dfrac{-i\alpha' e^{i\varphi}}{E^{(1)}(k_z,l)-E_{\pm}+\Delta'}\end{pmatrix} \tag{7.1.386}$$

It is important to note that the energy shift as well as the profile of the Eigen functions will be affected by the presence of the term(s) which carries the magnetic field, $\Delta',\Delta=\Delta'(\omega_c),\Delta(\omega_c)$. We predict that the amplitude of the Eigen functions shall be attenuated (damped) by the presence of a parallel magnetic field.

7.2 Selected limiting values and their impact on the character of the Eigen energies.

Recall that the ground-state Eigen energy assumes, for $\vec{B}=0$, the following form:

$$E^{(0)}(k_z,l)=\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{l}{\rho}\right)^2 \tag{7.2.387}$$

Where, in Eqn. (7.1.333) we took the liberty of making the replacement $k\to l$. Now, in the limit as $\rho\to+\infty$, Eqn. (7.2.387) becomes

$$\underset{\rho\mapsto\infty}{Lim}\left\{E^{(0)}(k_z,l)\right\}=\underset{\rho\mapsto\infty}{lim}\left\{\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\left(\frac{l}{\rho}\right)^2\right\}$$

$$=\underset{\rho\mapsto\infty}{lim}\left\{\frac{\hbar^2}{2m^*}k_z^2\right\}+\underset{\rho\mapsto\infty}{lim}\left\{\frac{\hbar^2}{2m^*}\left(\frac{l}{\rho}\right)^2\right\}$$

$$E^{(0)}(k_z,l)=\frac{\hbar^2}{2m^*}k_z^2+\frac{\hbar^2}{2m^*}\underset{\rho\mapsto\infty}{lim}\left\{\left(\frac{l}{\rho}\right)^2\right\} \tag{7.2.388}$$

Furthermore, as $\rho\to+\infty$ the ratio in the second summand, $\dfrac{l}{\rho}$ becomes continuous.

Let us call this pseudo-continuous function k_l, say. Hence,

$$\lim_{\rho \mapsto \infty} \left\{ \left(\frac{l}{\rho} \right)^2 \right\} = k_l^2 \tag{7.2.389}$$

Back-substituting Eqn. (7.2.389) into Eqn. (7.2.388) yields

$$E^{(0)}(k_z, l) = \frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} k_l^2 \tag{7.2.290}$$

Where k_l may now be regarded as the magnitude of the wave vector $\vec{k}_l$ in the plane.

By similar arguments, one also finds that for

$$\begin{aligned}
\underset{\rho \mapsto \infty}{Lim} \left\{ E^{(0)}(k_z, l-1) \right\} &= \lim_{\rho \mapsto \infty} \left\{ \frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left(\frac{l-1}{\rho} \right)^2 \right\} \\
&= \lim_{\rho \mapsto \infty} \left\{ \frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left\{ \left(\frac{l}{\rho} \right)^2 - 2 \frac{l}{\rho} \cdot \frac{1}{\rho} + \frac{1}{\rho^2} \right\} \right\} \\
&= \lim_{\rho \mapsto \infty} \left\{ \frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} \left\{ \lim_{\rho \mapsto \infty} \left(\frac{l}{\rho} \right)^2 - 2 \lim_{\rho \mapsto \infty} \frac{l}{\rho} \cdot \frac{1}{\rho} + \lim_{\rho \mapsto \infty} \frac{1}{\rho^2} \right\} \right\} \\
&= \frac{\hbar^2}{2m^*} k_z^2 + \frac{\hbar^2}{2m^*} k_l^2 \\
&= \frac{\hbar^2}{2m^*} \left\{ k_z^2 + k_l^2 \right\}
\end{aligned} \tag{7.2.391}$$

Chapter 8

Numerical Results & Conclusions.

In Fig. 1, we plot the plasmon dispersion relations for a pair of nanotubes $(N=2)$ with $L=0$. The electron effective mass is $m^*=0.25m_e$, where m_e is the free-electron mass, $\varepsilon_F=0.6$ eV for both tubules, the background dielectric constant $\varepsilon_b=2.4$, the radius of the inner tubule is $10.0\,\mathring{A}$ while the radius of the outer tubule is $20.0\,\mathring{A}$. The plasmon modes on the coaxial tubules are coupled by the Coulomb interaction. The modes are acoustic plasmons and were obtained at T=0 K. On the same graph we plot the phase velocity straight lines $\omega=vq_z$ for different values of the charged particle velocity v. Whenever one of these straight lines crosses one of the plasmon branches, or it comes through the particle-hole continuum shown in Fig. 2, we have transfer of energy between the charged particle and the electron gas on the tubules according to Eqn. (16). The plasmon modes lie in the pockets of the single-particle excitations which are responsible for Landau damping.

In Figs. 3 and 4, we plot the energy transfer due to plasmon excitations and single-particle excitations for the same material parameters used in the calculations for the pair of coaxial tubules in Figs. 1 and 2. The charged particle is an electron. Several values of the impact parameter, ρ_0, were chosen. Our calculations showed that the height and shape of each curve depend on the impact parameter. In the energy transfer plots for the single-particle excitations, there are only peaks. However, for the plasmons, the plot in Fig. 3 has both a peak and a dip. The locations of the peaks and dips are unchanged as ρ_0 is varied. They occur over the same range of $\frac{v}{v_F}$. This is particularly evident in the dip around $\frac{v}{v_F} = 1.45$. Since we interpret positive values of $\frac{dW}{dt}$ to indicate energy transferred from the moving charged particle to the electron gas, negative values of $\frac{dW}{dt}$ represent the flow of energy from the plasma to the charged particle. Therefore the negative peak for $v = 1.45 v_F$ indicates that our electron gas becomes unstable [48]. From Fig. 1 we see that the plasmon branch responsible for this instability is the second from the top most energetic plasmon. A possible explanation for this instability is that in the long wavelength limit the group velocity of this plasmon branch is constant and equals to $1.45 v_F$ for a wide range of q_z. Our calculations show that there is no plasmon instability arising for a single-walled nanotube when a current of charged particles is used to excite the modes. We conclude that the three-dimensional nature of the Coulomb interaction between tubules facilitates this instability.

In Fig. 5, we plot the plasmon contribution to the absorption coefficient when $L = 0$ and $q_z = 0.15 k_F$ as a function of the incident photon energy. The radius of the inner tubule is $R_1 = 10.0\,\mathring{A}$ and several radii R_2 were chosen for the outer tubule for a pair of coaxial tubules. The parameters used in our numerical calculations for the electron effective mass, the Fermi energy and the background dielectric constant were the same as Fig. 1 [14]. Figure 5 shows that the number of peaks depends on the ratio, $R_2 : R_1$. The intensity (oscillator strength) of each peak depends on the plasmon energy. Consistently, the highest peak has the largest oscillator strength [14]. Some of the less energetic plasmon modes have such weak coupling to the external electric field that they are not visible on the scale we used in Fig. 5. The energies of the two highest plasmon branches increase with R_2. On the other hand, the lowest modes decrease in energy as the radius of the outer tubule is increased. Because of the subband structure in Eqn. (13), more energy Eigen values can be occupied for a chosen Fermi energy as the tubule radius is made larger. This means that as R_2 is increased, there are more plasmon branches appearing. In Fig. 6, we plot the contribution to the absorption coefficient from the $L = 0$ (intra-band transitions) particle-hole modes when $q_z = 0.15k_F$ for the pair of coaxial tubules in Figs. 1 and 2. Since the imaginary part of $D_{L=0}$ is zero in the pockets where the undamped plasmon modes exist, this explains why there gaps in Fig. 6 along the frequency axis. Unlike the plasmon contribution in Fig. 5, the particle-hole modes contribute over a wider range of frequency. The plasmon excitations occur within pockets between the particle-hole modes where they are Landau damped [14]. Numerical results for plasma excitations between subbands for which $L \in \mathbb{Z}_+$ may also be obtained from our formula for the absorption coefficient as well as the energy loss induced by a current of charged particles.

In its current form, the dispersion formula, Eqn. (3.4.96) represents an infinite one-dimensional array of concentric nanotubes. However, for ease of computation we reduced the concentricity of tubules to one while maintaining the dimension of the array by setting $i = i' = 1$ in Eqn. (3.4.96). Consequently, we were able to generate the excitation spectra depicted in Figs. 9 and 10 for distinct values of angular momentum transfer, *m.* One will notice in the figures that the rationalized energy vs. momentum characteristic profiles are markedly dissimilar. The reason is that as *m,* increases the radicand of the Fermi momentum, $k_F(l)$ in Eqn. (2.1.17b) gets smaller and will eventually tend toward negative values when $\frac{2m^*\varepsilon_F}{\hbar^2} < \frac{l^2}{R^2}$. This produces the rather pronounced piecewise defined profile that appears in Fig. 10.

In Fig. 14, the peak positions of the Plasmon excitation energies for a pair of coaxial tubules are drawn as a function of $\frac{R_2}{R_1}$ for fixed $R_1 = 10\,\mathring{A}$. The parameters used in our calculations were for the electron effective mass $m^* = 0.25m_e$, where m_e is the free-electron mass, $\varepsilon_F = 0.6$ eV for both tubules, the background dielectric constant $.\varepsilon_b = 2.4$. We plotted the peak positions of the plasmon excitations, since the less energetic plasmon modes have such weak coupling to an external electric field that they are not at times easily observed as in a previous scaled plot. Due to the coupled modes on the two tubules are split by the Coulomb interaction. The energies of the two highest plasmon branches increase with R_2. On the contrary, the lowest modes decrease in energy as the radius of the outer tubule is increased. In light of the subband structure, more Eigen energies can be occupied for a chosen Fermi energy as we increase the radius of the tubule. This accounts for the emergence of more plasmon branches as we increase R_2 in Fig. 14. However, the two highest acoustic Plasmon branches exist throughout the range of plots which were obtained at $T = 0^\circ K$.

In this paper, we presented formalisms for calculating the rate of transfer of energy from a current of charged particles and the light absorption coefficient for a pair of coaxial tubules. The calculations were carried out using a self-consistent field theory for the induced potential and density fluctuations on the tubules. Our results are given in terms of the electron-electron interaction on each tubule and between the two tubules. The effective dielectric function $D_L(R_1, R_2; q_z; \omega)$ for the pair of tubules is expressed in terms of the dielectric functions $\varepsilon_L^{(1)}(q_z;\omega)$ and $\varepsilon_L^{(2)}(q_z;\omega)$ for each tubule, as shown in Eqn. (40). The electron gas model for each tubule was used to simplify the calculations. However, a more realistic model whose energy bands are obtained using a tight-binding approximation, for example, would be incorporated through the susceptibility $\chi_L^{(1)}(q_{z,}\omega)$ and $\chi_L^{(2)}(q_{z,}\omega)$ for each tubule. We showed that the loss function $\Im m\left\{D_L^{-1}(R_1,R_2;q_z;\omega)\right\}$ can be separated into contributions due to plasmon excitations and particle-hole modes. Figures 2 and 6 show that there are pockets within the particle-hole continuum where there is no Landau damping of the collective plasmon excitations. These regions could only be determined by separating the contributions to the loss function from the plasmon and single-particle excitations, as we described above. This separation would allow direct comparison between theory and experimental results of the absorption spectrum for plasma excitations on nanotubes.

Our calculations show that there is a crucial difference between the spectra for light absorption and the energy transfer from a beam of charged particles for a pair of coaxial tubules. In both loss functions, the single-particle excitation spectrum contains peaks, indicating that the energy absorbed from the perturbing source is used to excite the particle-hole modes. The peaks in either spectrum could be used to identify the energy range for the excitation spectrum. The plasmon spectrum for light absorption show only peaks corresponding to the collective mode excitation. However, some of the plasmon modes excited by a charge current become unstable and give up their energy after being excited. This phenomenon is displayed by the dips, as shown in Fig. 3 [15, 16, 17]. This plasmon instability is not observed in the energy loss spectrum for a single-walled nanotube. Therefore, the plasmon instability depends on the type of perturbation employed as well as the number of tubules making up the nanotube.

Ofttimes, the experimentalist would use a magnetic field to control the spin of an electron, our results suggests that this type of magnetic field reliance can be obviated by the Rashba effect. Indeed, our calculations show that this type of 'spin-switching' can be achieved by utilizing the intrinsic electric field brought about by taking the gradient of the average potential.

List of Figures (Plots)

Figure 5: The $L=0$ plasmon contribution to the absorption coefficient (arbitrary units) versus photon energy for $q_z = 0.15k_F$, where $k_F = \sqrt{\frac{2m^*\varepsilon_F}{\hbar^2}}$ with the radius of the inner tubule being $R_1 = 10.0\,\mathring{A}$ and several values of R_2. For clarity, the curves are shifted. From below, the curves correspond to $R_2 = 20.0, 30.0$ and $40.0\,\mathring{A}$. The parameters used in the calculation are given in the text for m^*, ε_F and ε_b.

Figure 6: The $L=0$ particle-hole mode contribution to the absorption coefficient (arbitrary units) versus photon energy for $q_z = 0.15k_F$. The radius of the inner tubule is $R_1 = 10.0\,\mathring{A}$ and $R_2 = 20.0\,\mathring{A}$ is the radius of the outer tubule. Only the frequency range where there are particle-hole modes contributes to the absorption. The gaps on the frequency axis correspond to pockets where plasmon excitations are not Landau damped. The parameters used in the calculation for m^*, ε_F and ε_b are the same as Fig. 1.

Figure 7: Intraband (m = 0) Plasmon spectrum for one-dimensional array of single-walled nanotubes. The Plasmon excitation energies, in units of Fermi energy, ε_F as a function of q_z, in units of Fermi wave vector number k_F in the ground (l = 0) subband, were obtained by solving Eqn. (4.5.174) at $q_x = 0$ for $i = i'$.

Figure 8: Intraband (m = 2,-2) Plasmon spectrum for one-dimensional array of single-walled nanotubes. The Plasmon excitation energies, in units of Fermi energy, ε_F as a function of q_z, in units of Fermi wave vector number k_F in the ground (l = 0)

subband, were obtained by solving Eqn. (4.5.174) at $q_x = 0$ for $i = i'$.

Figure 9: Excitation spectrum for a single-walled nanotube with $L = 0$ and $R = 10\,\mathring{A}$

Figure 10: Excitation spectrum for a double-walled nanotube with $L = 0$ and radii $R_1 = 10\,\mathring{A}$ and $R_2 = 2R_1\,\mathring{A}$, respectively.

Figure 11: The total density of states $\upsilon(E) = \upsilon_+(E) + \upsilon_-(E)$ as a function of energy E of a single-walled nanotube of radius $R = 11.0\,\mathring{A}$. Here, $\alpha = 0.001 meV\,\mathring{A}$, $m^* = 0.25 m_e$, where m_e is the free-electron mass.

Figure 12: The Plasmon dispersion of the excitation energy as a function of the wave number $\frac{q_z}{k_F}$ (in units of $k_F = \sqrt{\frac{2m\varepsilon_F}{\hbar^2}}$) along the axis of the nanotube. We chose the Fermi energy, $E_F = 0.6eV$ the electron effective mass $m^* = 0.25 m_e$, where m_e is the free electron mass and the background dielectric constant $\varepsilon_b = 2.4$. Here, $\alpha = 0.0001 meV\,\mathring{A}$. The third branch from above is the intra $(L = 0)$ -SO Plasmon. The inter-SO Plasmon branches are those above the intra-SO Plasmon.

Figure 13: The Plasmon dispersion of the excitation energy as a function of the wave number $\frac{q_z}{k_F}$ (in units of $k_F = \sqrt{\frac{2m\varepsilon_F}{\hbar^2}}$) along the axis of the nanotube. We chose the Fermi energy, $E_F = 0.6eV$ the electron effective mass

$m^* = 0.25m_e$, where m_e is the free electron mass and the background dielectric constant $\varepsilon_b = 2.4$. Here, $\alpha = 0.0001 meV\,\mathring{A}$. The branch labeled Ω_0 by is the intra-SO Plasmon. The inter-SO Plasmon branches are denoted by Ω_- and Ω_+

Figure 14: Dimensionless energy versus radial aspect ratio.

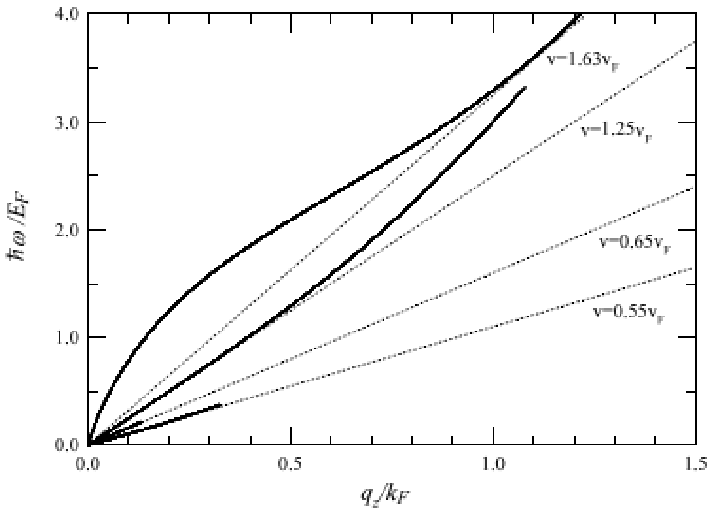

4.0
3.0
2.0
1.0
0.0
$\hbar\omega/E_F$
0.0
0.5
1.0
1.5
q_z/k_F
v=1.63v$_F$
v=1.25v$_F$
v=0.65v$_F$
v=0.55v$_F$

Fig. 1

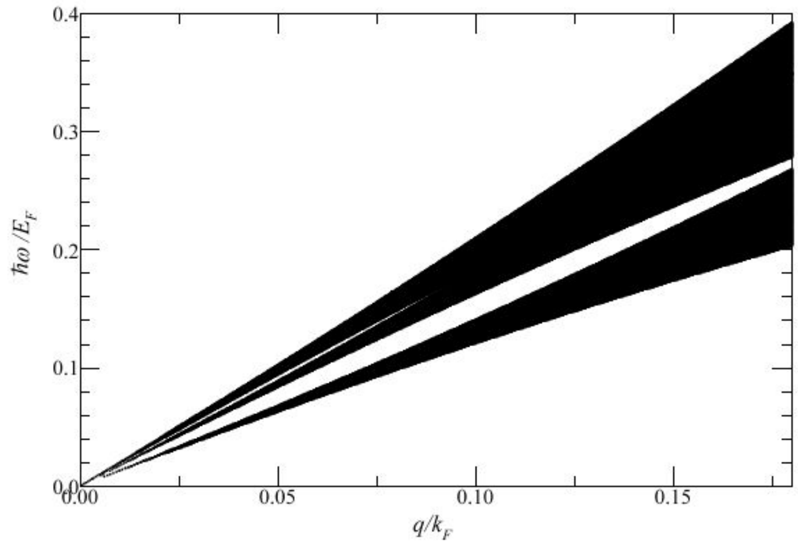


Fig. 2

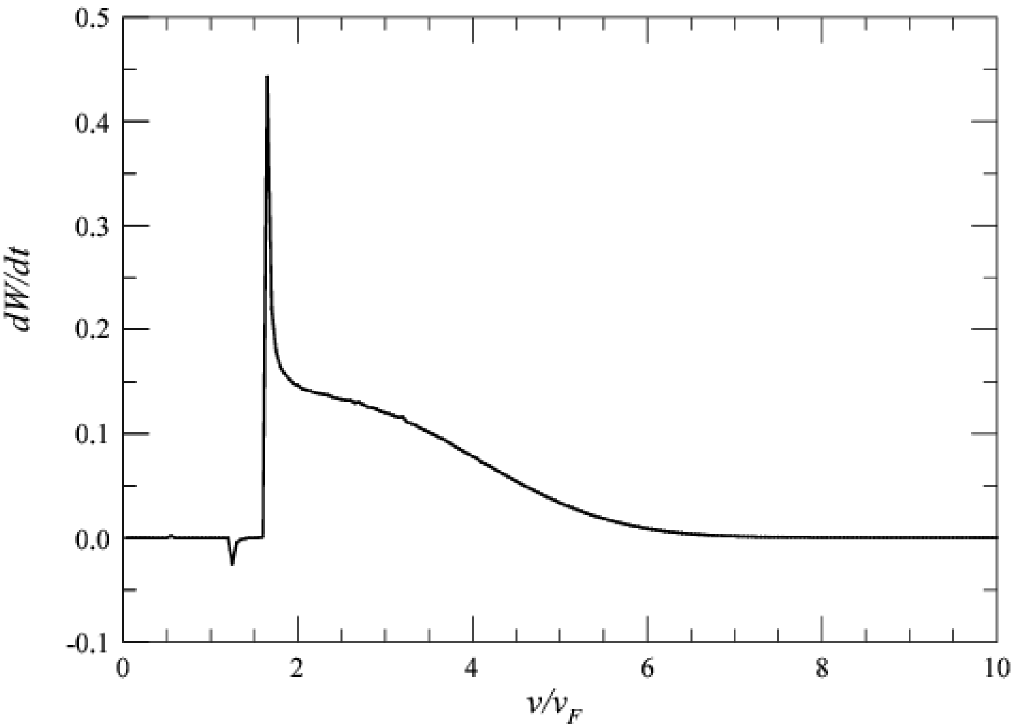


Fig.3

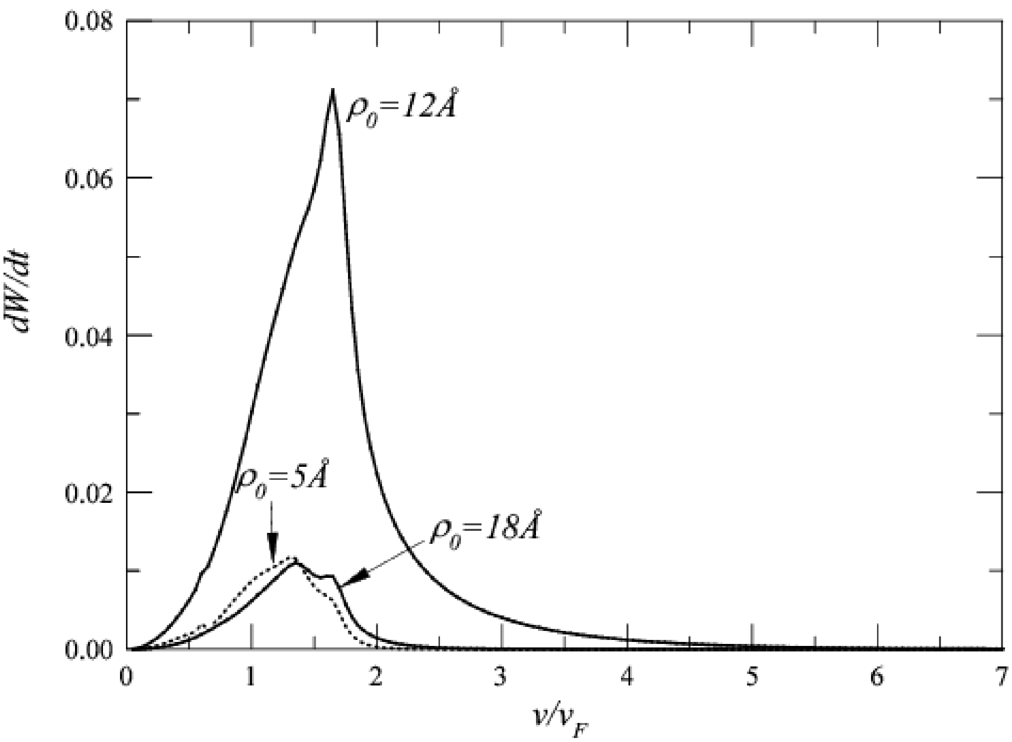

0.08
0.06
0.04
0.02
0.00
dW/dt
ρ_0=12Å
ρ_0=5Å
ρ_0=18Å
0
1
2
3
4
5
6
7
v/v$_F$

Fig.4

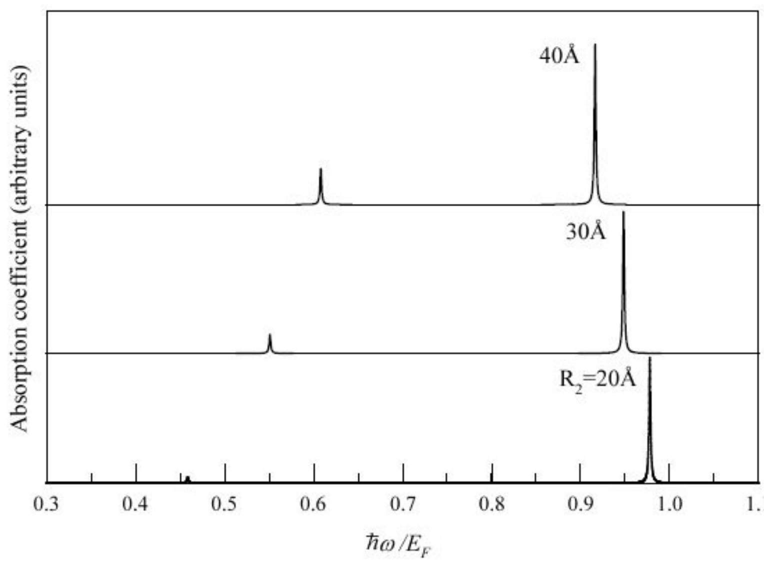
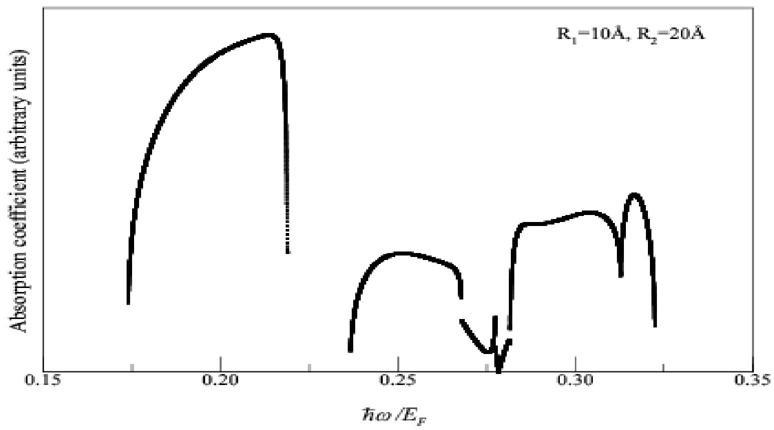

40Å
30Å
R_2=20Å
Absorption coefficient (arbitrary units)
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
$\hbar\omega/E_F$

Fig. 5



R_1=10Å, R_2=20Å
Absorption coefficient (arbitrary units)
0.15
0.20
0.25
0.30
0.35
$\hbar\omega/E_F$

Fig. 6

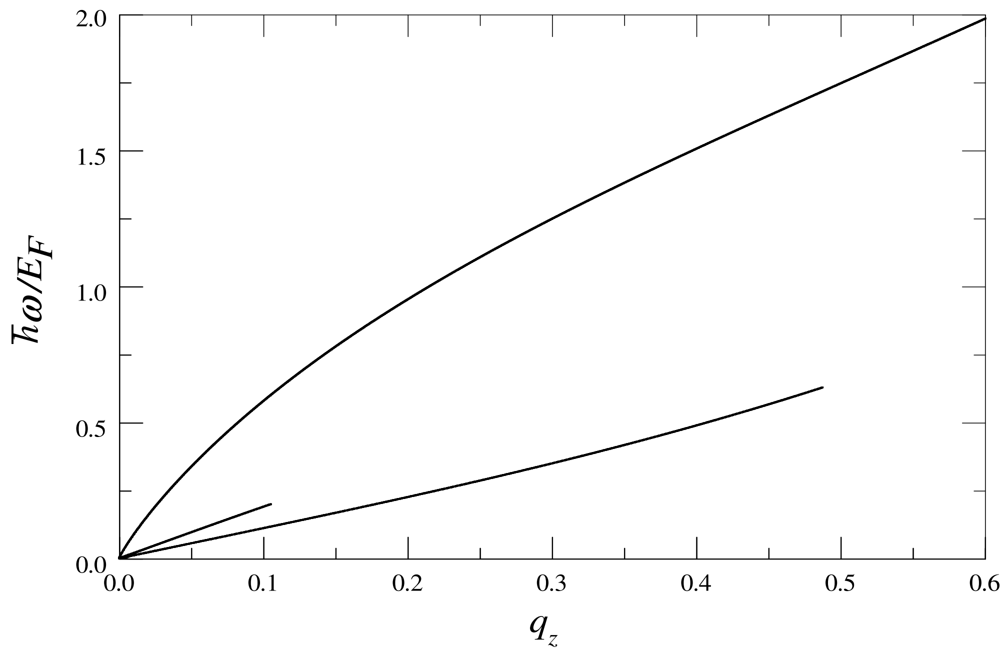


Fig. 7

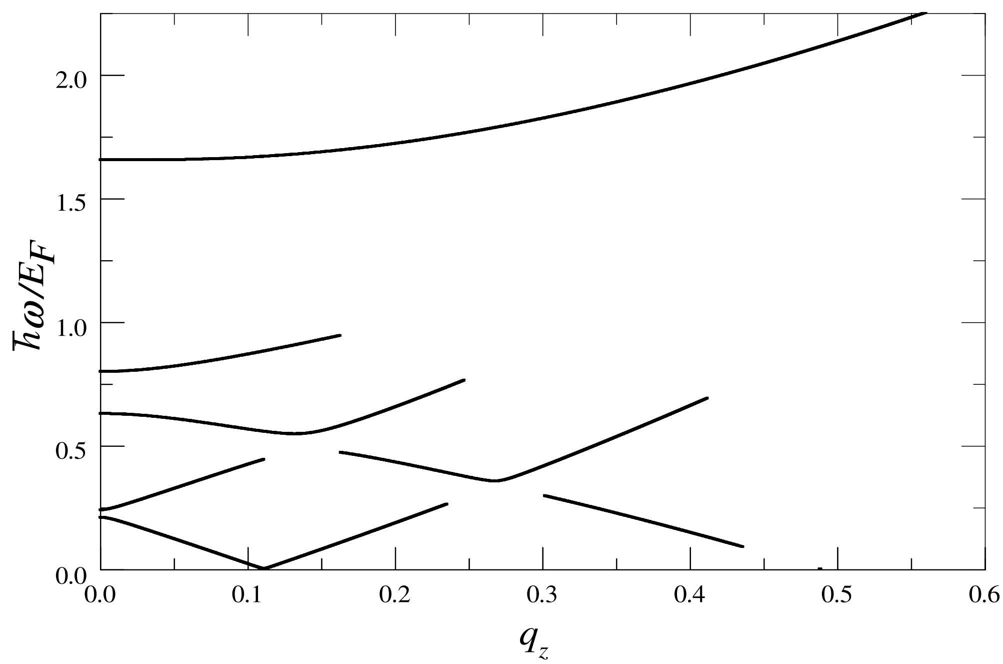


Fig. 8

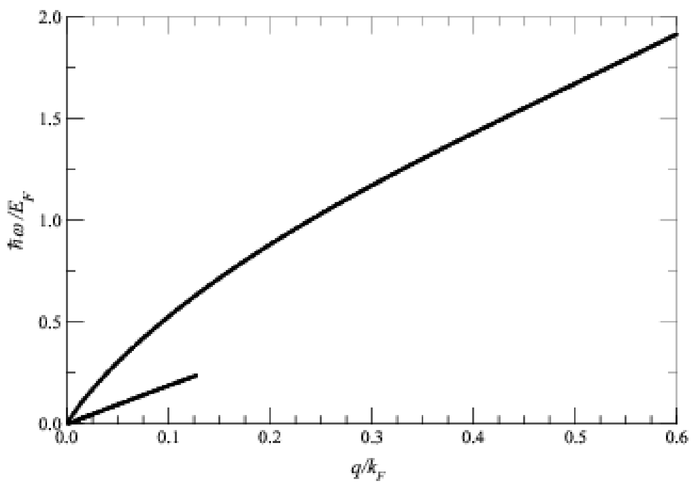


Fig. 9

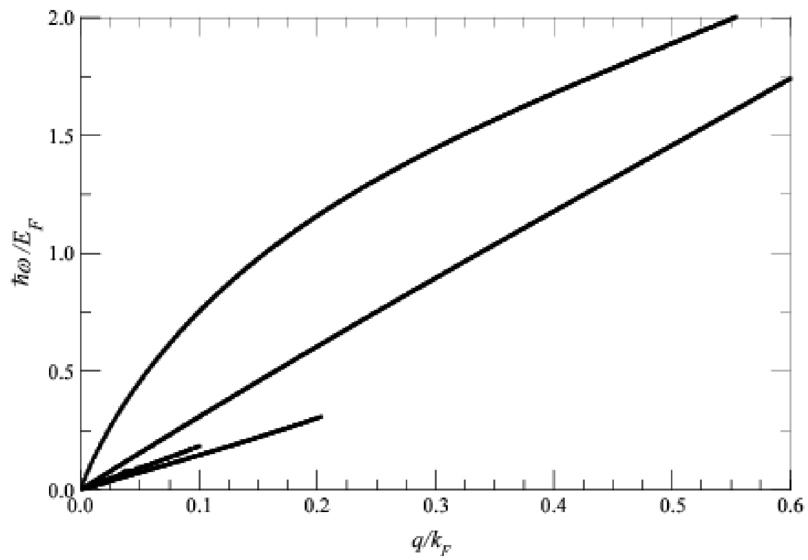


Fig.10

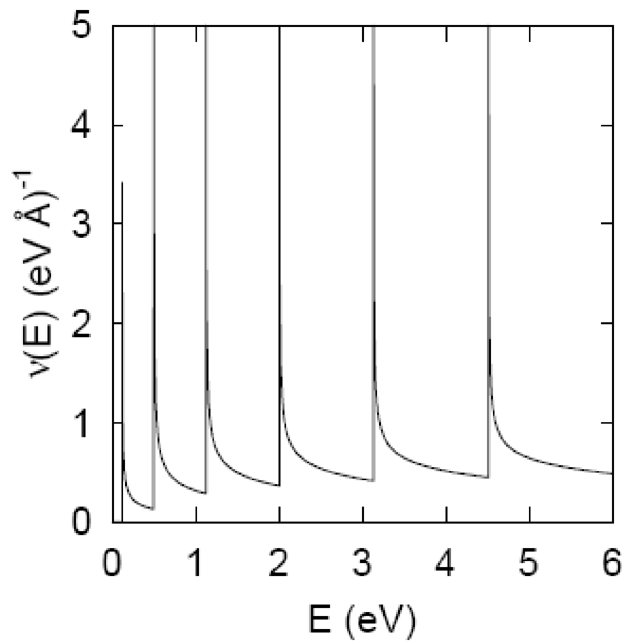


Fig. 11

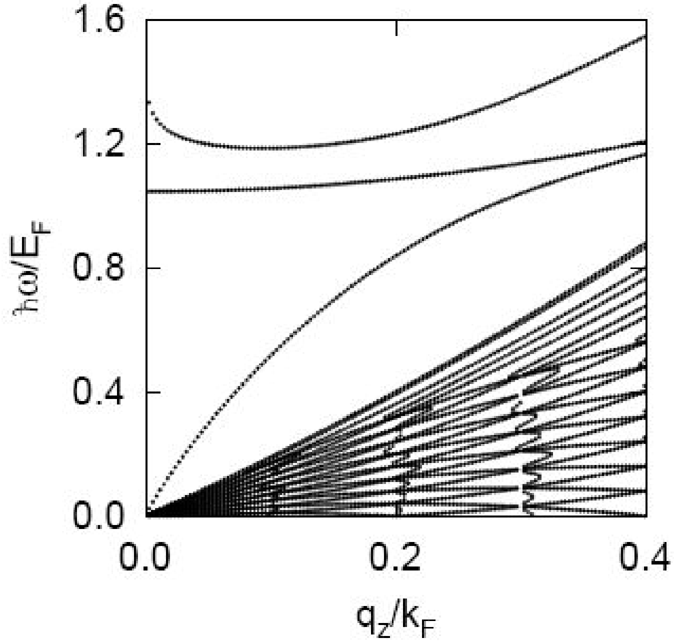


Fig.12

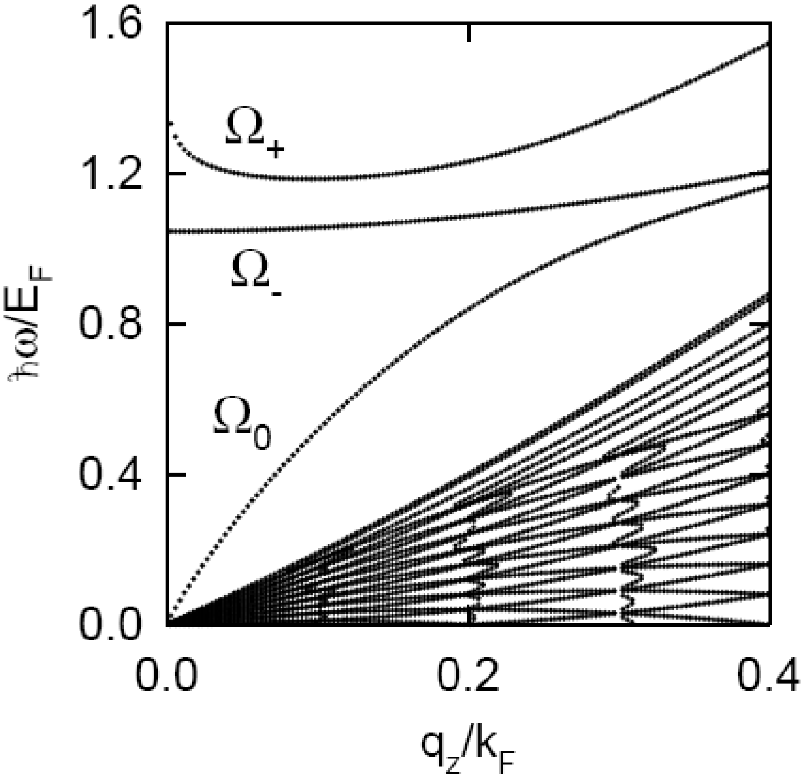


Fig. 13

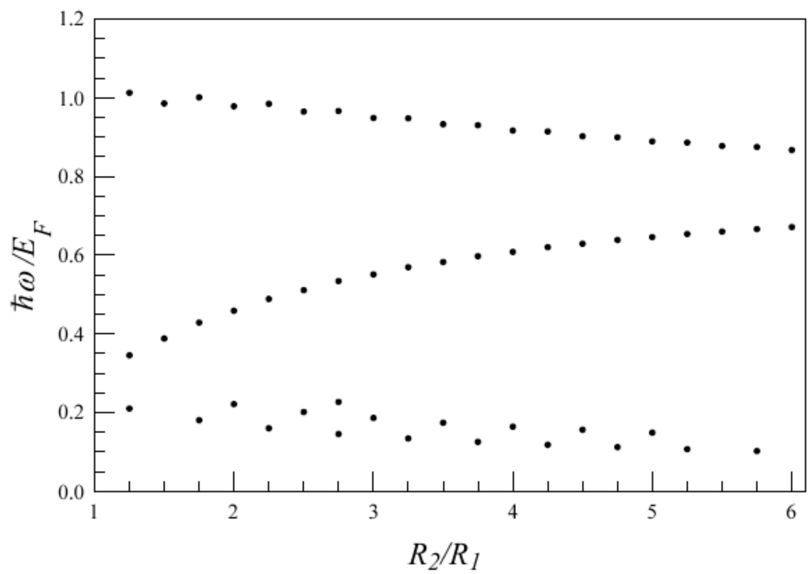


Fig. 14

```
c    SOLVING THE DISPERSION EQUATION FOR ONE NANOTUBE
c    ------------------------------------------------

     PROGRAM SDISPERSION1  ! Simple method,solve for plasmons.The tube is
                  ! embeded in a background of epsilon=2.4 (Lin's model)
     IMPLICIT NONE
        REAL(KIND=8),PARAMETER::kf0=0.198419D10,r=11.D-10
     INTEGER::m,l           ! Angular momentum transfer
        COMPLEX(KIND=8)::epsilo  ! Nanotube's dielectric function
     REAL(KIND=8)::q,wmin,wmax,w1,w2,wm,f1,f2,dq,dw,qmax,b
        INTEGER::nq          ! Number of steps for q
     INTEGER::nw          ! Number of steps for w
        REAL(KIND=8),DIMENSION(-2:2)::kf ! Fermi wavenumber of the l-th
subband
     WRITE(*,*)'Enter the angular momentum transfer m : '
        READ(*,*)m
     WRITE(*,*)'Enter numbers of steps nq and nw for q and w: '
        READ(*,*)nq,nw

        b=r*kf0
        qmax=0.6D0          ! Max value for q, wavelength
     dq=qmax/nq          ! Step size for q
     wmax=2.5D0          ! Max value for w, angular frequency
     dw=wmax/nw          ! Step size for w

        DO l=-2,2
        kf(l)=DSQRT(1.D0-(l/b)**2)
        END DO

        q=dq              ! Starting value for q ,it can not be 0 because of divergence
5    w1=dw              ! Starting value for w

c    START SEARCHING FOR THE 0'S OF THE DISPERSION EQUATION

     f1=DREAL(epsilo(m,kf,q,w1))
10   w2=w1+dw
     IF(w2>wmax) GO TO 20
     f2=DREAL(epsilo(m,kf,q,w2))

     IF(f1*f2<=0.D0) THEN
     wm=(w1+w2)/2.D0    ! This is a plasmon mode
     IF(DIMAG(epsilo(m,kf,q,wm))==0.D0) WRITE(28,*)q,wm
        END IF

15   w1=w2
        f1=f2
     GO TO 10

20   q=q+dq
     IF(q>qmax)GO TO 30
```

```
    GO TO 5

30  CONTINUE
    END PROGRAM


    COMPLEX(KIND=8) FUNCTION epsilo(m,kf,q,w) ! Define the dielectric
function
    USE NUMERICAL_LIBRARIES
    IMPLICIT NONE
        INTEGER,INTENT(IN)::m
        INTEGER::l,n,nl
    REAL(KIND=8),DIMENSION(-2:2)::kf
    REAL(KIND=8)::eminus,eplus,sum,b,pi
    REAL(KIND=8),PARAMETER::c=0.631573D0
!c=2*effectivemass*e^2/pi*epsilons*hbar^2*kf
        REAL(KIND=8),PARAMETER::kf0=0.198419D10,r=11.D-10
    REAL(KIND=8),INTENT(IN)::q,w
    REAL(KIND=8)::epsilon1,epsilon2,DBSI(m+1),DBSK(m+1)

    pi=4.D0*DATAN(1.D0)
    b=r*kf0
    sum=0.D0
        n=0

    DO l=-2,2
        eplus=(q**2+2.D0*q*kf(l))+(m**2+2.D0*m*l)/(b**2)
    eminus=(q**2-2.D0*q*kf(l))+(m**2+2.D0*m*l)/(b**2)

    sum=sum+DLOG(DABS((w**2-eplus**2)/(w**2-eminus**2)))

    IF((DABS(eminus)<w).AND.(w<DABS(eplus))) THEN
    nl=1
    ELSE IF((DABS(eplus)<w).AND.(w<DABS(eminus))) THEN
    nl=-1
    ELSE
    nl=0
    END IF
    n=n+nl
    END DO

        CALL DBSKS(0.D0,q*b,m+1,DBSK) ! gives the mth order modified Bessel
function of 3nd kind
    CALL DBSINS(q*b,m+1,DBSI) ! gives the mth order modified Bessel function
of 1st kind

    epsilon1=1.D0+(c/q)*DBSI(m+1)*DBSK(m+1)*sum ! real part of dielectric
function
    epsilon2=(c*pi/q)*DBSI(m+1)*DBSK(m+1)*n  ! imaginary part of dielectric
function
```

```
    epsilo=DCMPLX(epsilon1,epsilon2)

END FUNCTION
```

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