ELECTRICAL CONDUCTIVITY IN THIN FILMS

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This thesis deals with electrical conductivity in thin films. Classical and quantum size effects in conductivity are discussed including some experimental evidence of quantum size effects. The component conductivity along the applied electric field of a thin film in a transverse magnetic field is developed in a density matrix method.

Classical size effects are discussed for the cases of random and partially specular surface scattering. Fuchs' expression for the conductivity of a thin film with random scattering, Sondheimer's form of Fuchs' results for partially specular scattering, and Cottey's approximation for almost wholly specular scattering are discussed. Appropriate approximations to the cases of random and partially specular scattering are given. Two cases of the conductivity of films in magnetic fields are discussed, i.e. the case of a magnetic fields transverse to the film and the case of the magnetic field parallel to the applied electric field.

Sandomirskii's theory for quantum size effects in semimetal films is briefly reviewed. This theory predicts an oscillatory nature for the conductivity with a constant period on the order of half of the electron de Broglie wavelength in certain cases. The number density of charge carriers is also oscillatory.

The experiments by Orgen et al, Garcia, and Duggal and

Rup dealing with quantum size effects in thin bismuth films are reviewed. These experiments showed oscillatory electrical properties for films in and out of magnetic fields. The experiments of Komnik and Bukshtab dealing with quantum size effects in metal films are discussed. These showed oscillations with a very short period (7 to 8 A in tin and 28 A in antimony).

The componet of electrical current density along the direction of the applied electric field in a thin film in a transverse magnetic field is developed through a density matrix method reviewed by Kahn and Frederiske. The film surfaces are treated as an infinite square well. The free electron model is used. Wave functions and energy levels are calculated along with appropriate matrix elements of a velocity component. The density matrix method is shown and modified to apply to the thin film current density component. Scattering is approximated as δ-function potentials. This is averaged spacially.

Through these considerations an expression for the current density component is developed. This expression is non-ohmic. It goes to zero as either the electric field or the thickness goes to zero. It may be oscillatory. A method for extension of this development to the case of semimetals and semiconductors is mentioned. Further areas of investigation are suggested. These include more experimental investigation, other surface potentials, and specularity

ELECTRICAL CONDUCTIVITY IN THIN FILMS

THESIS

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By

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CHAPTER I

CLASSICAL AND QUANTUM SIZE EFFECTS IN THIN FILMS

Introduction

This thesis deals with quantum size effects in thin films. The major purpose of the thesis is a non-relaxation time, quantum mechanical development of the current density of a thin film in the direction of the electric field, while the film is in a transverse magnetic field. The thesis also contains introductory material concerning classical size effects, Sandomirskii's relaxation time development of quantum size effects in thin films, and a summary of several experiments concerning quantum size effects in thin films.

For this purpose there is an introductory chapter containing the material on the classical size effects, the relaxation time development of quantum size effects, and the experimental material concerning quantum size effects. There then follows a chapter for the theoretical development of the quantum size effects of the current density component.

Classical Size Effects

It is well known that in large bulk samples of materials, the conductivity is not a function of the dimensions of the sample. However, if the size of the sample is restricted in any direction, size effects begin to appear. This was first

noticed in thin plates during 1898 by J. J. Thompson[1], who suggested that this effect was due to restriction of the mean free path of charge carriers. Both Thompson and A. B. C. Lovell[2] did classical calculations of this effect. In both of these calculations statistical velocity distributions for the electrons envolved were ignored. And Thompson's calculation also did not include electrons starting from the surfaces of the plate, Fuchs[3,4] derived the form

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{4}\left[K - \frac{K^3}{12}\right] E_i(-K) - \frac{3}{8K}\left[1 - e^{-K}\right] \tag{1}$$

$$- \left[\frac{5}{8} + \frac{K}{16} - \frac{K^2}{16}\right] e^{-K}$$

where $$E_i(u) = -\int_u^\infty t^{-1} e^{-t}\, dt .$$

And where σ is the conductivity of the film along the direction of theelectric field, and where σ_0 is the bulk conductivity of the material. This equation is deriver under the assumption of a spherical Fermi surface, random surface scattering, an isotropic mean free path, and the Boltzman transport equation. The quantity K is the ratio of the film thickness to the mean free path of the electrons. Approximations to Fuchs' equation are

$$\frac{\sigma}{\sigma_0} = \frac{3K}{4}\left[\ln\left(\frac{1}{K}\right) + 0.423\right] \quad \text{for } K << 1 \tag{2}$$

and

$$\frac{\sigma}{\sigma_0} \simeq 1 - \frac{3}{8K} \qquad \text{for } K >> 1 . \quad (3)$$

Also for a larger range of K, the equation

$$\frac{\rho}{\rho_0} = \frac{\sigma_0}{\sigma} \simeq 1 + \frac{3}{8K} \qquad \text{for } K \gtrsim 1 . \quad (4)$$

is a better approximation to the inverse of Fuchs' equation (equation (1)), than is the inverse of equation (3). Thus for numerical calculations of the resistivity ρ or its reciprocal the conductivity σ, equation (4) is superior to equation (3) for film thicknesses of the order of the conduction electron mean free path.

Fuchs also developed an expression for the conductivity of a film with partially specular scattering at the surfaces of the film. This development requires a specularity parameter P, which is the fraction of electrons incident upon a surface which are scattered in a specular manner. The remaining electrons are assumed to be scattered randomly. When both surfaces have the same specularity parameter, E. H. Sondheimer expressed Fuchs' result as either[5]

$$\left(\frac{\sigma}{\sigma_0}\right)_{K,P} = 1 - \frac{3}{2K}(1-P)\int_1^\infty \left(\frac{1}{t^3} - \frac{1}{t^5}\right) \frac{1 - e^{-Kt}}{1 - P e^{-Kt}} dt \quad (5)$$

or in another interesting form

$$\left(\frac{\sigma}{\sigma_0}\right)_{K,P} = (1-P)^2 \sum_{n=1}^{\infty} n P^{n-1} \left(\frac{\sigma}{\sigma_0}\right)_{nK,P=0}. \qquad (6)$$

The quantity $\left(\frac{\sigma}{\sigma_0}\right)_{nK,P=0}$ is the same as equation (1) with nK substituted for K. Useful expressions for numerical work are

$$\frac{\rho}{\rho_0} = \frac{\sigma_0}{\sigma} = 1 + \frac{3}{8K}(1-P) \qquad \text{for } K >> 1 \qquad (7)$$

and for very thin films

$$\frac{\rho}{\rho_0} = \frac{\sigma_0}{\sigma} = \frac{4}{3}\left[\frac{1-P}{1+P}\right]\frac{1}{K \ln\left(\frac{1}{K}\right)} \qquad \text{for } K << 1. \qquad (8)$$

A. A. Cottey[6] also developed an approximate closed expression for equations (5) or (6) using a periodic boundry condition on the mean free path. This expression is

$$\left(\frac{\sigma}{\sigma_0}\right)_{\mu} = \frac{3\mu}{2}\left[\mu - \frac{1}{2} + (1-\mu^2)\ln\left(1+\frac{1}{\mu}\right)\right] \qquad (9)$$

where $$\mu = K/(1-P).$$

This expression is good in the region of $P=1$ and has a closed form.

It should be noted that both surfaces of a film need not have the same specularity parameter. Cottey derives an expression for this case using his technique. Also H. J. Juretschke[7] derives expressions for the thick and thin

limits using the Fuchs-Sondheimer technique. Juretschke also puts limits on an effective specularity parameter for this case which he claims works well for the thick limit.

There are three cases of films in magnetic fields in the classical study viz. 1) the magnetic field parallel to the current density, 2) the magnetic field perpendicular to the current density and parallel to the plane of the film, and 3) the magnetic field perpendicular to the current density and perpendicular to the plane of the film. Sondheimer[8] discussed the latter case. He found theoretically that

$$\frac{\rho_0}{\rho} = \frac{Re\,\phi(S)}{K} \tag{10}$$

where $S = K + i\beta$ and

$$\frac{1}{\phi(S)} = \frac{1}{S} - \frac{3}{8S^2} + \frac{3}{2S^2}\int_1^\infty \left(\frac{1}{t^3} - \frac{1}{t^5}\right) e^{-St}\,dt. \tag{11}$$

This is just an integral expression of equation (1) divided by K and with K replaced by S. The quantity β is related to the magnetic field H and the film thickness a by

$$\beta = \frac{a}{r} = \frac{a e H}{m \bar{v} c} \tag{12}$$

where $\bar{v}$ is the mean velocity of a conduction electron. Also for partially specular surface scattering

$$\left(\frac{\sigma_0}{\sigma}\right)_{K,P} = \frac{Re\,\phi_P(S)}{K} \qquad (13)$$

where

$$\frac{1}{\phi_P(S)} = \frac{1}{S} - \frac{3}{2S^2}(1-P)\int_1^\infty \left(\frac{1}{t^3} - \frac{1}{t^5}\right)\frac{1-e^{-St}}{1-Pe^{-St}}dt. \qquad (14)$$

This is similar to equation (5) with K replaced by S. These expressions, (10) and (13), for the conductivity of a film have an interesting consequence viz. the conductivity has an oscillatory nature as a function of the magnetic field. However the oscillations are not of uniform amplitude.

D. K. C. MacDonald and K. Sargenson[9] discussed the classical effects of a magnetic field on a conducting film when the field is perpendicular to the current density but in the plane ofthe film. They found two expressions for J/J_∞, the ratio of the current density to the bulk current density. One expression applies when $a > 2r$ where a is the film thickness and r is the radius of the path of unscattered elecrtons in a bulk sample when the bulk sample is in the magnetic field. Thus this expression applies to thicker films or stronger fields. The other expression to the case of $a < 2r$. That is thinner films or weaker fields. An interesting point concerning this case of magnetic field orientation is that the Hall electric field is across the thin dimension of the

film. Therefore the Hall field is a quickly varying field. This concludes the discussion of classical size effects in films.

A Quantum Size Effects Theory for Semimetals

Quantum size effects are those properties of materials which are dependent upon a material's dimensions being of the order of the de Broglie wavelength of particles or excitations within the material. V. B. Sandomirskii[10] discussed theoretically the quantum size effects in the electrical properties of semimetal films. His development of these effects was done in the relaxation time approximation. Sandomirskii used randomly distributed δ-function potential scattering centers. A critical parameter in his formulation is the quantity $\bar{a}$, the thickness of the film when the hole and electron bands change from overlapping to nonoverlapping. In cases where the hole effective mass greatly exceeds the electron effective mass $\bar{a}$ corresponds to half of the de Broglie wavelength of the electron, and vice versa. Sandomirskii's expressions for the conductivity of a thin semimetal film are

$$\frac{\sigma}{\sigma_0} = \frac{a}{\bar{a}} \frac{2n/n_0}{2A+1} \qquad \text{for } a > \bar{a} \qquad (15)$$

and

$$\frac{\Delta\sigma}{\sigma_0} = \frac{3kT}{\Delta}\left[\frac{m_n + m_p}{M}\right]^{1/2} e^{-\frac{\varepsilon_g}{2kT}} \qquad \text{for } a < \bar{a}. \qquad (16)$$

The electron and hole effective masses are m_n and m_p respectively. The inverse of the sum of the inverse effective masses is M. The energy band overlap in the bulky semimetal is Δ. While kT is the product of the Boltzman constant and the absolute temperature. The integer part of $a/\bar{a}$ is A. The quantity ε_g is the energy band gap which exist in extremely thin semimetal films. The number density of conduction band electrons is n, while that in a bulky semimetal is n_o. Note that both ε_g and n are functions of the semimetal film thickness a. Sandomirskii derived expressions for the ratio n/n_o through the density of states. By assuming the conduction electrons to be a degenerate gas for $a < \bar{a}$ he found the expressions

$$\frac{n}{n_o} = \frac{1}{4}\left(\frac{\bar{a}}{a}\right)^3 A\left[6\left(\frac{a}{\bar{a}}\right)^2 - (A+1)(2A+1)\right] \qquad (17)$$

for $a > \bar{a}$, and

$$\frac{n}{n_o} = \frac{3kT}{\Delta}\left[\frac{m_n + m_p}{M}\right]^{1/2} \frac{\bar{a}}{a}\, e^{-\frac{\varepsilon_g}{2kT}} \qquad (18)$$

for $a < \bar{a}$. Both of these expressions are continuous. But the derivative of equation (17) is discontinuous at each integer value of $a/\bar{a}$. Also equation (17) has a relative maximum in each interval $S < a/\bar{a} < S+1$ where S is an integer. Thus in this formulation both the conductivity and the number density of charge carriers are oscillatory

functions of a with period $\bar{a}$. Sandomirskii also stated results for the Hall constant and magnetoresistance. These are also oscillatory in thickness with period $\bar{a}$.

Experimental Evidence of Quantum Size Effects

The above work done by Sandomirskii was prompted by experimental work done by Orgin et al[11]. This was the first observation of quantum size effects. The work was done with bismuth films at 300, 78, and 4.2 K. The films were produced by sputtering bismuth onto a mica substrate heated to 70 to 80 C at a rate of about 50 Å/min. Measurements of the resistivity, Hall constant, and magnetoresistance were taken for film thicknesses of 200 Å to greater than 4000 Å. The resistivity, transverse magnetoresistance, Hall constant, and Hall mobility were found to have a periodic thickness dependence with a period of 400 to 500 Å for the 78 and 4.2 K cases. The series of measurements at 300 K shower very little if any oscillatory behavior. All three cases showed a sharp rise in resistivity below 400 Å. These results are in fair agreement with Sandomirskii's theory since using a representative electron effective mass of .01 m_e yields a thickness parameter $\bar{a}$ of 390 Å.

Other experimental work has been done with thin bismuth films. Two instances of interest are the work of N. Garcia[12] and that of V. P. Duggal and R. Rup[13]. Garcia grew his bismuth films epitaxially on a mica substrate by evaporation. The substrate was heated to a temperature of 100 C during

growth and annealing. Measurements were made at 12, 77, and 394 K. The growth rate was 60 Å/min. Garcia was careful to use a sequential growth and measurement procedure in order to prevent extreme structural changes in the film between measurements. Measurements were made for the resistivity, Hall effect, and transverse magnetoresistance. Garcia found oscillatory behavior with thickness variation only at 12 K. An electron micrograph of a film when 500 Å thick shows that the film is mot a single crystal, though an x-ray diffraction pattern does show that the orientation of the crystalites were quite similar. An electron micrograph of a film 1000 Å thick also shows a similar pattern, though the crystalites were somewhat larger.

Duggal and Rup also grew their bismuth films epitaxially by evaporation onto a mica substrate at 130 C. The evaporation rate here ranged from 400 to 600 Å/min. Measurements of the resistivity and Hall constant were taken at 90 and 300 K for films varying in thickness from 250 to 1700 Å. The major difference between this work and that of Garcia is that the resistivity and the Hall constant R_H were periodic in thickness even at 300 K. Duggal and Rup also did an x-ray analysis and made an electron micrograph study of their films. The electron micrograph study revealed that these films had grains with widths of one to three microns. They also discovered voids in films thinner than 600 Å. Furthermore the density of voids increased with decreasing film thickness. Thus quantum size

effects have been observed in the semimetal bismuth in the thickness range of 400 to 4000 A. They have also been observed in the temperature range of 4.2 to 300 K.

Yu. F. Komnik and E. I. Bakhshtab [14,15] have also observed quantum size effects in metals. They observed conductivity oscillations with a period of 28 A in antimony films. Quantum size effects were also observed in tin films. Komnik and Bukhshtab made electron microscopic and electron micrographic studies of their tin films. They found that a temperature dependent critical thickness exists. At this thickness the deposited tin changes from an amorphous structure to a crystaline structure. They observed that sharp channels or labyrinths exist in the crystal near this thickness. The critical thickness for tin is 200 to 250 A at room temperature. Tin was found to have a weak oscillatory thickness dependence in its conductivity. And a stronger oscillatory thickness dependence was found in the critical transition temperature associated with superconductivity. The oscillatory dependence in both cases has a double period. There are weaker oscillations with a period of 7 to 8 A and stronger oscillations with a period of 15 A. The smallness of the oscillatory periods in tin and antimony films illustrates well why most experiments dealing with quantum size effects have involved simimetals.

CHAPTER II

CURRENT DENSITY IN THIN FILMS

Introduction

This chapter contains a quantum derivation of the component of current density in a thin film along the direction of the applied electric field, when the thin film is in a magnetic field which is perpendicular to both the applied electric field and the plane of the film. The chapter also contains a discussion of the results of the derivation.

The model used here is the free electron model. As in Figure 1, the thin dimension of the film is along the z direction. The magnetic field is also along the z direction. The electric field is along the x direction. The plane of the thin film is along the x and y directions. The dimensions of

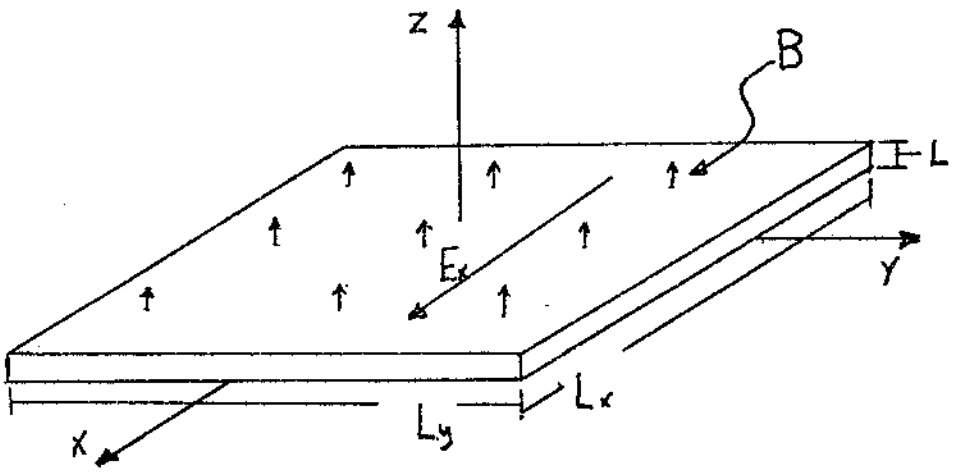

Fig. 1--Thin film orientation

the film along the x and y directions are considered to be almost infinite. The electrons encounter random scattering centers which are assumed to have δ-function potentials. And the sursaces of the film are approximated by an infinite square well at z=0 and z=L .

Wave Functions and Energies

In order to solve for single particle wave functions, the gauge of the magnetic field is chosen to be (0, Bx , 0). This vector potential yields a magnetic field of magnitude B along the z direction. With this gauge the Hamiltonian is

$$H = \frac{1}{2M}\left[P_x^2 + (P_y + M\omega x)^2 + P_z^2\right] + eE_x x \qquad (19)$$

where ω is the cyclotron frequency

$$\omega = \frac{Be}{Mc} . \qquad (20)$$

When solving the stationary state Schrodinger equation, the z dependence seperates immediately as the infinite square well problem. The x and y dependencies can be seperated if a free particle wave function is tried for the y direction. The remaining dependence is

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2}+\frac{M\omega^2}{2}\left(x+\frac{\hbar k}{M\omega}+\frac{eE_x}{M\omega^2}\right)^2\right]\phi(x)$$
$$=\left[E-\epsilon_z-\frac{M\omega}{2}\left(\frac{\hbar k}{M\omega}+\frac{eE_x}{M\omega^2}\right)^2\right]\phi(x). \tag{21}$$

This is the Schrödinger equation of a harmonic oscillator. The point of equilibrium for this oscillator is

$$x=-\frac{\hbar k}{M\omega}-\frac{eE_x}{M\omega^2}. \tag{22}$$

Thus the complete normalized wave function is

$$\psi_{nkm}=\sqrt{\frac{2}{L_y L}}\,\phi_n\left(x+\frac{\hbar k}{M\omega}+\frac{eE_x}{M\omega^2}\right)e^{iky}\sin\frac{m\pi z}{L} \tag{23}$$

where ϕ_n is the normalized harmonic oscillator wave function. The energy is

$$E_{nkm}=\left(n+\tfrac{1}{2}\right)\hbar\omega+\frac{\pi^2\hbar^2m^2}{2L^2M}-\frac{eE_x\hbar k}{M\omega}-\frac{e^2E_x^2}{2M\omega^2} \tag{24}$$

$$n=0,1,2,\ldots \qquad m=1,2,3,\ldots .$$

When the electric field is not turned on, the energy is

$$\epsilon_{nm}=\left(n+\tfrac{1}{2}\right)\hbar\omega+\frac{\pi^2\hbar^2m^2}{2L^2M}. \tag{25}$$

The matrix element $\langle n\,k\,m|\,v_x\,|n'k'm'\rangle$ will be needed to calculate the current density. Since v_x has no y or z dependence,

$$\langle n\,k\,m|\,v_x\,|n'k'm'\rangle = \langle n|v_x|n'\rangle\langle k|k'\rangle\langle m|m'\rangle. \quad (26)$$

Using the canonical momentum $p_x = M v_x$ and the harmonic oscillator creation and destruction operators $a^\dagger$ and a respectively, one obtains

$$\begin{aligned}\langle n|v_x|n'\rangle &= i\left(\frac{\hbar\omega}{2M}\right)^{\frac{1}{2}}\langle n|\,a^\dagger - a\,|n'\rangle \\ &= i\left(\frac{\hbar\omega}{2M}\right)^{\frac{1}{2}}\left[\langle n|a^\dagger|n'\rangle - \langle n|a|n'\rangle\right].\end{aligned} \quad (27)$$

This yields

$$\langle n|v_x|n'\rangle = i\left(\frac{\hbar\omega}{2M}\right)^{\frac{1}{2}}\left[\sqrt{n}\,\delta_{n',n-1} - \sqrt{n+1}\,\delta_{n',n+1}\right]. \quad (28)$$

Thus the entire matrix element is

$$\begin{aligned}\langle n\,k\,m|\,v_x\,|n'k'm'\rangle &= i\left(\frac{\hbar\omega}{2M}\right)^{\frac{1}{2}}\delta_{k'k}\,\delta_{m'm} \\ &\times\left[\sqrt{n}\,\delta_{n',n-1} - \sqrt{n+1}\,\delta_{n',n+1}\right].\end{aligned} \quad (29)$$

A Density Matrix Method

The method used at the begining of this development for a current density component of a thin film in a transverse magnetic field is similar to that reviewed by A. H. Kahn and H. P. R. Frederiske[16] in their treatment of transport effects in bulk conducting materials in magnetic fields. Thus the equation of motion of the density operator is

$$i\hbar \frac{\partial \rho}{\partial t} = [\rho, H_{KIN} + eE_x x + V] \tag{30}$$

where H_{KIN} is the Hamiltonian of an electron including the magnetic field but excluding the electric field. The total scattering potential is V.

Now a device employed by Kohn and Luttinger[17] is used. It entails "switching on" the electric field adiabatically by replacing E_x by $E_x e^{st}$. The switching parameter S is positive. Thus when the time $t = -\infty$ the electric field is completely off and when $t = 0$ the electric field is completely on. The abruptness of the switching is controled by the switching parameter. Later the limit as S changes from a small positive number to zero will be taken. This same device is used to describe the density operator. Therefore

$$\rho = \rho_0 + f e^{st} \tag{31}$$

where ρ_o is the density operator for the film at $t = -\infty$ in the magnetic field and in thermal equilibrium. Its matrix elements are

$$\rho_{o\,nkm,n'k'm'} = \left[e^{-\frac{\epsilon_{nm} - E_F}{k_o T}} + 1 \right]^{-1} \delta_{nn'} \delta_{kk'} \delta_{mm'} . \quad (32)$$

Substitution of equation (31) into equation (30), the density operator equation of motion, yields

$$\begin{aligned} -i\hbar s e^{st} f = & \left[\rho_o + f e^{st}, H_{KIN} + e \times E_x e^{st} \right] \\ & + \left[\rho_o + f e^{st}, V \right]. \end{aligned} \quad (33)$$

Taking the matrix elements of this at $t = 0$ with respect to the final state of the system gives

$$\begin{aligned} & \left(E_{nkm} - E_{n'k'm'} - i\hbar s \right) f_{nkm\,n'k'm'} \\ & = \left[\rho_o(\epsilon_{nm}) - \rho_o(\epsilon_{n'm'}) \right] V_{nkm,n'k'm'} + \left[f, V \right]_{nkm,n'k'm'}. \end{aligned} \quad (34)$$

One can see from equation (29) that one needs matrix elements which are diagonal in k and m, yet off diagonal in n. That is

$$[\hbar\omega(n-n') - i\hbar s] f_{nkm,n'km} = [f,V]_{nkm,n'km}$$

$$+ [\rho_o(\epsilon_{nm}) - \rho_o(\epsilon_{n'm})] V_{nkm,n'km}. \qquad (35)$$

The lowest order approximation in scattering which gives rise to a net current is now taken. To accomplish this the commutator in equation (34) is set to zero. Thus to the lowest order a general off diagonal matrix element of the correction to the density operator is

$$f_{nkm,n'k'm'} = \frac{[\rho_o(\epsilon_{nm}) - \rho_o(\epsilon_{n'm'})] V_{nkmn'k'm'}}{E_{nkm} - E_{n'k'm'} - i\hbar s}. \qquad (36)$$

This matrix element is put into the commutator to solve for the matrix elements of the correction to the density operator which gives rise to a net current. One gets

$$f_{nkm,n'km} = \frac{1}{\hbar\omega(n-n') - is\hbar} \sum_{n''k''m''} \left[\frac{\rho_o(\epsilon_{nm}) - \rho_o(\epsilon_{n''m''})}{E_{nkm} - E_{n''k''m''} - is\hbar} \right. \qquad (37)$$

$$\left. - \frac{\rho_o(\epsilon_{n'm}) - \rho_o(\epsilon_{n''m''})}{E_{n'km} - E_{n''k''m''} - is\hbar} \right] V_{nkmn''k''m''} V_{n''k''m''n'km}.$$

One now takes the limit as the switching parameter approaches zero. Again as in Kohn and Luttinger[17] one can use the relation

$$\lim_{s\to 0} \frac{1}{x - is} = P\left(\frac{1}{x}\right) + i\pi\,\delta(x) \tag{38}$$

where $P(u)$ indicates the principal part of u. With this the needed matrix element of the correction to the density operator becomes

$$f_{nkm,n'km} = \frac{i\pi}{\hbar\omega(n-n')} \sum_{n''k''m''} V_{nkm\,n''k''m''} V_{n''k''m''\,n'km} \times \left\{ \left[\rho_0(\epsilon_{nm}) - \rho_0(\epsilon_{n''m''})\right] \delta\left(E_{nkm} - E_{n''k''m''}\right) + \left[\rho_0(\epsilon_{n'm}) - \rho_0(\epsilon_{n''m''})\right] \delta\left(E_{n'km} - E_{n''k''m''}\right) \right\}. \tag{39}$$

Note that energy is conserved during collisions because of δ-function dependence on total energy.

It is at this point that this derivation begins to diverge more radically from the bulk problem. The above is now applied to the present goal of finding an expression for the x component of the current density. This is done by taking

$$J_x = -\frac{e}{\Omega} Tr\left(v_x \rho\right). \tag{40}$$

Next expand this in terms of final states at time $t = 0$

$$J_x = -\frac{e}{\Omega} \sum_{\substack{n k m, \\ n' k' m'}} \Big[\langle n k m | v_x | n' k' m' \rangle \langle n' k' m' | \rho_0 | n k m \rangle + \langle n k m | v_x | n' k' m' \rangle \langle n' k' m' | f | n k m \rangle . \tag{41}$$

The sum over the first product of matrix elements is zero since $\langle n' k' m' | \rho_0 | n k m \rangle$ envolves $\delta_{n'n} \delta_{k'k} \delta_{m'm}$ while $\langle n k m | v_x | n' k' m' \rangle$ envolves $\delta_{n', n-1}$ and $\delta_{n', n+1}$. Therefore putting the matrix elements into equation (41) and summing over the primed indicies yields

$$\begin{aligned} J_x = \frac{e\pi}{\Omega (2M\hbar\omega)^{\frac{1}{2}}} \sum_{\substack{n k m \\ n'' k'' m''}} \Big[& \sqrt{n+1}\; V_{n+1\,k m\, n'' k'' m''}\, V_{n'' k'' m'' n k m} \\ & \times \{ [\rho_0(\epsilon_{n+1\,m}) - \rho_0(\epsilon_{n'' m''}] \, \delta(E_{n+1\,k m} - E_{n'' k'' m''}) \\ & + [\rho_0(\epsilon_{n m}) - \rho_0(\epsilon_{n'' m''})] \, \delta(E_{n k m} - E_{n'' k'' m''}) \} \\ & + \sqrt{n}\; V_{n-1\,k m\, n'' k'' m''}\, V_{n'' k'' m'' n k m} \{ [\rho_0(\epsilon_{n-1\,m}) - \rho_0(\epsilon_{n'' m''})] \\ & \times \delta(E_{n-1\,k m} - E_{n'' k'' m''}) + [\rho_0(\epsilon_{n m}) - \rho_0(\epsilon_{n'' m''}) \delta(E_{n k m} - E_{n'' k'' m''}) \} \Big] . \end{aligned} \tag{42}$$

The index n is changed to $n-1$ in the first term of the summation above. The range of summation remains the same however. Also because the scattering potential V is Hermitian, one has

$$V_{n''\kappa''m''\,n\kappa m} = V^{\dagger}_{n''\kappa''m''\,n\kappa m} = V^{*}_{n\kappa m\,n''\kappa''m''}. \qquad (43)$$

Thus one writes equation (42) as

$$J_x = -\frac{e\pi}{\Omega(2M\hbar\omega)^{1/2}} \sum_{\substack{n\kappa m \\ n''\kappa''m''}} \sqrt{n}\,\Big\{\big[\rho_0(\epsilon_{n-1\,m}) - \rho_0(\epsilon_{n''m''})\big] \times \delta(E_{n-1\kappa m} - E_{n''\kappa''m''}) + \big[\rho_0(\epsilon_{nm}) - \rho_0(\epsilon_{n''m''})\big] \times \delta(E_{n\kappa m} - E_{n''\kappa''m''})\Big\} \mathrm{Re}\big[V_{n-1\kappa m\,n''\kappa''m''} V_{n''\kappa''m''\,n\kappa m}\big]. \qquad (44)$$

Scattering

Calculations of the current density made from the above equation, however, depend upon the exact locations of the scattering centers. A more useful quantity is the current density component for a randomly distributed set of scattering centers. Thus the quantity one seeks is

$$J_x = -\frac{e\pi}{\Omega(2M\hbar\omega)^{1/2}} \sum_{\substack{n\kappa m \\ n''\kappa''m''}} \sqrt{n}\,\Big\{\big[\rho_0(\epsilon_{n-1\,m}) - \rho_0(\epsilon_{n''m''})\big] \times \delta(E_{n-1\kappa m} - E_{n''\kappa''m''}) + \big[\rho_0(\epsilon_{nm}) - \rho_0(\epsilon_{n''m''})\big] \times \delta(E_{n\kappa m} - E_{n''\kappa''m''})\Big\} \big\langle \mathrm{Re}\, V_{n-1\kappa m\,n''\kappa''m''} V_{n''\kappa''m''\,n\kappa m}\big\rangle \qquad (45)$$

where the brackets $\langle \ldots \rangle$ indicate a statistical average over the scattering center locations.

It is now time to consider specifically the nature of the scattering. Since δ-function potential scattering is being used, the total scattering potential is

$$V = (2\pi)^{3/2} C \sum_i \delta(\vec{r} - \vec{R}_i) = C \sum_i \int e^{i\vec{q}\cdot(\vec{r}-\vec{R}_i)} d^3q. \tag{46}$$

Thus the product of matrix elements is

$$V_{nkm\,n''k''m''} V_{n''k''m'n-1\,km} = C^2 \int \sum_{ij} e^{-i(\vec{q}\cdot\vec{R}_i + \vec{q}'\cdot\vec{R}_j)} \times \langle nkm|e^{i\vec{q}\cdot\vec{r}}|n''k''m''\rangle\langle nkm|e^{i\vec{q}'\cdot\vec{r}'}|n-1\,km\rangle d^3q\, d^3q'. \tag{47}$$

Note that the scattering center position dependence has been isolated. To average over the scattering centers one needs to average only over the quantity

$$S = \sum_{ij} e^{-i(\vec{q}\cdot\vec{R}_i + \vec{q}'\cdot\vec{R}_j)}. \tag{48}$$

Thus the average of S for randomly distributed scattering centers is

$$\langle S \rangle = \frac{1}{\Omega^N} \int \sum_{ij} e^{-i(\vec{q}\cdot\vec{R}_i + \vec{q}'\cdot\vec{R}_j)} \, d^3R_1 \, d^3R_2 \ldots d^3R_N. \quad (49)$$

where N is the total number of scattering centers. One assumes an equal probability of any scattering center being anywhere within the film. Seperating the sum into the cases $i = j$ and $i \neq j$, one obtains

$$\langle S \rangle = \frac{N}{\Omega} \int e^{-i(\vec{q}+\vec{q}')\cdot R_1} \, d^3R_1 + \frac{N(N-1)}{\Omega^2} \int e^{-i(\vec{q}\cdot R_1 + \vec{q}'\cdot R_2)} \, d^3R_1 \, d^3R_2. \quad (50)$$

Hence in the sense of box normalization

$$\langle S \rangle = N \delta_{\vec{q},\vec{q}'} + N(N-1) \delta_{\vec{q},0} \delta_{\vec{q}',0}. \quad (51)$$

The second term here does not contribute to a net current since it corresponds to a potential which is constant throughout the film. Substituting $\langle S \rangle$ into equation (47) one gets

$$\langle V_{n\kappa m\, n''\kappa''m''}\, V_{n''\kappa''m''\, n-1\,\kappa m}\rangle = \frac{C^2N^2}{L_y^2L^2}\int \phi_n(x+\alpha)\,\phi_{n''}(x+\beta)$$

$$\times\,\phi_{n''}(x'+\beta)\,\phi_{n-1}(x'+\alpha)\,e^{-i\vec{q}\cdot\vec{r}-i\vec{q}'\cdot\vec{r}-iky+ik''y-ik''y'+iky'} \tag{52}$$

$$\times\,\sin\left(\frac{m\pi z}{L}\right)\sin\left(\frac{m''\pi z}{L}\right)\sin\left(\frac{m''\pi z'}{L}\right)\sin\left(\frac{m\pi z'}{L}\right)\delta_{\vec{q},\vec{q}'}\,d^3q\,d^3q'\,d^3r\,d^3r'$$

where

$$\alpha = \frac{\hbar k}{M\omega} + \frac{eE_x}{M\omega^2}\quad,\quad \beta = \frac{\hbar k''}{M\omega} + \frac{eE_x}{M\omega^2}\,. \tag{53}$$

Next, doing the $\vec{q}$ and $\vec{q}'$ integrations yields

$$\langle V_{n\kappa m\, n''\kappa''m''}\, V_{n''\kappa''m''\, n-1\,\kappa m}\rangle = \frac{4C^2N(2\pi)^3}{L^2L_y^2\Omega}\int \phi_n(x+\alpha)\,\phi_{n''}(x+\beta)$$

$$\times\,\phi_{n''}(x'+\beta)\,\phi_{n-1}(x'+\alpha)\,e^{-iky+ik''y-ik''y'+iky'}\,\delta(\vec{r}-\vec{r}') \tag{54}$$

$$\times\,\sin\left(\frac{m\pi z}{L}\right)\sin\left(\frac{m''\pi z}{L}\right)\sin\left(\frac{m''\pi z'}{L}\right)\sin\left(\frac{m\pi z'}{L}\right)\,d^3r\,d^3r'.$$

When the integration over $\vec{r}'$ is done, the averaged scattering matrix element product becomes

$$\langle V_{nkm\,n''k''m''} V_{n''k''m''n-1km} \rangle = \frac{32C^2\pi^3 N}{L^2 L_y^2 \Omega} \int \phi_n(x+\alpha)\ \phi_{n''}^2(x+\beta)$$

$$\times\ \phi_{n-1}(x+\alpha)\ \sin^2\left(\frac{m\pi z}{L}\right) \sin^2\left(\frac{m''\pi z}{L}\right) d^3r. \tag{55}$$

The integration over z gives

$$\int_0^L \sin^2\left(\frac{m\pi z}{L}\right) \sin^2\left(\frac{m''\pi z}{L}\right) dz = \frac{L}{4}\left(1+\tfrac{1}{2}\delta_{mm''}\right). \tag{56}$$

And since the harmonic oscillator wave functions are real, one has

$$\langle \mathrm{Re}\, V_{nkm\,n''k''m''} V_{n''k''m''n-1km} \rangle = \frac{8C^2\pi^3 N}{L_y L \Omega}\left(1+\tfrac{1}{2}\delta_{mm''}\right)$$

$$\times \int \phi_n(x+\alpha)\, \phi_{n''}^2(x+\beta)\, \phi_{n-1}(x+\alpha)\, dx. \tag{57}$$

for the scattering dependence of the x component of the current density.

With the above considerations for scattering, the x component of current density of a thin film in a transverse magnetic field is

$$J_x = -\frac{e\pi^4 C^2 8N}{L_y L \Omega^2 (2M\hbar\omega)^{1/2}} \sum_{\substack{n\,k\,m \\ n''k''m''}} \sqrt{n}\,\left(1+\tfrac{1}{2}\delta_{mm''}\right)\left\{\left[\rho_0(\epsilon_{n-1\,m}) - \rho_0(\epsilon_{n''m''})\right]\right.$$

$$\times \delta(E_{n-1\,k\,m} - E_{n''k''m''}) + \left[\rho_0(\epsilon_{nm}) - \rho_0(\epsilon_{n''m''})\right] \qquad (58)$$

$$\left.\times \delta(E_{n\,k\,m} - E_{n''k''m''})\right\} \int \phi_n(x+\alpha)\,\phi_{n''}(x+\beta)\,\phi_{n-1}(x+\alpha)\,dx.$$

The thin film is large in the y direction, thus the quantum numbers k and k'' are quasi-continuous. Hence one can replace the sum over k'' by $\frac{L_y}{2\pi}\int dk''$ and change the explicit dependence of the δ-functions from energy to k''. With these considerations the x component of the current density after integration over k'' is

$$J_x = \frac{-e\pi^3 C^2 4N}{L\Omega^2(2M\hbar\omega)^{1/2}} \frac{M\omega}{eE_x\hbar} \sum_{\substack{n\,k\,m \\ n''\,m''}} \sqrt{n}\,\left(1+\tfrac{1}{2}\delta_{mm''}\right)$$

$$\times \left\{\left[\rho_0(\epsilon_{nm}) - \rho_0(\epsilon_{n''m''})\right] \int_{-\infty}^{\infty} \phi_n(x+\alpha)\,\phi_{n''}^2(x+K)\,\phi_{n-1}(x+\alpha)\,dx \right. \qquad (59)$$

$$\left. + \left[\rho_0(\epsilon_{n-1\,m}) - \rho_0(\epsilon_{n''m''})\right] \int_{-\infty}^{\infty} \phi_n(x+\alpha)\,\phi_{n''}^2(x+K')\,\phi_{n-1}(x+\alpha)\,dx\right.$$

where

$$K = \frac{\hbar k}{M\omega} - \frac{1}{eE_x}\left[\hbar\omega(n-n'') + \frac{\pi^2\hbar^2}{2L^2M}(m^2 - m''^2)\right] + \frac{eE_x}{M\omega^2} \qquad (60)$$

and

$$K' = \frac{\hbar k}{M\omega} - \frac{1}{eE_x}\left[\hbar\omega(n-1-n'') + \frac{\pi^2\hbar^2}{2L^2M}(m^2-m''^2)\right] + \frac{eE_x}{M\omega^2}. \qquad (61)$$

To facilitate further simplification one makes the change of variables $x+\alpha=y$. Thus the first integral over x in equation (59) becomes

$$I = \int_{-\infty}^{\infty} \phi_n(y)\,\phi_{n''}^2(y+\eta)\,\phi_{n-1}(y)\,dy. \qquad (62)$$

A similar change occurs in the second integral with η replaced by η' where

$$\eta = \frac{1}{eE_x}\left[\hbar\omega(n-n'') + \frac{\pi^2\hbar^2}{2L^2M}(m^2-m''^2)\right]$$
$$\eta' = \frac{1}{eE_x}\left[\hbar\omega(n-n''-1) + \frac{\pi^2\hbar^2}{2L^2M}(m^2-m''^2)\right]. \qquad (63)$$

Note that neither η nor η' are dependent on k. Expressing the harmonic oscillator wave functions directly in terms of the Hermite polynomials, $H_j(u)$, one finds

$$I = \frac{C_n C_{n''}^2 C_{n-1}}{2^{\frac{2n+2n''-1}{2}}} \int e^{-(ay)^2-(ay+a\eta)^2} H_n(ay) \times H_{n''}^2(ay+a\eta)\, H_{n-1}(ay)\,dy \qquad (64)$$

where

$$C_n = \left(\frac{\sqrt{M\omega/\pi\hbar}}{n!}\right)^{\frac{1}{2}} \qquad a = \sqrt{M\omega/\hbar}\,. \tag{65}$$

There are several methods of doing this integral. The most obvious is to express the Hermite polynomials as a series or perhaps to use a generating series. A more direct method is to use an integral representation. Use the integral representation

$$H_j(u) = \int_{-\infty}^{\infty} (u+is)^j e^{-s^2} ds\,. \tag{66}$$

Thus one has

$$I = \frac{C_n C_{n''} C_{n-1}}{2^{\frac{2n+2n''-1}{2}} a} e^{-(a\eta)^2} \int e^{-2(ay)^2 - 2a^2\eta y - s^2} \cdot$$
$$\times e^{-t^2-u^2-v^2} (ay+is)^n (ay+a\eta+it)^{n''} \tag{67}$$
$$\times (ay+a\eta+iu)^{n''} (ay+iv)^{n-1} a\, ds\, dt\, du\, dv\, dy\,.$$

Expanding the algebraic terms in the integrand in a binomial expansion will facilitate the integration over y. Also make the change of variables $\theta = ay$. Therefore

$$I = \frac{C_n C_{n''}^2 C_{n-1}}{a\, 2^{\frac{2n+2n''-1}{2}}} \sum_{j=0}^{n} \sum_{l=0}^{n''} \sum_{p=0}^{n''} \sum_{q=0}^{n-1} \binom{n}{j}\binom{n''}{l}\binom{n''}{p}\binom{n-1}{q}$$
$$\times \int (is)^{n-j} (a\eta + it)^{n''-l} (a\eta + iu)^{n''-p}$$
$$\times (iv)^{n-q-1} \int e^{-2\theta - 2a\eta\theta - s^2 - t^2 - u^2 - v^2} \qquad (68)$$
$$\times\ \theta^{j+l+p+q}\, d\theta\, ds\, dt\, du\, dv.$$

Once the integration over θ is done and the dependencies on s, t, u, and v are examined one sees that[18]

$$I = \frac{C_n C_{n''}^2 C_{n-1}}{a\, 2^{\frac{2n+2n''-1}{2}}} \sqrt{\frac{\pi}{2}}\, e^{-\frac{(a\eta)^2}{2}} \sum_{jlpq} H_{n-j}(0)$$
$$\times H_{n''-l}(a\eta)\, H_{n''-p}(a\eta)\, H_{n-q-1}(0) \binom{n}{j}\binom{n''}{l}\binom{n''}{p} \qquad (69)$$
$$\times \binom{n-1}{q} \left(\frac{a\eta}{2}\right)^{j+l+p+q} \sum_{b=0}^{E\left(\frac{j+l+p+q}{2}\right)} \frac{(2a\eta)^{-b}}{(j+l+p+q-2b)!\, b!}$$

where $E(u)$ is the integer part of u.

Because η and η' do not depend on k, the summation over k simply involves an integration $\frac{L^2}{2\pi}\int dk$. The limits of this integration are not however infinite. The center of the harmonic oscillator wave function are dependent upon k. This center must be within the film since it corresponds to

the most probable position of electrons. The quantum number k is subject to condition[19]

$$-\frac{L_x}{2} \leq \frac{\hbar k}{M\omega} + \frac{eE_x}{M\omega^2} \leq \frac{L_x}{2}. \tag{70}$$

With this the k summation is performed as

$$\frac{L_y}{2\pi}\int_{-\frac{M\omega L_x}{2\hbar}-\frac{eE_x}{\hbar\omega}}^{\frac{M\omega L_x}{2\hbar}\frac{eE_x}{\hbar\omega}} dk = \frac{M\omega L_x L_y}{2\pi\hbar}. \tag{71}$$

With the considerations of the previous paragraphs the x component of the current density of a thin film in a transverse magnetic field is

$$\begin{aligned} J_x = {} & \frac{\pi^{3/2} C^2 M^2 \omega^2 N}{L^2 \Omega E_x \hbar^3} \sum_{\substack{n\,n'' \\ m\,m''}=1}^{\infty} \frac{n!\,n''!}{2^{\frac{2n+2n''-1}{2}}} \left(1+\tfrac{1}{2}\delta_{mm''}\right) \\ & \times \sum_{j=0}^{n}\sum_{l=0}^{n''}\sum_{p=0}^{n''}\sum_{q=0}^{n-1} \frac{H_{n-j}(0)\,H_{n-q-1}(0)}{(n-j)!\,(n''-l)!\,(n''-p)!\,(n-q-1)!\,j!\,l!\,p!\,q!} \\ & \times \left\{ \left[\rho_0(\epsilon_{n''m''}) - \rho_0(\epsilon_{nm})\right] e^{-\frac{(a\eta)^2}{2}} \left(-\frac{a\eta}{2}\right)^{j+l+p+q} H_{n''-l}(a\eta) \right. \\ & \times H_{n''-p}(a\eta) \left[\sum_{b=0}^{E\left(\frac{j+l+p+q}{2}\right)} \frac{(2a\eta)^{-b}}{(j+l+p+q-2b)!\,b!}\right] + \left[\rho_0(\epsilon_{n''m''}) - \rho_0(\epsilon_{n-1m})\right] \\ & \times e^{-\frac{(a\eta')^2}{2}} \left(-\frac{a\eta'}{2}\right)^{j+l+p+q} H_{n''-l}(a\eta')\, H_{n''-p}(a\eta') \\ & \left. \times \sum_{b=0}^{E\left(\frac{j+l+p+q}{2}\right)} \frac{(2a\eta')^{-b}}{(j+l+p+q-2b)!\,b!} \right\}. \end{aligned} \tag{72}$$

Conclusions

This result for the x component of the current density, which is based on the method reviewed by Kahn and Frederiske, has several interesting aspects. First, all of the explicit temperature dependence is contained in the two terms which are the differences of Fermi distributions. This does not appear to be a simple temperature dependence however because all values of the quantum numbers n, n'', m, and m'' are summed over.

Second, if the method reviewed by Kahn and Frederiske is applicable to thin films it certianly indicates a non-ohmic dependence upon the applied electric field. The quantities η and η' both contain inverse elecrtic field dependence. Thus the current density component does go to zero at zero electric field due to the exponential involving η and η' squared. However this elecrtic field dependence deserves further study, which we hope to consider in the future.

Third, the thickness dependence of the x component of the current density is rather complex. The current density goes to zero as the thickness goes to zero. Yet each term involving either temperature or electric field is also thickness dependent. The sum over Hermite polynomials suggests that the current density may be oscillatory with respect to film thickness. But the nature of these oscillations is not obvious. It should be noted that the experimental situation with respect to these oscillations of magnetoresistance is ill-defined at

present. Many experimenters have claimed a regular period to these oscillations. However Garcia's experiments tend to throw some doubt on this. Additional experiments are required to clarify the nature of these oscillatory quantum size effects.

The expression developed here for the x component of the current density is directly applicable only to metals. It can be extended to semimetals and semiconductors by adding a similar expression for holes and replacing the mass by hole and electron effective masses. The two parts of the extended current density expression will have to be connected by the neutrality condition.

Finally, the surface conditions existing at the film surfaces have certainly been highly idealized in this development by use of an infinite square well. The finite square well and the harmonic oscillator potentials deserve consideration. Also the question of specular versus partially specular scattering needs consideration.

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