NON-EQUILIBRIUM THERMO FIELD DYNAMICS AND THE TRANSPORT OF ELECTRONS IN MAGNETIC AND ELECTRIC FIELDS

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by

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Abstract

The superoperator formalism of non-equilibrium Thermo Field Dynamics is extended to consider a system of electrons in contact with a thermal reservoir in a homogeneous crossed electric and magnetic field. Particular attention is paid to the role of gauge invariance. A brief overview of the development of a non-equilibrium, finite time, temperature dependent field theory is included, as well as an outline of the construction of the superoperator formalism of non-equilibrium thermo field dynamics. The relationship between the two point electron Green's functions and the probability distribution function appearing in the semi-classical Boltzmann equation is established.

As an illustration of how the transport coefficients are found from the Boltzmann equation, the case of the Chamber's solution for the electrical conductivity is considered. The position dependence of the conductivity tensor in the presence of a domain wall is evaluated numerically, and the trends are verified analytically.

Future extensions of the present work are discussed.

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Chapter I: Introduction

Quantum field theory has evolved to become more suitable to deal with problems in solid state physics, in addition to those in the physics of elementary particles, for which it was originally developed. The development of the most consequence to many-body theory is the use of a quantum space whose states are defined by the action of creation and annihilation operators on a vacuum state. The theory can then be discussed in terms of physical or "incoming" fields which correspond to the quasiparticles or physical quanta that are connected to the observable phenomena of solid state physics, such as phonons and magnons. The interaction between these quanta and macroscopic objects such as boundaries, that arises in many-body theory can be discussed in terms of a "self-consistent" potential that represents the object. This is where many quantum effects are manifest. At zero temperature, quantum field theory gives exact solutions for these sorts of many-body problems. The importance of field theory in solid state physics has increased with its new developments that extend it to the treatment of finite temperature and non-equilibrium effects.

The semi-classical approach to transport theory is concerned with specifying the distribution function of the particles. This is represented by the function $f_{\mathbf{k}}(\mathbf{x},t)$, which represents the probability of a particle being in momentum state $\mathbf{k}$, at position $\mathbf{x}$, at time t. The Boltzmann equation is a self-consistent equation for the classical single

particle distribution function. It describes the balance between the influence of an accelerating external field, and the thermal diffusiop and scattering. The effect of external fields is present through perturbations of the distribution function (Callaway, 1976; Ziman, 1979), and has been thoroughly studied for magnetic fields (see for example, Bailyn, 1962; Stinchcombe, 1961, for homogeneous fields, or Moliner and Simons, 1957; Man'kov, 1962; and Berger, 1984 for inhomogeneous fields), and electric fields (Sarker *et al*, 1986). The full expression with electric and magnetic fields in the relaxation time approximation is

$$\partial_t f_k - [\mathbf{E}+\nabla\times\mathbf{B}]\cdot\nabla_k f_k = [f_k^0 - f_k]/\tau_k,$$

where f_k^0 denotes the equilibrium distribution with no perturbing external electric and magnetic fields, at temperature, T, and τ denotes the relaxation time, arising from inter-particle collisions.

The transport coefficients have been obtained by solving the Boltzmann equation, and their calculation forms the main link between the statistical mechanics and the various quantum field theoretical treatments of transport theory.

Kubo Formalism: Zero and Finite Temperature

Another approach to transport more deeply rooted in quantum mechanics is the so-called Kubo formalism or linear response theory for many-body systems (Kubo, 1957; Kadanoff and Baym, 1962), which relates transport properties to correlation functions. It is assumed that the response of a system is linearly proportional to the applied field. The magnitude of the response provides a measure of the corresponding transport coefficient. The Kubo formula was first derived for electric fields, where the induced

current is proportional to the applied electric field. It was found that the total current was made up of two terms, the first proportional to the field, and the second, to the expectation value of the local current operator which arises from the interaction between the field and the system particles. This expectation value is in fact directly related to the electric field by a time correlation function called the Kubo formula.

$$\sigma_{ij} = \frac{1}{kT}\int_0^\infty < j_i(t)\, j_j(0) > dt + \frac{n_0 e^2}{mkT}\delta_{ij} \qquad (1.1)$$

The brackets represent the average of the expectation value of the operators contained, over the equilibrium ensemble. The i and j components of the current operator are the denoted by $j_i(0)$, at time $t=0$, and $j_j(t)$ at a later time, t, and n_0 represents the equilibrium density of particles of mass m.

At zero temperature, the correlation function is just an expectation value with respect to the ground state of the system. It can be computed using such standard techniques of quantum field theory as perturbation theory and Feynman diagram techniques, through Wick's theorem, for time-ordered Green's functions (Bogoliubov and Shirkov, 1980).

Perturbation theory is established from the fact that most interesting systems consist of particles whose exact state is not precisely known. Working in the interaction representation, the system is divided into two parts; an exactly solvable unperturbed part, that is, the one whose eigenfunctions and eigenenergies are known, and a part containing the effect of the interaction considered as small perturbations of the first subsystem.

Wick's theorem is a mathematical construction which allows the replacement of the operators in multi-operator expectation values by creation and annihilation operators.

The commutation relations between such operators must be known, so that by a series of commutations, the annihilation operators can be gathered to the right of the expectation value, thereby annihilating the vacuum, leaving simpler terms that arise from the commutations. For example, the pairing of two creation and annihilation operators to be used in the time-ordered ground state expectation value is

$$<0|\ T\ [a_n^{\dagger}(t)\ a_m(t')]\ |\ 0>.$$

The commutation relations between the two define the way a product of operators is contracted. The end result of this sort of pairing is a sum of all possible paired products, or an expansion in terms of unperturbed single-particle Green's functions.

A combination of these techniques provides a well-defined calculation procedure of the correlation function, at zero temperature, that arises from the Kubo formalism in relation to a particular transport coefficient.

Finite temperature introduces a mean energy and a thermal average of observables. The correlation function in equation (1.1) becomes a trace over a thermal distribution. The solution can be found by the imaginary time technique of Matsubura (Matsubara, 1955). The complication of the thermal effect comes from the fact that the perturbing part of the Hamiltonian will appear twice; once in the time exponential factor, $e^{\pm iHt}$, as in the zero temperature situation, and again in the density operator $e^{-\beta H}$. This complicates the problem a great deal, as the second term must be expanded perturbatively. Because both terms are arguments of an exponential, the problem is resolved if the two could be combined, so the Matsubara method treats β and t as the real and imaginary parts of a complex temperature. The Matsubara Green's functions, then, contain an

imaginary time, τ.

The main problem with the Matsubara formalism is that once an imaginary time solution is achieved, an analytic continuation to the real time is required. The continuation tends to be unwieldy, and in the actual analysis of transport properties, approximation procedures must be used which are unsatisfactorily simple. This was demonstrated in the analysis by Kadanoff and Baym (1962). The extension to non-equilibrium is not obvious.

An approach that extends the Matsubura technique to consider both real time and finite temperature is the Path Ordering Technique (Mills, 1969), which will be discussed later.

Real Time Methods at Finite Temperature

1. Thermo field dynamics

In a field theory, dynamical observables are associated with an an operator average, in some specially defined space. This average can be evaluated from many different standpoints such as using a Greens function approach to finding the expectation value of the operator, or solving a density matrix that completely defines the system at any time.

Thermo Field Dynamics (TFD) was founded on the attempt to compute this time dependent ensemble average without recourse to the imaginary time formalism of Matsubura. The procedure is based on replacing or expressing the trace thermal average of an observable by its expectation value in terms of some "thermal vacuum", or thermal wavefunction.

$$<\beta|\ A\ |\beta> = Tr[e^{-\beta H} A] \,/\, Tr[e^{-\beta H}] \qquad (1.2)$$

with $e^{-\beta H}$ is the equilibrium density operator. TFD had its origins in superconductivity, (Leplae *et al*, 1974), and was detailed by Takahashi and Umezawa (1975) where the name was coined and the creation and annihilation operators for this thermal "vacuum" were constructed.

The original construction of TFD began with introducing a mirror space having a single particle operator $\tilde{a}$, obeying the same canonical commutation relations as the operators, a, of the normal Hilbert space.

$$[a_n, a_m^\dagger] = [\tilde{a}_n, \tilde{a}_m^\dagger] = \delta_{nm} \qquad (1.3)$$

The temperature dependent operator is defined as the linear combination of a_n and $\tilde{a}_n$.

$$\begin{aligned} \alpha_n(\beta) &= c_n(\beta)\ \tilde{a}_n + d_n(\beta) a_n^\dagger \\ \tilde{\alpha}_n(\beta) &= c_n(\beta)\ a_n - d_n(\beta) \tilde{a}_n^\dagger \end{aligned} \qquad (1.4)$$

If it is required that these new operators obey the canonical commutation relations,

$$[\alpha_n(\beta), \alpha_m(\beta)^\dagger] = [\tilde{\alpha}_n(\beta), \tilde{\alpha}_m(\beta)^\dagger] = \delta_{nm} \qquad (1.3.1)$$

then the mapping is the Bogoliubov transformation. The constants must satisfy

$$c_i(\beta)^2 + d_i(\beta)^2 = 1 \qquad (1.5)$$

hence may be written as

$$\begin{aligned} c_n &= \cos\theta_n \\ d_n &= \sin\theta_n \end{aligned} \qquad (1.4.1)$$

The parameter θ_n will be determined from the requirement given in equation (1.2). The thermal vacuum or thermal wavefunction is defined so that the following relationship with the annihilation operators is true.

$$\alpha(\beta)\,|\,\beta> = \tilde{\alpha}(\beta)\,|\,\beta> = 0. \qquad (1.6)$$

The requirement (1.2) is equivalent to

$$<\beta|\ a_n^\dagger a_m\ |\beta> = \frac{\delta_{nm}}{e^{\beta\epsilon_n} + 1},$$

given that $\tan\theta_n = e^{\beta\epsilon_n/2}$. The term on the right hand side is the Fermi-Dirac distribution for particles, since the particles of the system which will be discussed are electrons, however if the operators were defined to obey anticommutation relations, the corresponding expectation value would give the Bose-Einstein distribution. The Bogoliubov transformation and the thermal wavefunction are now fully defined. Substituting expansion (1.4) into relation (1.6) yields the thermal state condition that relates the mirror or tilde space to the non-tilde space, by defining the thermal behavior of the system.

$$a_n \mid \beta> = e^{\beta\epsilon_n/2}\, \tilde{a}_n^{\dagger} \mid \beta> \qquad (1.7)$$

Equation (1.6) defines creation and corresponding annihilation operators obeying commutation relations (1.3.1), in a space built from the thermal wavefunction $\mid \beta>$. Having them, a Wick's theorem can be constructed.

The doubling of the degrees of freedom of the system by the introduction of a mirror space can be interpreted physically. At finite temperature, a certain number of thermally excited states will always exist. The thermal wavefunction represents the lowest possible number of excited states, meaning that the ground state of the system includes these "hole" thermal states. An excitation of the system may then be described as either the creation of an excited state or the annihilation of a hole state. The doubling of the system space accounts for this duality. The conditions that ensure the equivalence of the descriptions, are that the operators of the two spaces have a one-to-one correspondence, and that the annihilation of particles corresponds to the creation of holes. The latter is called the thermal state condition, and has been derived as equation (1.7).

This type of construction has recently been extended to dissipative TFD (see for

example Umezawa *et al*, 1987).

2. Superoperators

Another construction of a method wherein the trace average can be replaced by an expectation value is Fano (1957) and Crawford's (1958) superoperator formalism where a new "double" space is defined, that is called the thermal Liouville space. This was shown to be an equivalent formulation to TFD by Schmutz (1978).

The Hilbert space of the system has a set of basis kets $| n >$. Define a new space whose basis states are

$$| n,m >> = | \{ | n > < m | \} >>. \tag{1.8.1}$$

$$<< n,m | = | n,m >>^{\dagger} = << \{ | n > < m | \} |. \tag{1.8.2}$$

If the inner product is defined in the following way,

$$<< n'm' | nm >> = < n' | n > < m | m' > \tag{1.9}$$

and the completeness condition holds,

$$\sum_{nm} | nm >> << nm | = \hat{1}$$

then the operators in this space also form a linear space. This new space is referred to as the Liouville space. The definition of the action of operators $\mathbf{A}$ in this space (or "superoperators" to distinguish them from the operator states) is defined in terms of the Hilbert space operator A.

$$\mathbf{A} | n\tilde{m} >>' <-> | A | n > < m | >>,$$

Also, the following states can be defined on the Liouville space.

$$| A >> = \sum_{nm} | nm >> < m | A | n >$$

$$<<A| = \sum_{nm} <m|A|n><<nm|$$

Then the expectation value of any operator with respect to state $|1>>$ defined from the Hilbert space identity operator may be written as the trace of the operator.

$$<<1|A|1>> = Tr\ A. \tag{1.10}$$

By the same token, a new state may be defined from the equilibrium density operator so that the expectation value is a trace thermal average.

$$<<1|A\rho|1>> = Tr\ A\rho$$
$$<<1|A|\rho>> = Tr\ A\rho$$

The operator ρ is the density operator in an equilibrium system, or $e^{-\beta H}$, which appears in the thermal average, in equation (1.2). The thermal wavefunctions in the superoperator formalism are a little different from those of TFD, but the thermal average has been replaced by an expectation value in a new space.

There are two more points of equivalence between the two methods. The duality of this representation is apparent through the fact that operators α_i and $\tilde{\alpha}_i$ may be defined as the annihilation of state $|n>$ of the original Hilbert space, or the creation of state $<m|$.

$$\alpha_i |n\tilde{m}>> = |\{\alpha_i |n><m|\}>>$$

$$\tilde{\alpha}_i |n\tilde{m}>> = \sigma^{\mu+1}|\{|n><m|\alpha_i^\dagger\}>>$$

with $\mu = \sum_i (m_i - n_i)$, m_i and n_i representing the number of electrons, $a_i^\dagger a_i |n> = n_i |n>$. The second important point is that creation and annihilation operators and their commutation relations can be defined in this space, and hence a Wick's theorem may be constructed in the same way as in TFD. Relations

$$\gamma_i |\rho_0>> = 0$$
$$\tilde{\gamma}_i |\rho_0>> = 0 \tag{1.11}$$

are true if the operators are defined from the Hilbert space operators as

$$\gamma_i = z_i^{1/2}[\alpha_i - e^{\beta\epsilon_i}\tilde{\alpha}_i^\dagger] \tag{1.12.1}$$

$$\tilde{\gamma}_i^\dagger = z_i^{1/2}[\tilde{\alpha}_i^\dagger + \alpha_i] \tag{1.12.2}$$

The normalization factor $z_i^{1/2}$ is determined from the canonical commutation relations, and is given by

$$z_i^{1/2} = 1 + \frac{f_i}{1+f_i}$$

with $\{\gamma_i, \gamma_j^\dagger\} = \{\tilde{\gamma}_i, \tilde{\gamma}_j^\dagger\} = \delta_{ij}$

This establishes the correspondence between the superoperator formalism, TFD and Green's functions techniques.

The thermal state condition for this formalism may be found by substituting (1.12.1) into (1.11):

$$\alpha_i \,|\, \rho_0 >> = f_i \,\tilde{\alpha}_i^\dagger \,|\, \rho_0 >>$$

where $f_i = e^{\beta\epsilon_i}$. The time dependence can be introduced through the operators as $\alpha_i(t) = e^{i\hat{H}t}\,\alpha_i\, e^{-i\hat{H}t}$. The time dependent thermal state condition is as follows.

$$\alpha_i(t) \,|\, \rho_0 >> = f_i \,\tilde{\alpha}_i^\dagger(t) \,|\, \rho_0 >> \tag{1.13}$$

This formulation is a little easier to use than the Bogoliubov transformation construction, and the extension to non-equilibrium systems is clearer.

3. Path ordering and other finite temperature methods

A generalization of the Matsubara technique that includes real time is the Path Ordering Technique (Mills, 1969). The technique replaces the time-ordering of the Matsubura technique by a contour ordering, by extending the integration along the imaginary axis, running from 0 to $i\beta$ to a contour starting at some time t_0 on the real axis and following a path in the complex time plane to the point $t_0 - i\beta$, subject to the

constraint that the contour must increase monotonically in the imaginary time, and that it have a real component. This gives a complex contour, monotonic along the imaginary axis that can be parametrized piecewise by a real parameter. If the real time limits are extended to infinity, the parts of the contour along the imaginary axis can be shown to have a vanishingly small contribution. The remaining real contour doubles back on itself, because of the conditions on it. Thus a doubling of degrees of freedom arises naturally from the attempt to calculate the real-time Green's function.

The equivalence of these techniques has been fairly extensively examined and discussed (Ojima, 1981; Araki and Woods, 1963; Niemi and Semenoff, 1984a; 1984b) and it has been established that other real time formulations are equivalent. The c^*-algebra approach (Araki and Woods, 1963), which was shown by Ojima (1981) to be equivalent to the TFD method. Niemi and Semenoff (1984a; 1984b) have shown how TFD can be expressed in the Feynman path integral formulation. TFD allows us to exploit many of the other properties of usual quantum field theory such as the Feynman diagram method, and the operator formalism. For a detailed history of finite temperature field theory, see the review by Landsman and van Weert (1987).

4. Non-Equilibrium Thermo Field Dynamics

The Kubo formalism technique of calculating transport properties is limited by the fact that only the response of a system to an external perturbation may be treated. This restricts the type of non-equilibrium systems that can be studied, since all systems cannot be treated in this fashion. It is important, then, to look at the extension of these real time formulations of quantum statistical mechanics to consider the general class of

non-equilibrium situations.

Non-equilibrium thermo field dynamics (NETFD) examines the relaxation of a system that is initially perturbed in some way through thermal effects. The scattering mechanism, and thermal effects serve to return the system to thermodynamic equilibrium.

The extension of TFD to non-equilibrium situations can be constructed in the superoperator formalism. The thermal state condition must be redefined to include a more general distribution kernel which evolves in time. The difference is that a non-equilibrium system can no longer be described by an equilibrium ensemble of states, so that the equilibrium density operator $e^{-\beta H}$, is not sufficient to describe the system. That is, the tilde and non-tilde fields are no longer related by a simple factor, but by a distribution function that evolves in time for a spatially inhomogeneous particle distribution.

$$\alpha_i(t) \mid \rho_0 >> = \sum_j f_{ij}(t)\, \tilde{\alpha}_j^{\dagger}(t) \mid \rho_0 >> \tag{1.14}$$

The creation and annihilation operators of the non-equilibrium thermal wavefunction are defined so that

$$\gamma_i(t) \mid \rho >> = 0$$
$$<<1 \mid \tilde{\gamma}_i^{\dagger\dagger}(t) = 0,$$

in terms of the electron operators.

$$\begin{cases} \gamma_i(t) = [\alpha_i(t) - \sum_j f_{ij}(t)\, \tilde{\alpha}_j^{\dagger}(t)] \\ \tilde{\gamma}_i^{\dagger\dagger}(t) = \sum_j [1 + f(t)]_{ij}^{-1} [\tilde{\alpha}_j^{\dagger}(t) + \alpha_j(t)], \end{cases}$$

As in the equilibrium situation, this means that the Wick's theorem can be used with these creation and annihilation operators. The quasiparticle operators obey the

canonical commutation relations

$$[\gamma_i(t), \gamma_j^{\dagger}(t)] = \delta_{ij} .$$

From these relations, and the definitions of the creation and annihilation operators in terms of $a_i^{\dagger}(t)$ and $a_i(t)$, the expectation value of the number operator, $a_i^{\dagger}(t)a_j(t)$, denoted by $n_{ij}(t)$, can be found using Wick's theorem to write all the annihilation operators to the right and all the creation operators to the left.

$$n_{ij}(t) = \sum_j f_{ij}(t) [1 + \sum_j f_{ij}(t)]^{-1} \qquad (1.15.1)$$

$$n_{ij}(t) = \frac{<<1 \mid a_i^{\dagger}(t)\, a_j(t) \mid \rho(t_0)>>}{<<1 \mid \rho(t_0)>>} \qquad (1.15.2)$$

If the particle density is homogeneous, $f_{ij} = f_i \delta_{ij}$, the expectation value of the number operator indicates the number of particles that occupy a state i. It would seem that there is some correspondence between this quantity which will be called the density function, and the distribution function that is described in the semi-classical Boltzmann equation.

In the next chapter, the application of this formalism to the evaluation of the conductivity tensor of a system of electrons in crossed electric and magnetic fields will be discussed, as an example of the type of calculation of transport properties that is possible. A simple form of relaxation of the system is being investigated, where the electrons are coupled to a thermal reservoir. Since only the transport properties of the electrons are of interest, the reservoir degrees of freedom will be projected out by means of the coarse graining procedure. This involves the manipulation of the Schrödinger equation solution to give an equation of motion for the new electron system state. The end result is a master equation for the wave function of the electrons in terms of an effective Hamiltonian that describes the dynamics of the electronic system. It should be noted that

this projection procedure gives rise to a dissipative term that couples the tilde and non-tilde fields that have been defined in the TFD formalism. A detailed discussion of the coarse graining technique will follow in chapter II.

The approach of quantum field theoretical techniques to study transport equations has been the subject of a number of recent reports. (Arimitsu, 1987; Mahan, 1987; Kreiger and Iafrate, 1987) Arimitsu uses an evolved form of the Bogoliubov transformation construction to derive a quantum transport equation, and Mahan follows a derivation using Green's functions, finding additional terms.

The importance and development of a quantum field theoretical treatment of non-equilibrium systems has been discussed. The simplicity and elegance of NETFD was seen in the case of the non-trivial extension to non-equilibrium systems, but will not become fully apparent until it is seen in use. The purpose of this investigation is to see how a transport equation emerges from this general non-equilibrium field theoretical formulation, and how transport properties, namely electrical conductivity, can be evaluated from the solution of such an equation. The parallels with the corresponding semi-classical calculations will be drawn, once the transport equation has been found.

The connection to the gauge invariant Boltzmann equation is not obvious because of the inherent gauge dependence of a system with a magnetic field. There seems to be some connection through the number operator expectation value, however. It should be interesting to see how a Boltzmann-type equation emerges, and what considerations the gauge invariance introduces. Finally, in order to see how the transport properties are affected by a spatial discontinuity in the field, the semi-classical solution of the

Boltzmann equation will be used to study the electrical conductivity in the presence of a domain wall.

Chapter II: The Transport Equation

Introduction

The problem under consideration is the derivation of a transport equation for a non-equilibrium system influenced by both a magnetic and an electric field, using perturbation theory. The difficulty arises from the fact that the magnetic field introduces a gauge dependence, and hence is difficult to treat perturbatively. The electric field will be chosen to be the perturbation $V = e\phi$, and the unperturbed Hamiltonian will be diagonal in a space which will be defined in terms of a maximal set of commuting observables of the system of electrons in a magnetic field. Again, a careful eye must be kept on the gauge, in the choice of these operators. It is important that any measureable quantities that arise from a theoretical calculation, namely the expectation values of the operators, not depend on the gauge, which is a purely mathematical construct.

Treated as an initially perturbing effect, the electric field will have excited the particles in the magnetic field, that is, the equilibrium energy level occupation will be disturbed, at time t=0. The perturbation competes with the scattering process, and eventually a steady state will be achieved. This restoration to equilibrium is the "relaxation" of the system, and as previously discussed, the simplest sort of relaxation mechanism (thermal) will be considered.

The first step in the calculation is to quantize the field. This entails the choice of three operators, which is the number required by dimensionality to completely specify but not give too much information about a the system. Gauge invariance is an important consideration here, and will be discussed in relation to the appropriate choice of the quantum numbers. The quantization of the field together with the choice of interaction between the electrons and the reservoir leads immediately to a general definition of the reservoir particle operators, since the specific relaxation mechanism will be a coupling between the electrons and reservoir particles. While the reservoir operators will be projected out, and hence it is not necessary to know their exact nature, it is required that the coupling be gauge invariant, which is a non-trivial consideration. Once the gauge invariant creation and annihilation operators are known, the coarse graining technique, following the method by Arimitsu and Umezawa (1985; 1987) can be applied to project the reservoir operators from the Schrödinger equation which will result in a master equation for the system.

The master equation is transformed into a transport equation by using the thermal state condition to introduce the distribution kernel $F(t)$. Once the transport equation has been derived, the electronic conductivity for a homogeneous magnetic field will be found from the solution for the transport equation. This chapter is concluded with a discussion of the relation between the distribution kernel from the thermal state condition, and the distribution function of the Boltzmann equation, the two of which would intuitively be expected to correspond in some way.

Quantizing the Field

The formulation of NETFD that will be used is expressed in the number operator representation that specifies, by means of the appropriate creation and annihilation operators, the number of electrons in each energy state, or the occupation numbers of the states. The electron and reservoir creation and annihilation operators need to be defined, and the fields written in terms of those operators.

1. Electron Operators

The Hamiltonian of an electron in the presence of the magnetic, $\mathbf{B}=\nabla\times\mathbf{A}$, and electric, $\mathbf{E}=-\nabla\phi$, fields is

$$\hat{H} = \frac{\Pi^2}{2m} + e\,\phi, \tag{2.1}$$

where $\Pi=\hat{p}-\frac{e}{c}\hat{\mathbf{A}}$ is the kinematical momentum, related directly to the electron velocity, as opposed to the canonical momentum, $\hat{p}$, defined by the canonical commutation relations with the position operator. The unperturbed Hamiltonian has been chosen to be $\hat{H}_0=\Pi^2/2m$, thus the basis states will be determined by observables that commute with $\hat{H}_0$. The magnetic field is chosen to be in the $\hat{z}$ direction,

$$\mathbf{B} = B\ \hat{\mathbf{e}}_z \tag{2.2}$$

so two obvious choices of labels for the states of the system are the energy, E, and the momentum in the direction of the field, p_z. In general, however, $\frac{\Pi^2}{2m}$ and the Π_i's do not commute, for $i=x,y$, hence the problem is non-trivial. The eigenstates of $\hat{H}_0$ are the Landau levels (Landau and Lifshitz, 1965) and these would seem to be the logical basis states.

Now consider the equation of motion of the kinematical momentum operator, $\dot{\Pi}=\frac{e}{2mc}[\Pi^2,\Pi]$. Then using the canonical commutation relation $[\hat{x}_i\,,\,\hat{p}_j\,]=i\,\delta_{ij}$, results in the following equation for a constant magnetic field,

$$\dot{\Pi}=\frac{e}{c}\dot{\mathbf{x}}\times\mathbf{B},$$

which gives the following constants of motion

$$\frac{d}{dt}[\Pi-\frac{e}{c}\mathbf{x}\times\mathbf{B}]=0.$$

The constants of motion in the x and y directions are gauge invariant operators that each commute with the Hamiltonian.

$$[\hat{H}_0,\hat{x}_0]=[\hat{H}_0,\hat{y}_0]=0$$

$$\hat{y}_0=\frac{\Pi_x}{m\,\omega_c}+y$$

$$\hat{x}_0=\frac{\Pi_y}{m\,\omega_c}-x$$

It will be seen that classically, these represent the centers of circular orbits.

If a specific choice of gauge is made, letting $\mathbf{A}=B\,[-y\,,0,0]$, then the maximal set of commuting operators which define this space is $\{\hat{H}_0,\ \hat{p}_z\,,\ \hat{p}_x\,\}$, where, in order simplify the notation, the operator

$$\hat{y}_0=\Pi_x+\frac{eB}{mc}y$$

has been denoted in terms of the canonical momentum,

$$\hat{p}_x=\Pi_x+\frac{eB}{c}y$$

and thus the solution for the Shrödinger equation is given in appendix I, as

$$\psi_n(\mathbf{p})=Ae^{[i(p_x x+p_z z)]}e^{[-eB(y-y_0)^2/2c]}H_n[\frac{\sqrt{eB}}{\sqrt{c}}(y-y_0)]. \qquad (1.5)$$

The vector $\mathbf{p}$ denotes a two dimensional vector operator, $\mathbf{p}=\hat{p}_x+\hat{p}_z$ (see appendix I for

the details of the calculation). In fact, the form of the wavefunction will not change significantly if another gauge is chosen.

To illustrate the role of the gauge transformation, consider the three possible symmetric gauges for this choice of magnetic field, where A, the vector potential has the following forms;

$$\begin{cases} A^{(1)} = B_0\,(-y\,,\,0,\,0) \\ A^{(2)} = B_0\,(0,\,x\,,\,0) \\ A^{(3)} = B_0/2\,(-y\,,\,x\,,\,0) \end{cases} \tag{2.3}$$

In the gauge where the potential has the form $A^{(1)}$, that is, in which the wave function was calculated in appendix I,

$$\hat{\Pi}_x + \frac{e}{c}\hat{A}_x = \hat{p}_x\,.$$

Transforming to the second gauge, (2.3b), the following changes occur.

$$\begin{aligned} A^{(1)} &\rightarrow A^{(2)} = A^{(1)} + \nabla\Lambda \\ \psi^{(1)} &\rightarrow \psi^{(2)} = \psi^{(1)} \exp\left(\frac{ie}{c}\Lambda\right) \\ \hat{p}_x^{(1)} &\rightarrow \hat{p}_x^{(2)} = \hat{p}_x^{(1)} - \nabla\Lambda \end{aligned}$$

with $\nabla\Lambda = By\hat{i} + Bx\hat{j}$, and so we have $\Lambda = Bxy$. As $\hat{p}_x^{(1)}$ is a constant of motion in this gauge, call it simply $\hat{p}_x$. This gives us the following in the new gauge:

$$\hat{p}_x^{(2)} = \hat{p}_x - \frac{eB}{c}y$$

$$\psi_n^{(2)}(x\,,y\,,z\,,\mathbf{p}) = e^{\frac{ieB}{c}xy}\; e^{i\left[p_x x + p_z z\right]}\; e^{-\frac{eB}{2c}(y-y_0)^2} H_n\left[\sqrt{\frac{eB}{c}}\,(y-y_0)\right],$$

where $y_0 = \dfrac{c\;p_x}{e\;B}$

The wave function changes only by a simple phase factor. It can be shown that although $\hat{p}_x^{(2)}$ changes in this gauge, its eigenvalue does not; the change of gauge does not affect the actual eigenvalue spectra.

$$\hat{p}_x^{(2)} = -i\frac{\partial}{\partial x}\psi^{(2)}$$

$$= \left[p_x + \frac{eB}{c}y - \frac{eB}{c}y\right]\psi^{(2)}$$

$$\hat{p}_x^{(2)} = p_x\ \psi^{(2)}$$

In the third gauge, given by expression (2.3c), p_x is still an eigenvalue of the transformed $\hat{p}_x^{(3)}$.

$$\psi^{(1)} \longrightarrow \psi^{(3)} = \psi^{(1)}\, exp\,(\frac{ieB}{2c}xy)$$

$$\hat{p}_x^{(1)} \longrightarrow \hat{p}_x^{(3)} = \hat{p}_x^{(1)} - \frac{eB}{2c}y$$

$$\hat{p}_x^{(3)}\psi^{(3)} = \left[(\frac{eB}{2c}y + p_x) - \frac{eB}{2c}y\right]\psi^{(3)} = p_x\psi^{(3)}$$

In all possible gauges in rectangular coordinates, $\hat{p}_x$ is an invariant of the motion, and more importantly, $p_x^{(1)}$ is always its eigenvalue. All calculations have the same result independent of gauge, so for simplicity, when an explicit vector potential is required, the first gauge, given by equation (2.3a) will be chosen. It has been shown that specifying the gauge does not actually change the eigenvalue spectra, and introduces only a simple phase factor in the wave function. The maximal set of commuting operators has been chosen in a gauge invariant way. The note at the end of the appendix, on degeneracy, reflects the existence of many possible sets of suitable operators.

As indicated in appendix I, the Hamiltonian eigenvalues are the energies of the Landau levels, labelled by the integer n. The complete set of basis states are labelled by the three gauge invariant quantum numbers are n, p_x, and p_z. The position space operator field, $\Psi(\mathbf{x})$, that destroys an electron at position $\mathbf{x}$, with momentum $\mathbf{p}$, and

energy ϵ_n can be expanded in these quantum numbers as follows;

$$\Psi(\mathbf{x}) = \sum_n \int d^2p \; a_n(\mathbf{p})\, \psi_n(\mathbf{p},\mathbf{x}). \tag{2.4}$$

where the coefficients $a_n(\mathbf{p})$ denote the single particle annihilation operator, and the integration $\int d^2p$, is over p_x and p_z. The operators $a_n(\mathbf{p})$ eliminate a single electron with momentum $\mathbf{p}$ and energy E_n, and obey the following commutation relation.

$$\left\{ a_n(\mathbf{p}),\, a_m^\dagger(\mathbf{k}) \right\} = \delta_{n,m}\; \delta(\mathbf{p}-\mathbf{k}) \tag{2.5}$$

From this relation, the commutation relation for the operator fields is

$$\left\{ \Psi(\mathbf{x}),\, \Psi^\dagger(\mathbf{x}') \right\} = \delta(\mathbf{x}-\mathbf{x}')$$

Thus the space has been defined by gauge invariant basis states which give rise to electron creation and annihilation operators.

2. Reservoir Operators

Before expanding the fields in terms of the electron creation and annihilation operators, it would be appropriate to briefly discuss the reservoir creation and annihilation operators, as they too appear in the full Hamiltonian.

The simplest interaction between the electrons and the thermal reservoir may be represented by the following interaction Hamiltonian.

$$\dot{H}_{\int} = g \int d\mathbf{x} \left\{ \Psi(\mathbf{x})\, R^\dagger(\mathbf{x}) + R(\mathbf{x})\, \Psi^\dagger(\mathbf{x}) \right\} \tag{2.6}$$

where $\Psi^\dagger(\mathbf{x})$ is the operator field for the electrons, $R^\dagger(\mathbf{x})$ denotes the operator field for the reservoir, which creates a reservoir particle at $\mathbf{x}$, and g is a coupling constant. Substituting the expansion for $\Psi(\mathbf{x})$ in the Landau state basis, equation (2.4), into equation (2.6), yeilds the result

$$\hat{H}_{\int} = g\sum_{n}\int d^2p \int d^3x \left\{ a_n(\mathbf{p})\psi_n(\mathbf{x})R^{\dagger}(\mathbf{x}) + R(\mathbf{x})\, a_n^{\dagger}(\mathbf{p})\psi_n^{\dagger}(\mathbf{x}) \right\}. \quad (2.7)$$

If the gauge invariant creation and annihilation operators are defined

$$R_n^{\dagger}(\mathbf{p}) \equiv \int d^3x \;\; \psi_n(\mathbf{x},\mathbf{p})\, R^{\dagger}(\mathbf{x})$$
$$R_n(\mathbf{p}) \equiv \int d^3x \;\; \psi_n(\mathbf{x},\mathbf{p})\, R(\mathbf{x})$$

then the interaction Hamiltonian can be expressed as a function of the single particle operators.

$$\hat{H}_{\int} = g\sum_{n=1}^{\infty}\int d\mathbf{p} \left\{ a_n(\mathbf{p})\, R_n^{\dagger}(\mathbf{p}) + R_n(\mathbf{p})\, a_n^{\dagger}(\mathbf{p}) \right\}. \quad (2.8)$$

The reservoir is present to provide a relaxation mechanism for the system. It must satisfy two requirements. The first is that the reservoir particle creation and annihilation operators be gauge invariant, which is achieved if the reservoir operator fields transform as

$$R(\mathbf{x}) \rightarrow R'(\mathbf{x}) = R(\mathbf{x})\, e^{\frac{ie}{c}\Lambda}. \quad (2.9)$$

Secondly, the reservoir particles are built from the vacuum state in the same way as the electrons; the commutation relations between the tilde and non-tilde superoperators and between the reservoir and system operators are as follows.

$$\{R_n(\mathbf{p}),\, R_m(\mathbf{k})\} = 0 = \{a_n(\mathbf{p}),\, R_m(\mathbf{k})\} \quad (2.10)$$

It should also be noted that the thermal state conditions are similar to those of the system superoperators, except that they are defined with respect to the reservoir bra vector.

$$\begin{cases} <<1_R \mid R_n^{\dagger}(\mathbf{p}) = <<1_R \mid R_n(\mathbf{p}) \\ <<1_R \mid \tilde{R}_n^{\dagger}(\mathbf{p}) = -<<1_R \mid \tilde{R}_n(\mathbf{p}) \end{cases}$$

Or, adding time dependence of the operators,

$$\begin{cases} <<1_R \mid R_n^{\dagger}(\mathbf{p},t) = <<1_R \mid \tilde{R}_n(\mathbf{p},t) \\ <<1_R \mid \tilde{R}_n^{\dagger}(\mathbf{p},t) = -<<1_R \mid R_n(\mathbf{p},t). \end{cases} \quad (2.11)$$

As long as the thermal reservoir has these properties, its exact nature is otherwise insignificant.

3. Expansion

The unperturbed Hamiltonian, $\hat{H}_0$ can be expressed in terms of these single electron creation and annihilation operators $a_n(\mathbf{p})$ and $a_n^\dagger(\mathbf{p})$, as follows:

$$\begin{aligned}\hat{H}_0 &= \int d^3x\, \Psi(\mathbf{x})\, \hat{H}_{mag}\, \Psi^*(\mathbf{x}) \\ &= \sum_{n,n'=0}^{\infty} \int_{-\infty}^{\infty} d^2p \int_{-\infty}^{\infty} d^2k\; H_{n,n'}^{\mathbf{p},\mathbf{k}}\; a_{n'}^\dagger(\mathbf{k})\, a_n(\mathbf{p})\end{aligned} \tag{2.12}$$

where $H_{n,n'}^{\mathbf{p},\mathbf{k}} = [(n+\frac{1}{2})\,\omega_c + \frac{p_z^2}{2m}]\delta_{n,n'}\delta(\mathbf{p}-\mathbf{x})$.

To write the electric field perturbation in this representation, consider the case for which the electric field is perpendicular to the magnetic field. The choice of gauge that has been made gives the field the form $\mathbf{E}=E\,\hat{\mathbf{e}}_y$, but this does not represent a serious loss of generality, as it can be shown that the same expansion in the creation and annihilation operators occurs for the gauges given in (2.3). The scalar potential ϕ of the electric field in equation (2.1) can then be written in the position representation.

$$\phi = \mathbf{E}\cdot\mathbf{x} = E\,y$$

Expanding this field in terms of the single particle operators, as in equation (2.8), introduces the matrix elements $E_{n,n'}^{\mathbf{p},\mathbf{k}}$. This integral is evaluated exactly, using the generating function for the Hermite polynomials.

$$\begin{aligned}E_{n,n'}^{\mathbf{p},\mathbf{k}} &= e\;E \int_{-\infty}^{\infty} d\mathbf{r}\; \psi_{n'}^*(\mathbf{k})\; y\; \psi_n(\mathbf{p}) \\ &= eE \int_{-\infty}^{\infty} dx\; e^{i(p_x-k_x)x} \int_{-\infty}^{\infty} dz\; e^{i(p_z-k_z)z} \int_{-\infty}^{\infty} dy\; e^{\frac{eB}{2c}[(y-y_0)^2-(y-y'_0)^2]} \\ &\quad \times y\; H_n\Big[\sqrt{\frac{eB}{c}}(y-y_0)\Big]\, H_{n'}\Big[\sqrt{\frac{eB}{c}}(y-y'_0)\Big]\end{aligned}$$

$$= eE\ \delta(p_z - k_z)\,\delta(p_z - k_z)\int_{-\infty}^{\infty} dy\ e^{\frac{eB}{2c}[(y-y_0)^2-(y-y'_0)^2]}$$

$$\times\ y\ H_n[\sqrt{m\omega_c}(y-y_0)]H_{n'}[\sqrt{m\omega_c}(y-y'_0)]$$

And so the electric field part of the Hamiltonian, $\dot{H}_{pert}$, is given by integrating this expression,

$$\dot{H}_{pert} = eE\sum_{n,n'}\int_{-\infty}^{\infty} d^2p \int_{-\infty}^{\infty} dy\ a_n^{\dagger}(\mathbf{p})\ e^{-m\omega_c(y-y_0)^2} y\, H_{n'}\left[\sqrt{m\omega_c}(y-y_0)\right] \times H_n\left[\sqrt{m\omega_c}(y-y_0)\right] a_n(\mathbf{p})$$

with the result that

$$\dot{H}_{pert} = \frac{eE}{\sqrt{2m\omega_c}}\sum_{n,n'=0-\infty}^{\infty}\int^{\infty} d^2p\ \ a_n^{\dagger}(\mathbf{p})[\sqrt{n'}\delta_{n,n'-1}+\sqrt{n+1}\delta_{n,n'+1}]a_n(\mathbf{p}).$$

Combining equations (2.12) and (2.13) yields a gauge invariant expression for the complete second quantized Hamiltonian given in equation (2.1), in terms of the creation and annihilation operators, $a_n^{\dagger}(\mathbf{p})$ and $a_n(\mathbf{p})$, of the Landau levels of the electrons,

$$\dot{H}_S = \sum_{n=0-\infty}^{\infty}\int^{\infty} d^2p\ \left[(n+\frac{1}{2})\omega_c + \frac{p_z^2}{2m}\right] a_n^{\dagger}(\mathbf{p})\ a_n(\mathbf{p}) - \frac{\sqrt{e^2E^2(n+1)}}{\sqrt{2m\omega_c}}\left[a_n^{\dagger}(\mathbf{p})a_{n+1}(\mathbf{p}) + a_{n+1}^{\dagger}(\mathbf{p})a_n(\mathbf{p})\right]$$

which, because it describes the system of electrons, will be called the system Hamiltonian, $\dot{H}_S$. The Hamiltonian of the full finite temperature system includes the reservoir degrees of freedom which are represented by the creation and annihilation operators $R_n(\mathbf{p})$ and $R_n^{\dagger}(\mathbf{p})$ in the following expression.

$$\dot{H} = \sum_{n=0-\infty}^{\infty}\int^{\infty} d^2p\ \{\left[(n+\frac{1}{2})\omega_c + \frac{p_z^2}{2m}\right] a_n^{\dagger}(\mathbf{p})\ a_n(\mathbf{p}) - \frac{\sqrt{e^2E^2(n+1)}}{\sqrt{2m\omega_c}}\left[a_n^{\dagger}(\mathbf{p})a_{n+1}(\mathbf{p}) + a_{n+1}^{\dagger}(\mathbf{p})a_n(\mathbf{p})\right]$$

$$+ g\,[a_n(\mathbf{p})R_n^{\dagger}(\mathbf{p}) + R_n(\mathbf{p})a_n^{\dagger}(\mathbf{p})$$

The Hamiltonian has a kinetic term, an off-diagonal term that arises from the presence of the perturbing electric field, an interaction term that represents the relaxation of the system through a thermal reservoir, and a term describing the thermal reservoir. is known only through its effect on the electron system, and hence the last term of the Hamiltonian will be projected out. Knowing the relevent parts of the Hamiltonian, then, a master equation may now be derived for the states of the finite temperature system.

The Master Equation

The underlying purpose to this investigation is to find transport coefficients by evaluating the trace average, or, in NETFD, the expectation value, of the observables. It would seem important, then, to examine the average $<<1 \mid A_S \mid W(t)>>$ of some system observable A_S, where $\mid W(t)>>$ is the state generated at any time by the Hamiltonian acting on the thermal vacuum. $W(t)$ is the density operator. A definition for a new system thermal wavefunction will emerge.

The system Hamiltonian given in equation (2.14) includes both the electron and the reservoir degrees of freedom. The reservoir is only present to provide a relaxation mechanism for the electronic system hence the detailed nature of the dynamics of the associated variables is largely irrelevant aside from the requirement that gauge invariance is observed, and that the characteristic relaxation time is short enough to regard the reservoir to be in thermal equilibrium. The afore-mentioned coarse graining technique (Arimitsu and Umezawa, 1987) will now be used to show how the reservoir degrees of freedom are projected out, and consequently, how the evolution of the system can be described in terms of an effective Hamiltonian for the electrons. Following the treatment by Arimitsu and Umezawa, (1987), temperature dependence and dissipation will emerge in a self-consistent way.

The first step is to note that the ket $<<1 \mid$, defined by equation (1.10), can be decomposed, or that at $t = 0$, the system state is separable.

$$<<1 \mid = <<1_R \mid \times <<1_S \mid$$

and hence any expectation value of operators involving only the electronic system may

be written as

$$<<1|A_S \mid W(t)>> = <<1_S \mid A_S \mid W_S(t)>>$$
$$\text{where} \quad \mid W_S(t)>> = <<1_R \mid W(t)>>. \tag{2.15}$$

The reservoir degrees of freedom are projected out in this way, and the ket defined above may be considered as an effective time dependent wave-function involving only the electronic degrees of freedom.

Having defined $\mid W_S(t)>>$, its governing equation can now be found. The master equation for the system is derived by projecting out the reservoir operators from the Schrödinger equation for the system states. The Schrödinger equation for the interaction Hamiltonian then takes the following form.

$$\partial_t \mid W(t)>>_I = -ig \; e^{-i\hat{H}_0(t-t_0)}\hat{H}_I \, e^{i\hat{H}_0(t-t_0)} \mid W(t)>>_I \tag{2.16}$$

The central operator on the right-hand side of the equation is just the Schrödinger representation operator, but all three can be combined as $\hat{H}_I(t)$, the Dirac interaction representation of the interaction Hamiltonian. Also, the ket vector can be transformed from the interaction to the Schrödinger representation, using the same unitary operator.

$$\mid W(t)>>_I = e^{i\hat{H}_0(t-t_0)} \mid W(t)>>. \tag{2.17}$$

The solution of equation (2.16) involves the time ordering operator T:

$$\mid W(t)>>_I = \hat{Z}(t,t_0) \mid W(t_0)>>$$
$$\text{where} \quad \hat{Z}(t,\tau) = T \exp\left[-ig\int_{\tau}^{t} ds \; \hat{H}_I(s)\right] \tag{2.18}$$

Then the projecting out of the system vacuum state using the expression for the system state (2.15), and the solution of the Schrödinger equation, equation (2.18), gives the following relationship.

$$\mid W_S(t)>>_I = <<1_R \mid T\exp[-ig\int_{t_0}^{t} ds \; \hat{H}_I(s)] \mid W(t_0)>> \tag{2.19}$$

The equation of motion for the state $|W_S(t)>>$, or the master equation, can be found from this result. The derivation is outlined in appendix II.

$$\partial_t \mid W_S(t)>> = -i\,[\hat{H}_S + i\hat{K}(t)] \mid W_S(t)>> \qquad \text{(II.4)}$$

where $\hat{K}(t)$ represents the effect of the reservoir on the electrons and which may be calculated to lowest order in the coupling constant to give

$$\hat{K}(t) = -g^2 \int_{t_0}^{t} dt_1 <<1_R \mid \hat{H}_I(t_0)\hat{H}_I(t_1 - t + t_0) \mid W_R>>$$

In order to use the master equation (II.4) in an actual calculation, the form of $\hat{K}(t)$ must be made workable, and reservoir operators must be defined.

The first assumption made about the system is that the thermalizing effect of the reservoir is very quick. That is, the system is initially perturbed, but settles back to thermal equilibrium almost immediately. Thus $\hat{K}(t)$ can be simplified by expanding in the long time limit. If the effect of the thermal reservoir is treated as a perturbation, $\hat{K}(\infty)$ is just the first non-zero term of the expansion given below in (2.20).

$$\hat{K}(\infty) = \lim_{t - t_0 \to \infty} (-ig)^2 e^{-i\hat{H}_S(t-t_0)} \hat{K}_I^{(2)}(t)\, e^{i\hat{H}_S(t-t_0)}$$

$$= -\lim_{t - t_0 \to \infty} g^2 \int_{t_0}^{t} dt_1 <<1_R \mid \hat{H}_I(t_0)\hat{H}_I(t_1 - t + t_0) \mid W_R>> \qquad (2.20)$$

To restate the master equation in the long time limit, equation (II.4) may be rewritten,

$$\partial_t \mid W_S(t)>> = -i\,[\hat{H}_S + i\hat{K}_1(\infty)] \mid W_S(t)>>$$

where $\hat{K}_1(\infty)$ is given by equation (2.20).

The interaction part of the master equation (II.4) can now be written in terms of the superoperators $a_n(\mathbf{p})$, $R_n(\mathbf{p})$, and their adjoints. As the form of $\hat{H}_S$ has been determined, we are now concerned with the interaction part of (II.4). To begin with,

substitute (1.3) and (2.8) into (2.20). As $a_n(\mathbf{p})$ and $a_n^\dagger(\mathbf{p})$ have no effect on the reservoir vacuum states, they can be taken outside the bra and ket vectors, using the commutation relations (2.10). All terms which violate number conservation, *i.e.*

$$<<1_R \mid R_n(\mathbf{p},t')\, R_n(\mathbf{p},t) \mid W_R>> = 0.$$

have been dropped, and the time translation $t \to t_1 - t \to -t$ has been made after substituting $a_n(t) = a_n e^{i\epsilon_n t}$. Then,

$$\dot{K}(\infty) = -g^2 \sum_{n,m} \int d^2k \int d^2p \int dt\ \dot{K}(\infty)^{\mathbf{pk}}_{n,m}$$

where the integrand is given by the rather complicated expression

$$\begin{aligned}
\dot{K}(\infty)^{\mathbf{pk}}_{n,m} = \{ & a_n^\dagger(\mathbf{p})[<<1_R \mid R_n^\dagger(\mathbf{p},t) R_m(\mathbf{k}) \mid W_R>> a_m^\dagger(\mathbf{k}) \\
& + <<1_R \mid R_n^\dagger(\mathbf{p},t) \tilde{R}_m^\dagger(\mathbf{k}) \mid W_R>> \tilde{a}_m(\mathbf{k})] \\
& - \tilde{a}_n^\dagger(\mathbf{p})[<<1_R \mid \tilde{R}_n(\mathbf{p},t) a_m(\mathbf{k}) \mid W_R>> R_m^\dagger(\mathbf{k}) \\
& + <<1_R \mid \tilde{R}_n(\mathbf{p},t) \tilde{R}_m^\dagger(\mathbf{k}) \mid W_R>> a_m(\mathbf{k})] \\
& + a_n^\dagger(\mathbf{p}) \Big[<<1_R \mid R_n(\mathbf{p},t) R_m^\dagger(\mathbf{k}) \mid W_R>> a_m(\mathbf{k}) \\
& + <<1_R \mid R_n(\mathbf{p},t) \tilde{R}_m(\mathbf{k}) \mid W_R>> \tilde{a}_m^\dagger \\
& - \tilde{a}_n(\mathbf{p}) \Big[<<1_R \mid \tilde{R}_n^\dagger(\mathbf{p},t) R_m^\dagger(\mathbf{k}) \mid W_R>> a_m(\mathbf{k}) \\
& + <<1_R \mid \tilde{R}_n^\dagger(\mathbf{p},t) \tilde{R}_m(\mathbf{k}) \mid W_R>> \tilde{a}_m^\dagger
\end{aligned}$$

This can be simplified by using the thermal state conditions given in (2.11), together with the Kubo-Martin-Schwinger correlation.

$$<<1_R \mid R_n(\mathbf{p},t)\, R_m^\dagger(\mathbf{k}) \mid W_R>> = <<1_R \mid R_m^\dagger(\mathbf{k})\, R_n(\mathbf{p},t+i\beta) \mid W_R>> \tag{2.21}$$

This is where time appears in the formulation.

The time retarded and advanced correlation functions, $<<1_R \mid R_n(\mathbf{p},t) R_n(\mathbf{k}) \mid W_R>>$ and $<<1_R \mid R_n(\mathbf{k}) R_n^\dagger(\mathbf{p},t) \mid W_R>>$, may be expressed in terms of a single function $L^{\mathbf{pk}}_{nm}$ as follows.

$$\int_0^\infty dt \,<<1_R \mid R_n^\dagger(\mathbf{p},t)R_m(\mathbf{k}) \mid W_R>> e^{-i\epsilon_n t} \tag{2.22}$$

$$= \frac{1}{\pi}\int_0^\infty dt \int_{-\infty}^\infty du \; e^{iut} L_{nm}^{pk}(u)\, e^{-i\epsilon_n t} \tag{2.23}$$

$$\int_0^\infty dt \,<<1_R \mid R_m(\mathbf{k})R_n^\dagger(\mathbf{p},t) \mid W_R>> e^{-i\epsilon_n t} \tag{2.24}$$

$$= \frac{1}{\pi}\int_0^\infty dt \int_{-\infty}^\infty du \; e^{iut} L_{nm}^{pk}(u)\, e^{\beta u} e^{-i\epsilon_n t} \tag{2.25}$$

Temperature has appeared in a natural way. In terms of this function, then, the full expression for the dissipation is

$$\dot{K}(\infty) = \sum_{nm}\int d^2p \int d^2k \int_{-\infty}^\infty du \tag{2.26}$$

$$L_{nm}^{pk}[-\left(\delta(\epsilon_m - u)e^{\beta\epsilon_m} - \delta(\epsilon_n - u)\right)\left(a_n^\dagger(\mathbf{p})a_m(\mathbf{k}) + \tilde{a}_n^\dagger(\mathbf{p})\tilde{a}_m(\mathbf{k})\right) - \left(\delta(\epsilon_m - u) + \delta(\epsilon_n - u)\right)$$

$$\times\left(e^{\beta u}\,\tilde{a}_n(\mathbf{p})a_m(\mathbf{k}) + \tilde{a}_n^\dagger(\mathbf{p})a_m^\dagger(\mathbf{k})\right) + 2\delta_{nm}\,\delta(\mathbf{p}-\mathbf{k})]\}$$

Equation (2.26) consists of an imaginary part that is just the renormalized electron system Hamiltonian, and a real part that represents the thermally dissipative approach of the system to equilibrium. The real part of (2.26), which will be denoted by Π, is just

$$\Pi(\infty) = \sum_{nm}\int d^2p \int dk \int_{-\infty}^\infty du \;\; L_{nm}^{pk}(u)\{-\left[\delta(\epsilon_m - u)e^{\beta\epsilon_m} - \delta(\epsilon_n - u)\right]\left[a_n^\dagger(\mathbf{p})a_m(\mathbf{k}) + \tilde{a}_n^\dagger(\mathbf{p})\tilde{a}_m(\mathbf{k})\right]$$

$$-\left[\delta(\epsilon_m - u) + \delta(\epsilon_n - u)\right]\left[e^{\beta u}\,\tilde{a}_n(\mathbf{p})a_m(\mathbf{k}) + \tilde{a}_n^\dagger(\mathbf{p})a_m^\dagger(\mathbf{k})\right] + 2\delta_{nm}\,\delta(\mathbf{p}-\mathbf{k})\} \tag{2.27}$$

One last assumption will be made now, and it is to let the correlation function be symmetric.

$$L_{nm}^{pk} = L_n(\mathbf{p})\,\delta(\mathbf{p}-\mathbf{k})\delta_{nm}.$$

This is the same as the assumption that each mode is mutually independent. $L_n^p(\epsilon_n)$ can be factored out. The distribution function is defined as

$$\eta(\epsilon_n) = -\left[1 + e^{\beta\epsilon_n}\right]^{-1}. \tag{2.28}$$

Having made these substitutions, we have the simple form for the real part of the dissipation:

$$\Pi(\infty) = -\sum_{nm}\int d^2p \int dk\ L_n^p(\epsilon_n)\,[1+e^{\beta\epsilon_n}]\{[1-2\eta(\epsilon_n)][a_n^\dagger(\mathbf{p})a_m(\mathbf{k})+\tilde{a}_n^\dagger(\mathbf{p})\tilde{a}_m(\mathbf{k})]$$
$$-\,2[1-\eta(\epsilon_n)]\tilde{a}_n(\mathbf{p})a_n(\mathbf{p}) + 2\eta(\epsilon_n)\tilde{a}_n^\dagger(\mathbf{p})a_n^\dagger(\mathbf{p}) - 2\eta(\epsilon_n)\} \tag{2.29}$$

Let the function $\chi_n(\mathbf{p})$ be the prefactor.

$$\chi_n(\mathbf{p}) \equiv [1+e^{\beta\epsilon_n}]L_n^p(\epsilon_n)$$

The imaginary part is just the relabeled Hamiltonian relating to the system, $-i\,\Delta\hat{H}_S$.

$$\hat{K}_0(\infty) = -i\,\Delta\hat{H}_S + \Pi$$

Adding the electric and magnetic parts of the Hamiltonian, (2.13) and (2.12), to (2.29), gives the second quantized Hamiltonian of the temperature-dependent electric and magnetic fields,

$$\hat{H} = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d^2p\ \{\epsilon_n[a_n^\dagger(\mathbf{p})a_n(\mathbf{p})-\tilde{a}_n^\dagger(\mathbf{p})\tilde{a}_n(\mathbf{p})]$$
$$-\frac{eE}{\sqrt{m\,\omega_c}}[a_n^\dagger(\mathbf{p})a_{n+1}(\mathbf{p}) + a_{n+1}^\dagger(\mathbf{p})a_n(\mathbf{p}) - \tilde{a}_n^\dagger(\mathbf{p})\tilde{a}_{n+1}(\mathbf{p}) + \tilde{a}_{n+1}^\dagger(\mathbf{p})\tilde{a}_n(\mathbf{p})]$$
$$-\,i\,\chi_n(\mathbf{p})\,[1-2\eta(\epsilon_n)][a_n^\dagger(\mathbf{p})a_n(\mathbf{p})+\tilde{a}_n^\dagger(\mathbf{p})\tilde{a}_n(\mathbf{p})]$$
$$+\,i\,\chi_n(\mathbf{p})\left[2[1-\eta(\epsilon_n)]\,\tilde{a}_n(\mathbf{p})a_n(\mathbf{p}) - 2\eta(\epsilon_n)\tilde{a}_n^\dagger(\mathbf{p})a_n^\dagger(\mathbf{p}) - 2\eta(\epsilon_n)\right]\}$$

which is just the Hamiltonian in the master equation

$$i\,\partial_t\,|\,W_S>> = \hat{H}\,|\,W_S>> \tag{2.30}$$

The first term arising from the magnetic field is just the kinetic part of the Hamiltonian, the electric field introduces some off-diagonal terms, and the dissipative terms couple the tilde and non-tilde operators through the distribution function $\eta(\epsilon_n)$.

The Distribution Function

The thermal reservoir variables have been projected out of the Schrödinger equation, giving the master equation (2.30), but it is possible to further simplify it, by removing the tilde field. The relationship between the tilde and the non-tilde fields is defined by the thermal state condition which was originally given in equation (1.13) in the non-equilibrium case, relating single electron operators $a_n(\mathbf{p})$ and $\tilde{a}_{n'}(\mathbf{p})$ through a distribution kernel $f_{nn'}(\mathbf{p},t)$,

$$a_n(\mathbf{p},t) \mid W_S >> = \sum_{n'} f_{nn'}(\mathbf{p},t)\, \tilde{a}_{n'}^{\dagger}(\mathbf{p},t) \mid W_S >> \qquad (1.13)$$

for an inhomogeneous particle distribution. The master equation has been written in the Schrödinger representation with base states that evolve in time. The evolution of the system may be described by the evolution of the system state, $\mid W_S >>$. The evolution, $\mid W_S(t) >>$, is described by the distribution kernel $f_{nn'}(t)$, according to the following thermal state condition.

$$a_n(\mathbf{p}) \mid W_S(t) >> = f_{nn'}(t)\, \tilde{a}_{n'}^{\dagger}(\mathbf{p}) \mid W_S(t) >> \qquad (2.31)$$

The time derivative of equation (2.31) is the expression

$$a_n(\mathbf{p})\, \partial_t \mid W_S(t) >> = [f_{nn'}(t)\, \tilde{a}_{n'}^{\dagger}(\mathbf{p}) + f_{nn'}(t)\, \dot{\tilde{a}}_{m}^{\dagger}((\mathbf{p}))] \mid W_S(t) >> \qquad (2.32)$$

into which the master equation (2.30) can be substituted. These two equations, (2.32) and (2.31), completely determine the distribution kernel, thus the substitution is made. Since $\hat{H}(a_n - f_{nn'}(t)\tilde{a}_{n'}^{\dagger}) \mid W_S(t) >> \geq 0$,

$$a_n\, \hat{H}\, \partial_t \perp W_S(t) >> = \tilde{a}_n^{\dagger} \hat{H}\, \partial_t \mid W_S(t) >> = 0.$$

$$\text{thus } \left[a_n(\mathbf{p}) - f_{nn'}(t)\tilde{a}_{n'}^{\dagger}(\mathbf{p}), \hat{H}\right] \mid W_S(t) >> = \dot{f}_{nn'}(t)\, \tilde{a}_{n'}^{\dagger} \mid W_S(t) >> \qquad (2.33)$$

The equation for the distribution kernel, (2.33), can be written as a matrix equation.

by substituting the Hamiltonian given in equation (2.30), using the commutation relations for a_n,

$$\begin{aligned} &[a_n, a_n^\dagger \tilde{a}_n] = a_n \\ &[a_n, \tilde{a}_n^\dagger \tilde{a}_n] = [a_n, \tilde{a}_n\, a_n] = 0 \\ &[a_n, \tilde{a}_n^\dagger a_n^\dagger] = \tilde{a}_n^\dagger, \end{aligned} \tag{2.34}$$

and introducing the following matrices:

$$\begin{aligned} &\epsilon = \epsilon_n\, \mathbf{I} \\ &F_{nn'} = f_{nn'} \\ &\chi = \chi_n(\mathbf{p})\, \mathbf{I} \\ &\eta = \eta(\epsilon_n)\, \mathbf{I} \\ &J_{nm} = \frac{1}{i}\delta_{n,m+1}\sqrt{\frac{n}{2}} \end{aligned} \tag{2.35}$$

Then using the matrix notation, and multiplying by F^{-1} from the left, we obtain

$$\begin{aligned} i\partial_t F^{-1} = i\Big\{ \frac{1}{i}[\epsilon, F^{-1}] + \frac{eE}{\sqrt{m\omega_c}}[F^{-1}, (J-J^\dagger)] \Big\} \\ + i\Big\{ \chi(F^{-1}+1) - (F^{-1}+1)\chi + 2\eta\chi(F^{-1}+1) + 2F^{-1}\eta\chi(F^{-1}+1) \Big\} \end{aligned} \tag{2.36}$$

With a little more manipulation, (2.36) may be written as an equation for $N(t)=[1+F^{-1}]^{-1}$, which, from the definition of the quasi particle creation and annihilation operators (see (1.8)) is simply the expectation value

$$\begin{aligned} n_{nm}(\mathbf{pk},t) &= \Big[<< 1 \mid a_n^\dagger(\mathbf{p},t)\, a_m(\mathbf{k},t) \mid W_S(t) >> \Big] \Big[<< 1 \mid W_S(t) >> \Big]^{-1} \\ &= N_{nm}^{\mathbf{pk}} \end{aligned} \tag{2.37}$$

The z_{lm} term corresponds to the factor $z_k^{1/2}$ from equation (1.8). We operate by $(1+F^{-1})^{-1}$ from both sides of the equation, using these three relations;

$$\begin{aligned} &A^{-1}[A, B]\, A^{-1} = [A^{-1}, B] \\ &A^{-1}\{A, B\}\, A^{-1} = \{A, B\} \\ &(1+F^{-1})^{-1}\partial_t (1+F^{-1})\, (1+F^{-1})^{-1} = -\partial_t (1+F^{-1})^{-1}, \end{aligned} \tag{2.38}$$

along with

$$[A\,,\,B] = [1 + A\,,\,B].$$

The final result is the transport equation;

$$\partial_t N(t) + \frac{1}{i}[N(t),\,\epsilon] = \{\chi,\,N_0 - N(t)\} + \sqrt{\frac{e^2E^2}{m\omega_c}}\,[N(t),\,J - J^\dagger] \quad (2.39)$$

where we have used

$$(1+F^{-1})^{-1}\partial_t(1+F^{-1})\,(1+F^{-1})^{-1} = \frac{F}{1+F}\left[\frac{\partial_t(1+F)}{F} - \frac{(1+F)\dot{F}}{F^2}\right]\frac{F}{1+F}$$

$$= \partial_t\left(\frac{F}{1+F}\right) = -\partial_t(1+F^{-1})^{-1}.$$

This is a purely quantum mechanical result, which is gauge invariant. The left hand side of the equation is the kinetic term, arising just from the motion of the electron. On the right hand side, the χ term represents the thermal dissipation of the system, characterizing the return to thermal equilibrium. The last term is the off-diagonal perturbation introduced by the presence of the crossed electric field.

The transport equation for electrons in crossed magnetic and electric fields has been obtained. The solution of the linearized equation can be readily obtained, and as an example of the emergence of transport coefficients from such a general expression, the conductivity will be evaluated from that solution.

The Conductivity Tensor Components σ_{yy} and σ_{yz}

The solution of the transport equation can be used to find the conductivity tensor elements in much the same way as the Chambers' solution will be used to find the conductivity using the classical trajectories. The conductivity tensor components are found by first linearizing the master equation, (2.39), in the energy, and then solving it for δN_{nm} which is the addition to the steady state (zero field) density function on the order $o(E)$ in the electric field. The expression for the current can then be found, and substituted into the expression for the conductivity.

The steady state density is as follows.

$$N_{nm}(p_z) = N^0_{nm}(p_z) = \delta_{nm}\frac{1}{e^{\beta\epsilon_n}+1} \tag{2.40}$$

where $\epsilon_n = (n+\frac{1}{2})\omega_c + p_z^2/2m$. Then, neglecting terms of higher than linear order in energy,

$$N_{nm} = N^0_{nm} + \delta N_{nm}, \quad E \neq 0. \tag{2.41}$$

Substituting back into the master equation (2.39), the following equation results:

$$\frac{1}{i}(E_n - E_m)\delta N_{nm} = (\chi_n + \chi_m)\delta N_{nm} + \frac{1}{i}\frac{eE}{\sqrt{2\omega_c}}\times$$
$$\left\{\sqrt{n}\,[\kappa(E_{n-1})-\kappa(E_n)]\delta_{n,m+1} + \sqrt{n+1}[\kappa(E_{n+1})-\kappa(E_n)]\delta_{n+1,m}\right\}$$

where $\kappa(E) = [e^{\beta E}+1]^{-1}$. The solution of δN_{nm} is found to be;

$$\delta N_{nm} = \frac{\delta_{n+1,m}}{i(\chi_n+\chi_{n+1})-\omega_c}\sqrt{\frac{n+1}{2}}[\kappa(E_{n+1})-\kappa(E_n)]\frac{eE}{\sqrt{m\omega_c}} - \frac{\delta_{n,m+1}}{i(\chi_n+\chi_{n-1})+\omega_c}\sqrt{\frac{n}{2}}[\kappa(E_n)-\kappa(E_{n-1})]\frac{eE}{\sqrt{m\omega_c}} \tag{2.42}$$

This is the small energy correction to the steady state density function, to order $o(E)$

in the field.

The current density can be calculated from the following expectation value.

$$\mathbf{J}=<<1\mid \frac{e}{2im}\nabla[\psi^{\dagger}(\mathbf{x})\psi(\mathbf{x})]-\frac{e^{2}}{mc}\mathbf{A}\psi^{\dagger}(\mathbf{x})\psi(\mathbf{x})\mid W_{S}>>$$

The x-component of the current in the gauge $\mathbf{A}=[-By,0,0]$ which is the gauge that has been used throughout this discussion, reduces to the expression

$$J_x = e^2E \int dp_z \sum_n \kappa(E_n) \frac{\omega_c^2\tau^2}{(1+\tau\omega_c)^2} \tag{2.43}$$

under two assumptions. At low temperature, T below the Fermi temperature, the derivative of the distribution $\kappa(E)$ will be localized in the region of energy E close to the Fermi energy. The relaxation time can be approximated as

$$\chi_n + \chi_{n+1} \approx 2\chi = 2/\tau.$$

Also, the infinite summation over the energy has been shifted from n to n+1. The effect should be very small considering not only the large number of states in the Fermi surface, but also the insignificant number of occupied states in the lowest Landau level.

The conductivity element σ_{xy} is given by this expression.

$$\sigma_{xy} = \frac{e^2\tau}{m}\,\omega_c\, m\,[\int dp_z \sum_n \kappa(E_n)]\frac{\tau\omega_c}{1+\tau^2\omega_c^2}$$

The term in square brackets is the sum over all states of the distribution function, hence the number of all occupied Landau levels, and $\omega_c\, m$ is the degeneracy per unit volume of each level (see appendix). The product of these terms yields the number of electrons per unit volume, n, and so

$$\sigma_{xy} = \frac{ne^2\tau}{m}\,\frac{\tau\omega_c}{1+\tau^2\omega_c^2}. \tag{2.44}$$

In the same manner, it can be shown that

$$\sigma_{yy} = \frac{ne^2\tau}{m} \frac{1}{1 + \tau^2\omega_c^2}. \tag{2.45}$$

These are the expected components of the conductivity tensor.

The master equation for the system of electrons in crossed magnetic and electric fields was derived quantum mechanically, and solved directly for a physically measurable quantity, the conductivity tensor element σ_{yy} and σ_{xy}. In a further discussion of this transport equation, it will be seen how the solution of the Boltzmann equation emerges from the quantum mechanical approach to non-equilibrium statistical mechanics.

The Boltzmann Equation

In order to establish the relationship between the Boltzmann equation and the quantum transport equation (2.39), the latter must be transformed into the position representation, then shifted to the center of mass coordinates in such a way that gauge invariance will be preserved. This will lead to a Fourier transformation into the momentum space.

Equation (2.39) can be rewritten in component form.

$$\dot{N}_{nm} + \frac{1}{i}(\epsilon_n - \epsilon_m)N_{nm} = (\chi_n + \chi_m)\,(N^0_{nm}\delta_{nm} - N_{nm})$$
$$+ \frac{1}{i}\frac{eE}{\sqrt{2m\omega_c}}[(\sqrt{n+1}N_{n+1,m} - \sqrt{m+1}N_{n,m+1}) - (\sqrt{n}N_{n,m-1} - \sqrt{m}N_{n-1,m})]. \tag{2.46}$$

First, how does the spatial distribution function transform? N_{nm} may be transformed to the position representation by multiplying from both sides by the Landau wave function (equation (4) of the appendix) and its complex conjugate, summing over the energy states and integrating over momentum. A position-dependent distribution function is defined

$$N(\mathbf{x},\mathbf{x}';t) = \sum_{nm}\int d^2p\, \psi_n^*(\mathbf{p},\mathbf{x})\, N_{nm}\, \psi_m(\mathbf{p},\mathbf{x}').$$
$$= \langle\langle 1 \mid \psi^\dagger(\mathbf{x},t)\,\psi(\mathbf{x}',t) \mid W_S \rangle\rangle$$

In effect, $N(\mathbf{x},\mathbf{x}';t)$ is the expectation value of the number operator in the position representation. Since the distribution function is related to the expectation value of the number operator, it should be gauge invariant, as well as translationally invariant. The quantity $N(\mathbf{x},\mathbf{x}';t)$ is not gauge invariant, but transforms as

$$N(\mathbf{x},\mathbf{x}';t) \rightarrow N'(\mathbf{x},\mathbf{x}';t) = exp\,[\frac{ie}{c}\,(\Lambda(\mathbf{x}') - \Lambda(\mathbf{x}))\,]N(\mathbf{x},\mathbf{x}';t).$$

The gauge dependence may be extracted if a new function $\overline{N}_P$ is defined, which shall be called the density function.

$$N(\mathbf{x},\mathbf{x}';t) = exp\left[-\frac{ie}{c}\int_P \mathbf{A}\cdot d\,\mathbf{x}\right] \overline{N_P(\mathbf{x},\mathbf{x}';t)}$$

$$\overline{N_P(\mathbf{x},\mathbf{x}';t)} = \int d^3q \ \exp[-\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')] \ \overline{N}_P\left(\mathbf{q};\frac{\mathbf{x}+\mathbf{x}'}{2};t\right) \tag{2.47}$$

where the gauge exponential factor is introduced to compensate for the factor that arises from the transformation. The path of integration, P, is the path beginning at position $\mathbf{x}$ and ending at $\mathbf{x}'$. In order to see how the path should be defined, consider the kinetic energy term of equation (2.46).

The position representation of the energy term is as follows.

$$(\epsilon_n - \epsilon_m)\, n_{nm}(t) = \sum_{nm}\int d^2p\left[\left(-i\nabla_x - \frac{e}{c}\mathbf{A}(\mathbf{x})\right)^2 - \left(\nabla_{x'} - \frac{e}{c}\mathbf{A}(\mathbf{x}')\right)^2\right] N(\mathbf{x},\mathbf{x}';t)$$

Substituting (2.47) yields a very long and complex term.

$$(\epsilon_n - i\epsilon_m t)N_{nm} = \int_P d^3q \ \ e^{i\int_P d\mathbf{x}\cdot\left[\mathbf{q}+\frac{e}{c}\mathbf{A}\right]}\{\mathbf{q}\cdot$$

$$\times\frac{e}{c}\left[(\nabla+\nabla')\int_P d\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x})-(\mathbf{A}(\mathbf{x})-\mathbf{A}(\mathbf{x}'))\right]nxm$$

$$-i\left[\mathbf{q}+\frac{e}{c}\{(\nabla-\nabla')\int_P d\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x})-(\mathbf{A}(\mathbf{x})+\mathbf{A}(\mathbf{x}'))\}\right]$$

$$\cdot\nabla\overline{N}_P\left(\mathbf{q};\frac{\mathbf{x}+\mathbf{x}'}{2};t\right)$$

$$-i\left[(\nabla^2-\nabla'^2)\int_P d\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x})-(\nabla\cdot\mathbf{A}(\mathbf{x})+\nabla'\mathbf{A}(\mathbf{x}'))\right]nxm$$

$$\frac{e^2}{c^2}\left[(\nabla-\nabla')\int_P d\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x})-(\mathbf{A}(\mathbf{x})+\mathbf{A}(\mathbf{x}'))\right]$$

$$\times\left[(\nabla+\nabla')\int_P d\,\mathbf{x}\cdot\mathbf{A}(\mathbf{x})-(\mathbf{A}(\mathbf{x})-\mathbf{A}(\mathbf{x}'))\right]nxm\ \}$$

with $nxm \equiv \overline{N}_P\left(\mathbf{q};\frac{\mathbf{x}+\mathbf{x}'}{2};t\right)$. This expression would simplify significantly if a path is

chosen to satisfy

$$(\nabla-\nabla')\int_P d\mathbf{x}\cdot\mathbf{A}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) + \mathbf{A}'(\mathbf{x}). \tag{2.48}$$

This assumption limits the choice of gauges in which it is possible to apply the method of calculation presented here, and may be more restrictive than desired, ideally, it should be possible to define P so that the relationship is satisfied for a large number of possible gauges.

The choice of gauge made for this calculation, $\mathbf{A}=[-By,0,0]$, satisfies this relationship. If the path is parametrized by t,

$$\mathbf{x}(t) = (\mathbf{x}_2-\mathbf{x}_1)t + \mathbf{x}_1$$
$$d\mathbf{x} = (\mathbf{x}_2-\mathbf{x}_1)dt$$

where $\mathbf{x}_1\equiv\mathbf{x}$ and $\mathbf{x}_2\equiv\mathbf{x}'$, then

$$\begin{aligned}(\nabla-\nabla')\int_P d\mathbf{x}\cdot\mathbf{A}(\mathbf{x}) &= \\ &= -(\nabla-\nabla')B\int_0^1 dt\,[\tfrac{1}{2}(y+y')t+y](x-x') \\ &= -\frac{B}{2}\left\{(y_2+y_1)\dot{x}+(x_2-x_1)\dot{y}-[-(y_2+y_1)\dot{x}+(x_2-x_1)\dot{y}]\right\} \\ &= \mathbf{A}(\mathbf{x})+\mathbf{A}(\mathbf{x}')\end{aligned} \tag{2.49}$$

The path for which the condition on the gauge holds true was found in a very straightforward manner, so it can be seen that the simplification assumption is readily satisfied in this gauge.

Returning to the energy term in position space, the expression simplifies, leaving only one term remaining.

$$(\epsilon_n-\epsilon_m)N_{nm} = 2\sum_{\mathbf{k}}[(\mathbf{k}\times\mathbf{B})\cdot\nabla_{\mathbf{k}}N_{\mathbf{k}}\; e^{i[\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')+\frac{e}{c}\int_P d\mathbf{x}\cdot\mathbf{A}(\mathbf{x})]} \tag{2.50}$$

Consideration of the dissipation term also yields an interesting physical insight to the problem. An intermediate path is introduced in the transformation to the position representation;

$$\sum_{nm}\int d^2p\ \psi_n^*(\mathbf{p},\mathbf{x})\chi_n N_{nm}\psi_n(\mathbf{p},\mathbf{x}')$$
$$= \sum_{nm}\int d^2p \int d\mathbf{x}''\ \psi_n^*(\mathbf{p},\mathbf{x})\chi_n\psi_n(\mathbf{p},\mathbf{x}'')\psi_n^*(\mathbf{p},\mathbf{x}'')N_{nm}\psi_n(\mathbf{p},\mathbf{x}')$$
$$= \int \chi(\mathbf{x},\mathbf{x}'')N(\mathbf{x}'',\mathbf{x}')\,d\mathbf{x}''$$

The dissipation function is allowed to transform in a fashion similar to that of the density function.

$$\sum_{nm}\int d^2p\ \psi_n^*(\mathbf{p},\mathbf{x})\chi_n^* N_{nm}\psi_n(\mathbf{p},\mathbf{x}') = \int N(\mathbf{x},\mathbf{x}'')\ \chi(\mathbf{x}'',\mathbf{x}')\ d\mathbf{x}''.$$

Let P_1 be the path from $\mathbf{x}$ to $\mathbf{x}''$, and P'_1 be the path from $\mathbf{x}''$ to $\mathbf{x}'$, so that the main path P is $P_1+P'_1$. Again, χ has an gauge dependence which may be compensated for, in the same way as the distribution function.

$$\int d\mathbf{x}''\chi(\mathbf{x},\mathbf{x}'')N(\mathbf{x}'',\mathbf{x}') = \int d\mathbf{x}'' e^{i\frac{e}{c}\int_{P_1+P'_1}\mathbf{A}(x)\cdot d\mathbf{x}}\overline{\chi(\mathbf{x}-\mathbf{x}'')}\overline{N(\mathbf{x}'',\mathbf{x}')},$$
$$\text{where } \chi(\mathbf{x},\mathbf{x}';t) = \exp\left[-\frac{ie}{c}\int_P \mathbf{A}(\mathbf{x})\cdot d\mathbf{x}\right]\overline{\chi(\mathbf{x}-\mathbf{x}')}$$

The momentum space representation of the dissipation function, can be defined

$$\widehat{\chi(\mathbf{x},\mathbf{x}')} = \int e^{i\int_P d\mathbf{x}\cdot[\mathbf{q}+\frac{e}{c}\mathbf{A}]}\chi(\mathbf{q};t)\,d\mathbf{q} \qquad (2.51)$$

In order to establish a correspondence with the Boltzmann equation in the relaxation time approximation, it is assumed that the correlations within the reservoir are of very short range. The length scale associated with the interactions must be less that the magnetic length scale, $\sqrt{B/\phi}$, with flux quantum ϕ, or non-local effects will arise. This is an important point, in that any quantum information is now lost in this approxima-

tion. The paths P_1 and P'_1 are small, so that the sum of the paths approaches P. The final result is

$$(\chi_n + \chi_m)(N^0_{nm}\delta_{nm} - N_{nm}) = 2e^{\frac{ei}{c}\int_P A(x)\cdot dx}\chi(q)\,\bar{N}_P(q;\frac{x+x'}{2};t).$$

The expression indicates that χ acts as a relaxation time. Let us call $\chi\ \tau^{-1}$, so that in the momentum representation,

$$(\chi_n + \chi_m)(N^0_{nm}\delta_{nm} - N_{nm}) = 2\sum_k e^{i\left[k\cdot(x-x')+\frac{e}{c}\left(\int_P' dx\cdot A(x) - \int_P dx\cdot A(x)\right)\right]}\chi_k N_k. \quad (2.52)$$

This assumption of very short correlation lengths represents the extraction of classical information from the quantum system. Long range interactions that arise in a purely quantum mechanical consideration are neglected.

The last term of the component transport equation, (2.46), may be simplified using the position-dependent ladder operators for the Hermite polynomials.

$$\Phi_n(\xi) = e^{-\xi^2/2}H_n(\xi)$$
$$\Phi_{n-1}(\xi) = [\xi - \nabla_\xi]\Phi_n(\xi)$$
$$\Phi_{n+1}(\xi) = [\xi + \nabla_\xi]\Phi_n(\xi)$$

An example of the position-space transformation is as follows.

$$\sum_{nm}\int d^2p\ \psi^*_n(\mathbf{p},\mathbf{x})N_{n,m+1}\psi_n(\mathbf{p},\mathbf{x}') = \sum_{nm}\int d^2p\ \psi^*_n(\mathbf{p},\mathbf{x})N_{n,m+1}[\mathbf{x}'+\nabla_{x'}]\psi_{m+1}(\mathbf{x}')$$
$$= [\mathbf{x}' + \nabla_{x'}]\,N(\mathbf{x},\mathbf{x}';t)$$

The position space term is

$$[(x'-\nabla_{x'})-(x'+\nabla_{x'})] - [(x-\nabla_x)-(x+\nabla_x)] = -2\,(\nabla_x - \nabla_{x'}),$$

so that the result, in center of mass and then in momentum space is

$$[(N_{n+1,m} - N_{n,m+1}) - (N_{n,m-1} - N_{n-1,m})] = \left\{[(x-x')+\nabla_{x-x'}]-[-(x-x')+\nabla_{x-x'}]\right\}\bar{N}_P(q;\frac{x+x'}{2};t)$$

$$[(N_{n+1,m} - N_{n,m+1}) - (N'_{n,m-1} - N_{n-1,m})] = \sum_k \nabla_k N_k e^{i\left[k\cdot(x-x')+\frac{e}{c}\left(\int_P dx\cdot A(x)\right)\right]} \quad (2.53)$$

The full expression, combining (2.51), (2.52), and (2.53), gives the momentum representation of (2.47).

$$\partial_t N_{\mathbf{k}} - [\mathbf{E}+(\mathbf{v}\times\mathbf{B})]\cdot\nabla_{\mathbf{k}} N_{\mathbf{k}} = \frac{N_{\mathbf{k}}^0 - N_{\mathbf{k}}}{\tau_{\mathbf{k}}} \qquad (2.54)$$

The correspondence between the quantum transport and Boltzmann equations has been established, through the semi-classical electron distribution function, and a quantum mechanical density function. These functions are distinct in the information they convey, indeed, $N_{\mathbf{k}}$ does not necessarily have a positive definite value, and hence is not strictly a probability as is the semi-classical distribution function. Since the form of the Boltzmann equation has been achieved, it should be possible to easily identify terms in the full quantum transport equation that represent quantum transport effects. The Boltzmann equation has been solved to give theoretical estimates of physically measureable quantities such as electrical resistivity, and so this correspondence with the quantum transport equation connects a purely field theoretically deived equation with an experimental result.

The condition that was made on the path, (2.49), is consistent with a transformation used by Mahan (1987) who has examined the transport equation by means of a Greens' function method.

Summary

In summary, a master equation for the distribution kernel $N_{nm}(t)$ has been derived, and it has been established that the associated position representation number operator $N(\mathbf{x},\mathbf{x}';t)(t)$ is explicitly gauge dependent. The correspondence with the Boltzmann equation for the distribution function has been established for a suitable

choice of path, with the introduction of a density function $\bar{N}(x,x',t)$ which absorbed the gauge dependence, and with the requirement of short correlation lengths associated with the reservoir modes.

It has been seen how the conductivity of electrons in a homogeneous magnetic field can be found directly from the quantum mechanical approach. The calculation can be readily extended to slowly varying fields, but for a rapid variations in the field such as those that occur at the walls separating magnetic domains, it is not obvious how to proceed, although it seems that quantum effects must arise for such a suddenly discontinuous field. However, it has also been seen that the quantum mechanical result has some parallels with the semi-classical Boltzmann equation. Quantum mechanical effects will not appear in a calculation of the conductivity from the solution to the Boltzmann equation, but once the system has been studied in this light, the correspondence between the Boltzmann equation and the quantum transport equation should readily allow the quantum effects of the domain wall to be studied.

Chapter III: Electrical Conductivity Near a Bloch Wall

Introduction

In the preceding chapter four things were accomplished. Firstly, a master equation was derived for a system of electrons in a homogeneous electric and magnetic field, in which the electrons couple to a thermal reservoir at a given temperature, T. This was done within the framework of non-equilibrium thermo field dynamics. The resultant equation, (2.45), provides the basis for the study of a quantum mechanical description of electron transport in the presence of a homogeneous magnetic field.

Next, in order to establish the correspondence between this result and the semi-classical Boltzmann equation discussed in the Introduction, the master equation was transformed to the position representation and the function $\overline{N}_q(\mathbf{x},t)$ was defined by means of equation (2.47). Establishing the interpretation of this function, it was shown that provided the correlation length associated with the reservoir degrees of freedom was small, then the equation (2.54) describing the evolution of $\overline{N}_q(\mathbf{x})$, was given by the Boltzmann equation in the relaxation time approximation. Thus the function $\overline{N}_q(\mathbf{x})$, which will be called the density function, can be associated with the distribution function $f_q(\mathbf{x},t)$ appearing in the semi-classical Boltzmann equation.

In this way the quantum mechanical origins of the Boltzmann equation can be understood, as well as the role it's solution performs in non-equilibrium statistical

mechanics through the thermal state condition. Furthermore, it was shown how the conductivity for a homogeneous external field could be obtained from the density function $\overline{N}_q(\vec{x})$.

In this chapter, the calculation of the conductivity for an inhomogeneous field will be discussed. The solution of the Boltzmann equation will be used to compute the effect of a Bloch type domain wall on the conductivity tensor. The way in which an expression for the conductivity tensor may be obtained by means of the Boltzmann equation will be discussed, and the standard expression for the Hall resistance will be briefly derived. It will then be shown how the introduction of a domain wall introduces a new class of classical trajectories into the problem, and the modification of the conductivity tensor due to these new trajectories will be calculated. Finally, in the light of the analysis presented in chapter II, the shortcoming of the present semi-classical analysis will be discussed, along with a brief discussion of how the calculation could be modified to include quantum mechanical effects.

Chambers' Solution

Boltzmann's equation can be solved semi-classically by the Chambers' method (Callaway, 1976). This comes from an intuitive proof but can be shown to be an exact solution.

The electrons in the system of interest are excited by an external field, and undergo a series of collisions, characterized by a relaxation time, τ, eventually returning to the equilibrium distribution. In a volume element of the conductor, consider electrons with wave vectors in phase space d^3k at t_0 which arrive with energy ΔE after passing

through a certain trajectory. The probability of an electron having followed that path from a time t previous to t_0, until time t_0, is given by the Poisson distribution, and so the distribution function, $f_q(\mathbf{x},t)$ can be found by adding the contributions from all electrons scattered into that trajectory at time t with energy $E-\Delta E(t)$, where ΔE is

$$\Delta E(t) = \int_t^{t_0} \mathbf{F}(t') \cdot \mathbf{v}(t')\, dt',$$

the energy gained during that time period. $\mathbf{F}$ is the force due to the field acting on the electron, that is, the Lorentz force in magnetic field, and $\mathbf{v}$ is its velocity. The trajectories introduced by this argument are classical paths the particles will follow, hence an effective path is given by the velocity of the particles intrgated over time, and weighted by the probability mentioned earlier.

$$\Lambda = \int_{-\infty}^{0} dt\ \mathbf{v}(\mathbf{k},t) \exp[-\int_{t}^{0} dt'\, 1/\tau(\mathbf{k},t')] \qquad (3.1)$$

The general Chambers' solution of the Boltzmann equation in the relaxation time approximation may be obtained from these considerations,

$$f = \int_{-\infty}^{t_0} \frac{dt}{\tau(\mathbf{k}(t))} f_0(E-\Delta E)\, e^{-\int_t^{t_0} dt'/\tau(\mathbf{k}(t'))}$$

but in order to obtain an expression for the conductivity, a term linear in the distribution function is needed. The linearized Boltzmann equation in the relaxation time approximation has the form

$$\mathbf{F}\cdot\nabla_p f = -(f - f_0)/\tau.$$

The solution of the linearized equation, which also derives from the expansion to first order in the energy of the general Chambers' solution, is the following.

$$f = f_0 - \frac{df_0}{dE} \int_{-\infty}^{t} \mathbf{F}\cdot\mathbf{v}(t')\, e^{-\int_t^{t'} ds/\tau(\mathbf{p}(s))}\, dt' \qquad (3.2)$$

The Chambers' solution of the Boltzmann equation has been found in the same manner as the solution of the transport equation (2.39), as discussed in the previous chapter.

In expression (3.2), the sum over all time of the velocity times the collisional exponential term can be interpreted as a trajectory. The electrons can be considered to be following classical trajactories. The sum over all the possible electron trajectories should then give the effective path of the electron.

The solution of the Boltzmann equation has been extensively applied to the calculation of various transport properties using a wide variety of approximations. As an example of such a calculation, it will be shown how the electrical conductivity at zero temperature is derived from the above solution, and how the Hall conductivity emerges.

The conductivity may be found from the electric current density $\mathbf{j}$ which is given as a function of the distribution function in the following manner.

$$\mathbf{j} = -e \int \mathbf{v}(\mathbf{k}) f(\mathbf{k},\mathbf{r})\, d^3k \qquad (3.3)$$

The distribution function must have a linear dependence on the field to use it in the calculation of the conductivity. Integrating the first order expansion of the Chambers' solution in ΔE yields a term $\partial f(0)/\partial E$.

$$\mathbf{j} = e^2 \int d^3k \frac{df}{dE} \mathbf{v}(\mathbf{k}) \int_{-\infty}^{0} \mathbf{E}\cdot\mathbf{v}(\mathbf{k},t)\, e^{\left[-\int_{t}^{0} dt'/\tau\right]} dt$$

Substituting this result with the Lorentz force

$$\mathbf{F} = -e\,(\mathbf{E} + \mathbf{v}\times\mathbf{B})$$

into the above expression gives the current density as an integral over phase space.

$$\sigma_{ij} = e^2 \int d^3k \frac{df_0}{dE} v_i(\mathbf{k}) \int_{-\infty}^{0} dt\; v_j(\mathbf{k},t)\, exp\left[-\int_{t}^{0} dt'/\tau(\mathbf{k}(t'))\right] \qquad (3.4)$$

The effective path of the electrons if the classical trajectories are integrated from some

time in the infinite past to time $t = 0$, has the form

$$\Lambda_j = \int_{-\infty}^{0} dt \; v_j(\mathbf{k},t) \exp\left[-\int_{\tau}^{0} dt' \tau^{-1}(\mathbf{k}(t'))\right]. \tag{3.5}$$

Two assumptions are made to simplify the calculation. At zero temperature, all the energy states below the Fermi surface will be occupied, so the expression $\partial f\,(0)/\partial E$ is zero except at the Fermi surface. It becomes a delta-function of the energy,

$$\sigma_{ij} = e^2 \int d^3k \; \delta(E - E_f) \; v_i(\mathbf{k}) \int_{-\infty}^{0} dt \; v_j(\mathbf{k},t) \exp\left[-\int_{\tau}^{0} dt' \tau^{-1}(\mathbf{k}(t'))\right]$$

and the states on the Fermi surface are projected out of the integration, and thus, since the surface will be assumed to be spherical, the energy states can be labelled by phase vectors expressed in spherical polar coordinates, with a fixed radium of k_f, the Fermi velocity. Thus the delta function of the energy becomes a delta function of the momentum. The integral over phase space of momenta on the Fermi surface can be replaced by an integral over the Fermi surface. The final form of the expression for the conductivity elements is the following.

$$\sigma_{ij} = \frac{e^2}{8\pi^3} \int dS \frac{v_i(\mathbf{k}) \, \Lambda_j(\mathbf{k})}{|\mathbf{v}(\mathbf{k})|}. \tag{3.6}$$

The Chambers' solution reduces to a familiar result in the limit as $\tau \to 0$. The relaxation time τ is taken to be very short, $\tau \ll 1$, and hence can be taken out of the exponential for integrations over small times; $\Lambda_i = v_i(\mathbf{k})\tau$. Thus,

$$\begin{aligned}
\sigma_{ij} &= e^2\tau \int d^3k \frac{\partial f_0}{dE} v_i v_j \\
&\doteq \frac{e^2\tau}{m} \int d^3k \frac{\partial f_0}{\partial v_i} v_j \\
&= \frac{e^2\tau}{m} \int d^3k \; f_0 \delta_{i,j} \; = \frac{n\tau e^2}{m}.
\end{aligned} \tag{3.7}$$

The conductivity tensor has been expressed in terms of the semi-classical Chambers' solution of the Boltzmann equation. The expression, given by equation (3.6), will be used in the semi-classical calculation of the electrical conductivity correction due to the presence of a Bloch type domain wall. It is instructive to first evaluate the conductivity tensor for a homogeous magnetic field. This will establish both the method of application of the Chambers' solution to the calculation of the conductivity, and the correspondence between the solution of the Boltzmann equation that has just been discussed, and that of the quantum mechanical transport equation, from the last chapter. Also, this will be directly related to the problem involving the domain wall, which we wish to treat.

Conductivity Tensor in a Homogeneous Magnetic Field

Electrons in the presence of a homogeneous magnetic field $\mathbf{B}=-B\ \hat{e}_z$ will traverse circular paths in the $x-y$ plane, of cyclotron radius, $r_c^2=c/eB$, with cyclotron frequency, $\omega_c=eB/mc$. The equation of motion for a single electron,

$$\dot{\mathbf{v}}=-\frac{e}{m}\,\mathbf{v}\times\mathbf{B} \tag{3.8}$$

in the $y>0$ domain yields the relations

$$\begin{cases} \dfrac{dv_x}{dt}=\omega_c\, v_y \\ \dfrac{dv_y}{dt}=-\omega_c\, v_x\,, \end{cases} \tag{3.9.1}$$

$$\begin{cases} \dfrac{dv_x}{dt}=-\omega_c\, v_y \\ \dfrac{dv_y}{dt}=\omega_c\, v_x\,. \end{cases} \tag{3.9.2}$$

If we rewrite the first of equations (3.9.1) as the time derivative $\frac{d}{dt}\left\{ v_x - \omega_c y \right\} = 0$, then the solutions to the equation (3.8) give the constants of motion which are simply the following.

$$v_x(t) - \omega_c y(t) = v_x^0 - \omega_c y_0$$
$$v_y(t) + \omega_c x(t) = v_y^0 + \omega_c x_0 \quad y > 0 \tag{3.10.1}$$
$$v_x(t) + \omega_c y(t) = v_x^0 + \omega_c y_0$$
$$-v_y(t) + \omega_c x(t) = -v_y^0 + \omega_c x_0 \quad y < 0 \tag{3.10.2}$$

This gives the velocity and position of an electron at any time in terms of the "initial" conditions. In fact, since the the effective path has been found from the integration of the electron trajectories from some time in the infinite past, the position and momentum at time $t = 0$ represent the final, rather than initial description of the electron, but as a matter of convention, y_0 and $\mathbf{v}_0$ will be called the initial conditions.

The calculation of the effective path

$$\Lambda_x = \int_{-\infty}^{0} dt \; v_x(t)\, e^{t/\tau}; \quad \Lambda_y = \int_{-\infty}^{0} dt \; v_y(t)\, e^{t/\tau} \tag{3.11}$$

can now be done by integrating the electron's orbit from the initial time, $t = 0$, tracing its trajectory back through time to $t \to -\infty$.

$$\begin{aligned}
\Lambda_x &= \int_{-\infty}^{0} dt \; v_x(t)\, e^{t/\tau} \\
&= -\frac{1}{\omega_c} \int_{-\infty}^{0} dt \; \frac{dv_y(t)}{dt}\, e^{t/\tau} \\
&= -\frac{v_y^0}{\omega_c} + \frac{1}{\omega_c \tau} \int_{-\infty}^{0} dt \; v_y(t)\, e^{t/\tau} \\
&= -\frac{v_y^0}{\omega_c} + \frac{1}{\omega_c \tau} \Lambda_y
\end{aligned}$$

And in the same fashion, a similar result may be derived for Λ_y.

$$\Lambda_y = \frac{v_y^0}{\omega_c} - \frac{1}{\omega_c \tau} \Lambda_x$$

Combining these two results yields the effective path in terms of the initial conditions.

$$\begin{aligned} \Lambda_x &= \frac{\tau}{1 + \omega_c^2 \tau^2} \left[v_x^0 - \omega_c \tau \, v_y^0 \right] \\ \Lambda_y &= \frac{\tau}{1 + \omega_c^2 \tau^2} \left[v_y^0 + \omega_c \tau \, v_x^0 \right] \end{aligned} \tag{3.12}$$

The effective path in the z-direction is just the usual mean free path and not affected by the presence of the domain wall, hence it need not be considered here.

Having the expressions for the components of the effective path, the conductivity can be derived using expression (3.12). Since the Fermi surface has been chosen to be spherical, the energy states on the phase space will be labelled by the angles θ and ϕ, the polar angles of the constant phase vector of length k_f. The element of phase space in the conductivity component expression, (3.6) becomes

$$dS = \sin\theta \, d\theta \, d\phi,$$

and the components of velocity are given by

$$\begin{cases} v_x = v_f \sin\theta \cos\phi \\ v_y = v_f \sin\theta \sin\phi \\ v_z = v_f \cos\theta. \end{cases}$$

The resultant components with $i, j = 1,2$, are;

$$\sigma = \frac{ne^2\tau}{(1 + \omega_c^2 \tau^2)} \begin{bmatrix} 1 & -\omega_c \tau \\ \omega_c \tau & 1 \end{bmatrix} \tag{2.13}$$

This result is the same as was derived from the solution for the quantum transport equation for a homogeneous field.

Conductivity Tensor for Bloch Type Domain Walls

A good example of a system that can be treated as a simple combination of homogeneous magnetic fields, yet is a very complex and interesting system is that of magnetic domains separated by Bloch type domain walls. A Bloch type wall of zero thickness at $y=0$ is placed between two infinite domains. This is not unreasonable on a macroscopic scale, neglecting boundary effects, although it represents a very sudden variation in the field. In the domain $y>0$, the homogeneous magnetic field in a direction antiparallel to the z-direction, and is parallel in the homogeneous domain $y<0$. The wall will essentially be treated as a discontinuous change in the magnetic induction field, and its effect on the conductivity will be determined.

This particular example was chosen because of the existence of similar calculations (Cabrera and Falicov, 1974a; 1974b; Zakharov and Man'kov, 1984) and the obvious extension to a treatment as an inhomogeneous magnetic field. The papers by both groups of authors use similar methods to find the electrical conductivity at the domain wall, with the difference that Zakharov and Man'kov (1984) use a cylindrical Fermi surface, as opposed to Cabrera and Falicov's (1974) spherical surface. The use of a cylindrical surface makes the calculation more straightforward to use due to the symmetry of the problem, but the spherical Fermi surface will be used here, being a more realistic approach. The present calculation encorporates parts of both treatments, ignoring Zakharov and Man'kov's rather drastic assumptions of the cylindrical Fermi surface, as well as of an equal number of particle and hole states, reducing the cross conductivity contribution to zero, and extending Cabrera and Falicov's study of conductivity which was limited to the region at the domain wall, that is, $y=0$.

The conductivity tensor has been derived for a homogeneous magnetic field. It will be found that there exists a condition on the initial position of the electron that determines the range of effect of the domain wall. It will be assumed that the electrons follow classical trajectories, neglecting scattering from the wall, and hence if the electrons are outside its influence, their contribution to the conductivity will be just the homogeneous conductivity as derived previously. The contribution from the remaining electrons will be calculated, using the Chambers' solution. Once the conductivity elements are known, the exact corrections to the conductivity due to the Bloch wall will be found, and solved numerically. Finally, the computational results will be verified analytically.

1. Effective Path

The conductivity has been derived in the homogeneous field case. It remains to be seen how the calculation proceeds for an inhomogeneous field, and that for electrons with initial positions at $y=0$, our results agree with those of Cabrera and Falicov (1974).

Consider a system of two homogeneous magnetic domains separated by an infinitely thin domain wall at $y=0$. The field in the $y<0$ domain is $\mathbf{B} = B\hat{e}_z$, and in the $y>0$ domain, $\mathbf{B} = -B\hat{e}_z$. Setting the problem up in the same way as in the homogeneous field case, the equations and constants of motion will change in the $y<0$ domain. Recall the constants of motion for $y>0$.

$$\begin{cases} \dfrac{dv_x}{dt} = -\omega_c v_y & y<0 \\ \dfrac{dv_y}{dt} = \omega_c v_x & y<0 \end{cases} \qquad (1)$$

$$\begin{cases} v_x(t) + \omega_c\, y(t) = v_x^0 + \omega_c\, y_0 \\ v_y(t) - \omega_c\, x(t) = v_y^0 - \omega_c\, x_0 \end{cases} \tag{3.10}$$

The states in phase space are labelled in the same manner as before.

With respect to this single domain wall, there are two types of trajectories the electron may describe. It could simply orbit in a circle of cyclotron radius, r_c . as in a uniform magnetic field, or it could cross and re-cross the domain wall in an open path, propagating in the positive x-direction (figure 1.1). In order to determine the condition for each possibility, consider the case when the electron travels in circular orbit that comes to just touch the wall at y=0 at time t, that is, $y(t)=0$. The velocity at that time is given be equation (3.10).

$$v_x(t) = v_x^0 - \omega_c\ y_0$$

Because the trajectory is circular, at the moment the electron's path is tangential to the wall, its motion is completely in the x-direction, or in phase space,

$$v_x(t) = -v_f\ \sin\theta$$

This gives the condition on the initial position of the electron.

$$\begin{aligned} -v_f\ \sin\theta &= v_f\ \sin\theta\cos\phi - \omega_c\, \overline{y}_0 \\ \omega_c\, \overline{y}_0 &= v_f\ \sin\theta\ \left[1 + \cos\phi\right] \end{aligned} \tag{3.13}$$

So if $y_0 > \overline{y}_0$, the electron trajectory will be a closed circular orbit of cyclotron radius, r_c, and does not encounter the domain wall, as shown in figure 1.1, and if $y_0 < \overline{y}_0$, the path will be the open orbit shown in figure 1.1 that crosses and recrosses the wall, as the direction of the electron's circular orbit in each homogeneous domain changes at each time the electron crosses the boundary. The maximum value of $\overline{y}_0$ can be determined from the fact that the phase angles labelling the energy states have the

range

$$0 < \theta < \pi, \text{ and } -\pi < \phi < \pi.$$

with $(\overline{y}_0)_{max} = 2\, v_f / \omega_c = 2\, r_c$. This implies an inherent limit of the phase space available to an electron influenced by the domain wall, since by condition (3.13),

$$\sin\theta\,[1 + \cos\phi] \leq \frac{y_0}{r_c}$$

In the case that $y_0 < \overline{y}_0$, the electrons describe closed orbits in the homogeneous fields of each domain, and derived in the same way as above, the resultant expressions for the effective path components are as follows.

$$\begin{cases} \Lambda_x = \dfrac{\tau}{1 + \omega_c^2 \tau^2} \left[v_x^0 - \omega_c \tau\, v_y^0 \right] \\ \Lambda_y = \dfrac{\tau}{1 + \omega_c^2 \tau^2} \left[v_y^0 + \omega_c \tau\, v_x^0 \right] \end{cases} \quad y > 0 \qquad (3.14.1)$$

$$\begin{cases} \Lambda_x = \dfrac{\tau}{1 + \omega_c^2 \tau^2} \left[v_x^0 + \omega_c \tau\, v_y^0 \right] \\ \Lambda_y = \dfrac{\tau}{1 + \omega_c^2 \tau^2} \left[v_y^0 - \omega_c \tau\, v_x^0 \right] \end{cases} \quad y < 0 \qquad (3.14.2)$$

The calculation of the effective path for open orbits is done using intuitive arguments about the electron's semi-classical trajectory. The equations of motion of the electron are different in the two domains and so the trajectory which crosses and re-crosses the domain boundary must be treated separately in each homogeneous domain by segmenting the path. The path is divided up into characteristic time units t_1 and Θ. The time t_1 represents the time elapsed during the electron's traveling from the last collision with the wall at $y = 0$, to its position $y = y_0$ at time $t = 0$. The second parameter Θ is the time between successive collisions with the domain wall.

$$\Lambda_x(t) = \left\{ \int_{-t_1}^{0} dt + \int_{-t_1-\Theta}^{-t_1} dt + \cdots \right\} v_x(t) e^{t/\tau} \qquad (3.15.1)$$

Along the y-direction, the electron encounters the wall. Ignoring the possibility of reflection for a moment, the trajectory will be sectioned in the same manner.

$$\Lambda_y(t) = \left\{ \int_{-t_1}^{0} dt + \int_{-t_1-\Theta}^{-t_1} dt + \cdots \right\} v_y(t) e^{t/\tau} \qquad (3.15.2)$$

Now, because the magnitude of the field does not change, Θ is constant for any point in the phase space. Consequently, the terms of the sum may be written in a more general form, by labelling them as $I_x^{(n)}(\Theta; t_1)$.

$$I_x^{(0)} \equiv \int_{-t_1}^{0} v_x(t) e^{t/\tau} dt; \quad I_x^{(n)} \equiv \int_{-(t_1+n\Theta)}^{-[t_1+(n-1)\Theta]} v_x(t) e^{t/\tau} dt, \; n \geq 1 \qquad (3.16)$$

$$I_y^{(0)} \equiv \int_{-t_1}^{0} v_y(t) e^{t/\tau} dt; \quad I_y^{(n)} \equiv \int_{-(t_1+n\Theta)}^{-[t_1+(n-1)\Theta]} v_y(t) e^{t/\tau} dt, \; n \geq 1$$

Thus the components of the effective path can be written in the following manner.

$$\Lambda_x = I_x^{(0)} + \sum_{n=1} I_x^{(n)}(\Theta, t_1)$$

$$\Lambda_y = I_y^{(0)} + \sum_{n=1} I_y^{(n)}(\Theta, t_1)$$

There are now just two different terms to solve in order to express the effective path in terms of v_0 and y_0.

First, using the same method as for the homogeneous field, let us solve $I_x^{(0)}$ and $I_y^{(0)}$.

$$I_x^{(0)} = -\frac{1}{\omega_c} v_y(t)\, e^{t/\tau} \Big|_{-t_1}^{0} + \frac{1}{\omega_c \tau} I_x^{(0)}$$

$$I_y^{(0)} = \frac{1}{\omega_c} v_x(t)\, e^{t/\tau} \Big|_{-t_1}^{0} - \frac{1}{\omega_c \tau} I_y^{(0)}$$

Combining,

$$I_x^{(0)} = \frac{\tau}{1+\omega_c^2\tau^2}\left\{[v_x^{(0)} - \omega_c \tau v_y^{(0)}(t)] - [v_x(-t_1) - \omega_c \tau v_y(-t_1)]e^{-t_1/\tau}\right\} \quad (3.17.1)$$

$$I_y^{(0)} = \frac{\tau}{1+\omega_c^2\tau^2}\left\{[v_y^{(0)} + \omega_c \tau v_x^{(0)}(t)] - [v_y(-t_1) + \omega_c \tau v_x(-t_1)]e^{-t_1/\tau}\right\} \quad (3.17.2)$$

To have $v_x(-t_1)$ as a function of the constant of motion, use the equation (3.9), and the fact that $y(-t_1)=0$.

$$v_x(-t_1) = v_x^0 - \omega_c y_0 \quad (3.18)$$

The dependence on x_0 may be removed by using the following condition

$$v_y^2(t) + v_x^2(t) = v_x^2(t) + v_f^2 \sin^2\theta. \quad (3.19)$$

When treating the remaining terms $I_x^{(n)}$ and $I_y^{(n)}$, it must be remembered that those of odd and even n indices correspond to the electron traveling in the $y<0$ and the $y>0$ domains, respectively, if, at $t=0$, the electron is in the $y>0$ domain. We see that by substituting (3.9) in the same way as before, and integrating by parts, we have

$$I_x^{(n)}(\Theta;t_1) = \frac{\tau}{1+\omega_c^2\tau^2}\left[\left(v_x(t) - (-1)^n \omega_c \tau v_y(t)\right) e^{t/\tau}\right]_{-(t_1+n\Theta)}^{-(t_1+(n-1)\Theta)}$$

$$I_y^{(n)}(\Theta;t_1) = \frac{\tau}{1+\omega_c^2\tau^2}\left[\left(v_y(t) + (-1)^n \omega_c \tau v_x(t)\right) e^{t/\tau}\right]_{-(t_1+n\Theta)}^{-(t_1+(n-1)\Theta)}$$

From this result, together with equation (3.17.1) and (3.17.2), the summation can be performed to give the final expression for the effective path for $y_0 < y_0$.

$$\Lambda_x(t) = \frac{\tau}{1+\omega_c^2\tau^2}\left\{v_x(t_1) + \omega_c \tau v_y(t_1)\left[1+\coth\frac{\Theta}{2\tau}\right]e^{-t_1/\tau}\right\} \quad (3.20)$$

Similarly,

$$\Lambda_y(t) = \frac{\tau}{1+\omega_c^2\tau^2}\left\{v_y(t_1) - \omega_c \tau v_x(t_1)\left[1+\tanh\frac{\Theta}{2\tau}\right]e^{-t_1/\tau}\right\} \quad (3.21)$$

These are the x and y components of the effective path of a single electron which

describes an open orbit in the influence of a single, infinitely thin domain boundary. Comparing these results to the equation (3.12), it can be seen that equations (3.20) and (3.21) consist of two parts; the homogeneous field effective path, and a y-dependent correction.

$$\Delta\Lambda_x(t) = \frac{\omega_c \tau^2 \, v_y(t_1)}{1+\omega_c^2\tau^2}\left[1+\coth\frac{\Theta}{2\tau}\right]e^{-t_1/\tau} \tag{3.22.1}$$

$$\Delta\Lambda_y(y) = -\frac{\omega_c \tau^2 \, v_x(t_1)}{1+\omega_c^2\tau^2}\left[1+\tanh\frac{\Theta}{2\tau}\right]e^{-t_1/\tau} \tag{3.22.2}$$

It can be seen that the effect of the domain wall is manifested by an additional term which depends on the time taken to complete a partial circular orbit in one domain, Θ, and the time elapsed since the electron's last contact with the wall, t_1. The correction is usually fairly small for short relaxation times. It remains to be seen what the exact form of the time parameters is, in terms of the initial conditions.

If $y<0$, the derivation of the effective path contribution follows the same procedure, giving the results,

$$\Delta\Lambda_x(t) = -\frac{\omega_c \tau^2 \, v_y(t_1)}{1+\omega_c^2\tau^2}\left[1+\coth\frac{\Theta}{2\tau}\right]e^{-t_1/\tau} \tag{3.23.1}$$

$$\Delta\Lambda_y(y) = \frac{\omega_c \tau^2 \, v_x(t_1)}{1+\omega_c^2\tau^2}\left[1+\tanh\frac{\Theta}{2\tau}\right]e^{-t_1/\tau} \tag{3.23.2}$$

2. Time Parameters

The expression for the effective path will be complete once it is known how the time parameters t_1 and Θ are found for a given state on the Fermi surface, characterized by the spherical polar angles θ and ϕ, and for a given position y_0. The previous analysis lends itself quite easily to a geometric interpretation which can be used as a

check on the results. This is particularly apparent when we come to finding the y_0 and v_z^0 dependence of the time t_1.

The equations of motion, (3.8), have the following solutions

$$\begin{cases} v_x(t) = A\cos\omega_c(t-t') + B\sin\omega_c(t-t') \\ v_y(t) = B\cos\omega_c(t-t') - A\sin\omega_c(t-t'). \end{cases} \tag{3.24}$$

which can be used to find the expressions for the time parameters in terms of the initial conditions, as outlined in appendix III.

The solutions for the equations of motion (3.8) can, on the other hand, be describe a circle of radius $r_c \equiv v_f \sin\theta/\omega_c$, and center

$$\begin{cases} y(t) - y' = r_c\cos(\phi-\omega_c t) \\ x(t) - x' = -r_c\sin(\phi-\omega_c t) \end{cases}$$

or

$$[y(t)-y']^2 + [x(t)-x']^2 = r_c^2 \tag{3.25}$$

where x' and y' are defined as

$$y' \equiv -\left[v_f \sin\frac{\theta}{\omega_c}\right]\cos\phi + y_0$$

$$x' \equiv \left[v_f \sin\frac{\theta}{\omega_c}\right]\sin\phi + x_0.$$

Thus the electron starts out from a point $y=y_0$, as in figure 1.2, at an angle ϕ from the positive x-direction, and travels counterclockwise in the $y>0$ domain (clockwise in the other domain), in a circle with center $r_c\cos\phi$ away from y_0, or

$$y = y' = y_0 - r_c\cos\phi.$$

Note that these cooridinates for the center of the orbit are the classical analogs of the operators $\hat{x}_0$ and $\hat{y}_0$ that emerged from the kinematical momentum operator equation of

motion in the previous chapter. Tracing the path backwards in time, the electron last intercepted the wall at a distance y' from the center of the orbit, and thus at an angle

$$\phi' = \frac{\pi}{2} + \sin^{-1}\left(\frac{y'}{r_c}\right) = \cos^{-1}\left(-\frac{y'}{r_c}\right), \tag{3.26}$$

from the positive x-direction. As can be seen in the diagram (figure 1.2), the time $\omega_c t_1$ corresponds to the angular distance between the initial position on the circle surrounding y', and the point at which the wall (y=0) intercepts the circle. This corresponds to the angle between velocities $\mathbf{v}_0$ and $\mathbf{v}(-t_1)$, which are tangential to the orbit at the those points, respectively. We then have

$$\omega_c t_1 = \phi' - \phi$$

or

$$\omega_c t_1 = \cos^{-1}\left[-\left(\frac{\omega_c y_0}{v_f \sin\theta} - \cos\phi\right)\right] - \phi, \tag{3.27}$$

which agrees exactly with the derivation given in appendix III.

Equation (3.27) has some interesting consequences. Consider three situations; $y_0=0$, $y_0=0.5\ r_c$ and $y_0=2r_c$. In the first case, a plot of t_1 as a function of the angle ϕ for a fixed θ, $\theta=\pi/2$, (figure 1.3.1) shows that t_1 is zero if the particle starts out with $v_y<0$, and increases monotonically, otherwise. This is what would intuitively been expected, since if $\phi<0$, the electron's path cannot be traced backward in time without crossing the domain boundary, that is, no time has passed since the last encounter with the wall, whereas if $\phi>0$, some finite time will have elapsed from the last contact. In fact, as ϕ decreases, the center of the orbit moves in the positive y-direction, thereby increasing the length of the path to be traversed back to $y=0$.

In the second situation, a plot of t_1 versus ϕ, (figure 1.3.2) again with $\theta=\pi/2$ indicates that t_1 gets cut off at extreme values of ϕ. As the electron moves farther away

from the wall, the possible paths that will take it to that point diminish. This corresponds to the loss of phase space wherein the electron does cross the wall ($y_0 < \bar{y}_0$). Finally at $y_0 = 2r_c$, the only non-zero value t_1 can take is π/ω_c, at $\phi = 0$. In fact, the domain of the θ parameter is also cut off at both ends for the same reasons, since $\sin\theta$ is small near the limits of $0 < \theta < \pi$, and the condition from (3.13) that

$$v_f \sin\theta \,[1 + \cos\phi] > \omega_c y_0$$

must be satisfied.

Following the same method in deriving t_1, equation (3.25) can be used to find Θ, with the following result.

$$\omega_c \Theta = 2 \cos^{-1}\left[\cos\phi - \frac{\omega_c y}{v_f \sin\theta}\right] \qquad (3.28.1)$$

This means that Θ corresponds to angle subtended between $\mathbf{v}(-t_1)$ and $\mathbf{v}(-t_1-\Theta)$, or, in terms of the angle ϕ' defined in equation (3.26),

$$\omega_c \Theta = 2\phi' \qquad (3.28.2)$$

The effective path has now been characterized for points on the Fermi surface. It is expressed as a function of the characteristic times t_1 and Θ, which have been determined in terms of the initial position y_0 for a given state on the Fermi surface, with t_1 and Θ given by

$$\omega_c t_1 = \cos^{-1}\left(\cos\phi - \frac{\omega_c y}{v_f \sin\theta}\right) - \phi \qquad (3.27)$$

$$\omega_c \Theta = 2 \cos^{-1}\left[\cos\phi - \frac{\omega_c y}{v_f \sin\theta}\right] \qquad (3.28.1)$$

The calculation of effective path in the $y < 0$ domain proceeds in a completely analogous manner, the only difference being that in order to account for the fact that the angles ϕ and θ are defined in the negative sense to those in the $y > 0$ domain, so that to

determine the time parameters, we have,

$$\tan^{-1}\left(\frac{v_y(t)}{v_x(t)}\right) = -\cos^{-1}\left(\frac{v_x}{v_f \sin\theta}\right).$$

The results are as follows:

$$\phi' = \cos^{-1}\left(\cos\phi - \frac{\omega_c y}{v_f \sin\theta}\right) \tag{3.29}$$

$$\omega_c t_1 = \phi' + \phi \tag{3.30}$$

$$\omega_c \Theta = 2\phi' \tag{3.31}$$

The expression for the effective path contribution that arises from the presence of a magnetic domain wall has been reduced to an integral over a spherical phase space parametrized by the angles ϕ and θ. The positional dependence of the effective path will remain, giving a domain wall correction that depends upon the distance from the wall.

3. Reflection at the Domain Wall

Thus far, only the effect of the Lorentz force on the electron has been considered in the analysis of the domain wall effect on the conductivity tensor. Introducing the exchange force will produce an effective potential at the wall, and the possibility of reflection arises.

Adding the possibility of reflection to the problem results in an additional multiplicative factor in the effective path, following the previous treatment of the problem by Cabrera and Falicov (1974a; 1974b). The reflection considered here will be specular reflection so that the electron will be perfectly reflected and not scattered into an arbitrary state. Reflection will not affect the effective path in the x-direction, Λ_x, but the possibility of the electron tracing out a mirror image of its unreflected orbit will certainly change Λ_y.

If the electron is reflected with probability R along a path P_2, or transmitted with probability $1-R$ along a path P_1, then each term in the division of the trajectory can be fairly simply expressed in the following way.

$$RP_2+(1-R)P_1 = R\int_{-t_1-n\Theta}^{-t_1-(n-1)\Theta} v_y\, e^{t/\tau}dt + (1-R)\int_{-t_1-n\Theta}^{-t_1-(n-1)\Theta}(-v_y)\,e^{t/\tau}dt$$

$$= (2R-1)\int_{-t_1-n\Theta}^{-t_1-(n-1)\Theta} v_y\, e^{t/\tau}dt.$$

Writing out the segmentation and multiplying out the factors, the expansion yields terms that increase in powers of $(2R-1)$ and $\exp(-\Theta/\tau)$, so in the same fashion as above, the summation in the y-direction yields the following,

$$\Lambda_y(t) = \frac{\tau}{1+\omega_c^2\tau^2}\left\{\left[v_y{}^0+\omega_c\tau v_x{}^0\right] - (2R-1)\omega_c\tau v_x(t_1)\left[1+\frac{1+e^{\Theta/\tau}}{1-(2R-1)e^{\Theta/\tau}}\right]e^{-t_1/\tau}\right\},$$

which, if the possibility of reflection is neglected, reduces to equation (3.21).

At the wall, $y=0$. The expressions for the time parameters, (3.27) and (3.28) simplify in the positive domain, giving

$$t_1 = \Theta = 2\phi/\omega_c .$$

If $\omega_c\tau$ is defined as $\chi\equiv\omega_c\tau$, and the above case is combined with equations (3.20) and (3.21) then the x and y components of the effective path have the form;

$$\Lambda_x(\theta,\phi) = \frac{v_f\sin\theta\tau}{(1+\chi^2)(1-e^{-2\phi/\chi})}\left\{e^{-2\phi/\chi}[\chi\sin\phi-\cos\phi] + \cos\phi + \chi\sin\phi\right\}$$

$$\Lambda_y(\theta,\phi) = \frac{(2R-1)v_f\sin\theta\tau}{(1+\chi^2(1-e^{-2\phi/\chi})}\left\{e^{-2\phi/\chi}[\chi\cos\phi-\sin\phi] + \sin\phi - \chi\cos\phi\right\}.$$

These are just equations (A13) and (A14) of Cabrera and Falicov (1974b), neglecting the reflection coefficient R. The results of this method of calculation reduce to a known expression.

4. Conductivity

In summary, the x and y components of the effective path are

$$\Lambda_x(t) = \frac{\tau}{1+\omega_c^2\tau^2}\left\{ \left[v_x^0 -+\omega_c\,\tau v_y^0\right] +- \omega_c\,\tau v_y(t_1)\left[1+\coth\frac{\Theta}{2\tau}\right]e^{-t_1/\tau}\right\} \quad (3.20)$$

$$\Lambda_y(t) = \frac{\tau}{1+\omega_c^2\tau^2}\left\{ \left[v_y^0 +-\omega_c\,\tau v_x^0\right] -+\omega_c\,\tau v_x(t_1)\left[1+\tanh\frac{\Theta}{2\tau}\right]e^{-t_1/\tau}\right\}, \quad (3.21)$$

where $-+$ and $+-$ indicate the sign varying between the $y>0$ and the $y<0$ domains, respectively. The homogeneous field paths with y-dependent corrections due to the presence of a domain boundary is

$$\Delta\Lambda_x(y) = \frac{\omega_c\,\tau^2\,v_y(t_1)}{1+\omega_c^2\tau^2}\left[1+\coth\frac{\Theta}{2\tau}\right]e^{-t_1/\tau} \quad (3.22)$$

$$\Delta\Lambda_y(y) = -+\frac{\omega_c\,\tau^2(2R-1)\,v_x(t_1)}{1+\omega_c^2\tau^2}\left[1+\tanh\frac{\Theta}{2\tau}\right]e^{-t_1/\tau} \quad (3.23)$$

where the time parameters Θ and t_1 given by equations (3.28) and (3.27), respectively. The conductivity matrix elements can now be found according to equation (3.6), knowing that the velocity components can be written in terms of ϕ and θ, the spherical polar angels, as follows:

$$\begin{cases} v_x &= v_f \sin\theta\cos\phi \\ v_y &= v_f \sin\theta\sin\phi \\ v_z &= v_f \cos\theta. \end{cases} \quad (3.32)$$

From the definition of $v_x(-t_1)$ given in equation (3.18), and the definition of ϕ', (3.26), for $y>0$, and from (3.10) and (3.29) for $y<0$, the velocities $v_i(-t_1)$ can be expressed in terms of the characteristic angle ϕ'.

$$\begin{cases} v_x &= v_f \sin\theta\cos\phi' \\ v_y &= \pm v_f \sin\theta\sin\phi' \end{cases} \quad (3.33)$$

Thus the domain wall corrections to the terms of the electronic conductivity, scaled by

the homogeneous field conductivity, defining $\chi=\omega_c \tau$, are the following.

$$\frac{\Delta\sigma_{xx}}{\sigma_0} = +-\int_0^{\pi}\sin^3\theta \; d\theta \int_{-\pi}^{\pi} d\phi[\cos\phi \; \sin\phi'][1+\coth\frac{\phi'}{\chi}]e^{(\phi-\phi')/\chi} \qquad (3.34)$$

$$\frac{\Delta\sigma_{yy}}{\sigma_0} = -+\int_0^{\pi}\sin^3\theta \; d\theta \int_{-\pi}^{\pi} d\phi[\sin\phi \; \cos\phi'][1+\tanh\frac{\phi'}{\chi}]e^{(\phi-\phi')/\chi} \qquad (3.35)$$

$$\frac{\Delta\sigma_{yx}}{\sigma_0} = \int_0^{\pi}\sin^3\theta \; d\theta \int_{-\pi}^{\pi} d\phi[\sin\phi \; \sin\phi'][1+\coth\frac{\phi'}{\chi}]e^{(\phi-\phi')/\chi} \qquad (3.36)$$

$$\frac{\Delta\sigma_{xy}}{\sigma_0} = -+\int_0^{\pi}\sin^3\theta \; d\theta \int_{-\pi}^{\pi} d\phi[\cos\phi \; \cos\phi'][1+\tanh\frac{\phi'}{\chi}]e^{(\phi-\phi')/\chi} \qquad (3.37)$$

The exact expressions for the conductivity tensor elements are complicated because of the explicit dependence of times t_1 and Θ on θ and ϕ, in which the path is parametrized. Hence the y-dependent contributions of the terms $\sigma_{i,j}$, with $i=x,y$ and $j=x,y$, cannot be calculated exactly. In order to determine the behavior of these corrections, the contribution to the conductivity due to the presence of the domain wall was calculated numerically as a function of position and plotted. The behavior of the corrections was verified analytically, from examining the limiting behavior of the conductivity both at the wall, and just at the edge of the range of the wall's effect.

Numerical results are given in figures 1.4 to 1.7, which are plots of the y-dependence of the conductivity corrections due to the wall, in units of $\omega_c \tau$. The calculation of the conductivity elements was performed on the Vax 11-70 computer, run by Newfoundland and Labrador Computer Services, using the pre-defined integration subroutines DMLIN and DBLIN in the IMSL subroutine library. The values assigned to the numerical factors involved, namely ω_c and τ, were chosen to give an order of magnitude rather than the exact values particular to an actual system. According to Kittel (1953), typical measurements for saturation magnetizations range from approximately 500 to

2500 gauss, and values of the Fermi velocity and the relaxation time are on the order of 1×10^{8} cm/sec and 1×10^{-14} sec and upward, respectively. Based on these values, ω_c was assigned a value of $\omega_c=1\times10^{10}$, and the τ parameter was varied in the computation of the contribution to the conductivity elements.

It was found that $\Delta\sigma$ showed interesting behavior only in the clean limit of very long inter-collisional lifetimes, that is, for high values of τ. For short relaxation times, the contribution to the conductivity was found to be relatively constant. It can be argued intuitively that if the inter-collisional lifetime is short, the wall's effect will be very localized since any information about the wall carried by the electrons will be lost in a very short time. An electron at an arbitrary position, then, will not recognize the presence of the wall, so that in the dirty limit, the only contribution to the conductivity will be some constant term, independent of position. The graphs given and discussed here were calculated using $\chi=\omega_c\,\tau=1$, with the conductivity being scaled by a factor of $ne^2\tau/2$, and the position given in units of $1/r_c$.

An interesting aspect of the longitudinal conductivity correction plots is that a maximum (or minimum) appears before and after $y=0$, rather than at $y=0$, as would be expected intuitively. This can be verified analytically by determining the slope of the curve at $y=0$, and just on either side. Because of the complexity of the expression for $\Delta\sigma$, the best possible way to verify the computational results analytically is to examine its behaviour in the limiting cases $|y|\to0$ and $|y|\to r_c$. In fact, it is possible to solve the expression for the conductivity tensor analytically at $y=0$.

4.1 The Tensor Component $\Delta\sigma_{zz}(y)$

The longitudinal conductivity contribution due to the presence of the domain wall is given in equation (3.34). From the previous discussion of the trajectories in the limit $y \to 2r_c$, the additional conductivity disappears as this distance from the domain wall is approached. Appendix IV discusses the limit as $y \to 0$ in some detail. The result is that at the wall, the expression for $\Delta\sigma_{zz}$ simplifies a great deal.

$$\lim_{y\to 0}\frac{\Delta\sigma_{zz}}{\sigma_0} = \frac{4\chi}{3}\int_{-\pi}^{\pi} d\phi \frac{\sin 2\phi}{1 - e^{-2\phi/\chi}} \tag{3.38}$$

$$= \Delta\sigma_{zz}(y>0 \to y=0).$$

Thus the sign of the change in conductivity due to the y-dependence does not vary as the electron crosses the wall, and $\Delta\sigma_{zz}$ tends toward the sames value whether the wall is approached from the $y>0$ domain, or the $y<0$ domain. The value that is approached is positive, and the numerical integration yeilds a value

$$\frac{4}{3}\int_{-\pi}^{\pi}\frac{\sin 2\phi\, d\phi}{e^{2\phi/\chi} - 1} = 1.43$$

that agrees with that found in calculating the points on the curve in figure 1.4. The contribution to the conductivity has been shown to be continuous across and symmetric about the domain wall for $\chi=1$.

The shape of the graph cannot be examined analytically, without knowing the slope of its equation. The general expression for the slope of the domain wall conductivity contribution curve has been be found to be (appendix V)

$$\frac{d\,\Delta\sigma_{zz}}{dy}(y>/<0) = \pm\chi\sigma_0\int\int d\theta\, d\phi \sin^3\theta\cos\phi\; e^{-(\phi'-/+\phi)/\chi}$$

$$\left\{[1\mp\coth\frac{\phi'}{\chi}][\cot\phi' - \frac{1}{\chi}] - \frac{1}{\chi\sinh^2\frac{\phi}{\chi}}\right\}$$

for electrons in the $y >/< $ domain. The behaviour of these derivatives is not obvious, so the limiting case of interest - $y \to 0$ - should be considered. At the wall, using the same sort of method as outlined in appendix IV, the slope reduces to this expression.

$$\lim_{y\to 0} \frac{d\,\Delta\sigma_{zz}}{dy}(y' >/< 0) = \pm \frac{4\chi\sigma_0}{3} \int_{-\pi}^{\pi} \left[\frac{2\cot\phi}{1-e^{-2\phi/\chi}} - \frac{1+e^{-2\phi/\chi}}{2\chi\sinh^2\frac{\phi}{\chi}} \right] \cos\phi\, d\phi \quad (3.39)$$

Under the transformation $\phi \to -\phi$ in either domain, the value to which the slope is tending changes sign, and so the derivative is discontinuous as can been seen in figure 1.4. The value of the expression in (3.39.1) which the slope is approaching is not obvious, indeed, at the wall, the slope would seem to have an infinite value, but from numerical integration it is found that the slope has a positive value just on the $y > 0$ side of $y = 0$.

$$\int_{-\pi}^{\pi} d\phi \left[\frac{\cot\phi}{1-e^{-2\phi}} - \frac{1+e^{2\phi}}{2\chi\sinh^2\phi} \right] = \overline{26.625} > 0$$

While approaching the same value at $y = 0$ from the $y < 0$ domain, the slope changes in sign, indicating a symmetric behavior. Since it has been determined that $\Delta\sigma_{zz} \geq 0$, the curve of the correction to the conductivity σ_{zz} decreases to some finite value at $y = 0$ in the $y < 0$ domain, and increases away from the wall in the $y > 0$ domain. Together with the knowledge of its behavior far from the wall, it has been shown that the conductivity contribution curve "dips" at the wall.

In summary, the $\Delta\sigma_{zz}$ component behaves as has been determined numerically. The position-dependent contribution will vanish away from the wall, and is continuous across the domain boundary. The curve rises to a maximum just before $y = 0$ in both $y < 0$ and $y > 0$ domains, and drops to a sharp dip that is tangentially discontinuous, that is, the first derivative is discontinuous at the wall.

4.2 The Tensor Component $\Delta\sigma_{yy}(y)$

The behavior of the correction to the transverse conductivity in the other direction, σ_{yy}, is quite similar to that of σ_{zz}. In the same way as was discussed in the previous case, the following can be derived.

$$\frac{\Delta\sigma_{yy}}{\sigma_0}(y>0\rightarrow y=0) = \frac{4\chi}{3}\int_{-\pi}^{\pi}\frac{\sin 2\phi\ d\phi}{1+e^{-2\phi/\chi}} \tag{3.40}$$

$$= \frac{\Delta\sigma_{yy}}{\sigma_0}(y<0\rightarrow y=0)$$

$$= -0.36\ \chi$$

The transverse additional conductivity is symmetric about the domain wall, as was true for the longitudinal conductivity. The first derivative with respect to y also behaves in the same manner as for $\Delta\sigma_{zz}$ at the wall.

$$\frac{d\,\Delta\sigma_{yy}}{dy}(y>0\rightarrow y=0) = \frac{4\chi\sigma_0}{6}\left\{\int_0^{\pi}\frac{1}{\chi}\cos\phi\,\tanh\frac{\phi}{\chi}+4\right\} \tag{3.41}$$

$$= 3.48\ \chi\ \sigma_0$$

$$= -\frac{d\,\Delta\sigma_{yy}}{dy}(y<0\rightarrow y=0)$$

Again, this is the same result as the calculation indicated by figure 1.5, the curve increases from zero to a maximum before $y=0$, then behaves symmetrically in the $y>0$ domain.

4.3 Cross-Conductivity

The corrections for the cross conductivity σ_{yx} and σ_{xy} are found in the same way as the longitudinal contributions. The results are

$$\frac{\Delta\sigma_{yx}}{\sigma_0}(y>0\to y=0) = \frac{8\chi}{3}\int_{-\pi}^{\pi}\frac{\sin^2\phi\, d\phi}{1-e^{-2\phi/\chi}} > 0 \qquad (3.42.1)$$

$$= 4.19\,\chi$$

$$= -\frac{\Delta\sigma_{yx}}{\sigma_0}(y<0\to y=0) \qquad (3.42.2)$$

$$\frac{\Delta\sigma_{xy}}{\sigma_0}(y>0\to y=0) = -\frac{8\sigma_0\chi}{3}\int_{-\pi}^{\pi}\frac{\cos^2\phi\, d\phi}{1+e^{-2\phi/\chi}} \qquad (3.43.1)$$

$$= 4.19\,\chi\,\sigma_0$$

$$= -\frac{\Delta\sigma_{xy}}{\sigma_0}(y>0\to y=0) \qquad (3.43.2)$$

And the first derivatives are

$$\frac{d\,\Delta\sigma_{yx}}{dy}(y>0) = -\frac{4\chi\sigma_0}{3}\int_0^{\pi}\left[\cos\phi\,\coth\frac{\phi}{\chi} - \frac{1}{\chi}\sin\phi\,\coth^2\frac{\phi}{\chi}\right]d\phi \qquad (3.44.1)$$

$$= 3.0\,\chi\,\sigma_0$$

$$= \frac{d\,\Delta\sigma_{yx}}{dy}(y<0) \qquad (3.44.2)$$

$$\frac{d\,\Delta\sigma_{xy}}{dy}(y>0) = \frac{4\chi\sigma_0}{3}\int_{-\pi}^{\pi}\left[\frac{2\cos\phi}{1+e^{-2\phi/\chi}} + \frac{\cos^2\phi(1-e^{2\phi/\chi})}{2\chi\cosh^2\frac{\phi}{\chi}\sin\phi}\right]d\phi \qquad (3.45.1)$$

$$= 1.0\,\chi\,\sigma_0$$

$$= \frac{d\,\Delta\sigma_{xy}}{dy}(y<0) \qquad (3.45.2)$$

The asymmetric nature of the curves in figures 1.5 and 1.6 is apparent from the limiting case of the analytic expressions for the additional conductivity given by equations (3.36) and (3.37), and their derivatives with respect to y. The additional cross conductivity reflects the dependence of the homogeneous field conductivity on the direction of the field (expression (2.13)).

The remaining terms of the y-dependent contributions to the conductivity matrix are zero. Λ_z has no correction due to the y-dependence, so

$$\Delta\sigma_{zz} = \Delta\sigma_{yz} = \Delta\sigma_{zz} = 0. \tag{3.45}$$

It also happens that since the velocity in the z-direction is $v_z = v_f \cos\theta$, the rest of the terms disappear.

$$\Delta\sigma_{zz} = \int_0^{\pi} \sin^2\theta \cos\theta \; d\theta [\; \cdots \;] = 0$$

$$\sigma_{zz} = \sigma_{zy} = 0 \tag{3.46}$$

We have, then, determined the general dependence of the electronic conductivity on the distance of the electron from the domain wall. Exact solutions for the correction are only possible right at $y=0$. Combining equations (3.38), (3.40), (3.42), and (3.43), the contribution to the conductivity matrix due to y-dependence is;

$$\Delta\sigma(y) = \frac{4\chi\sigma_0}{3} \begin{vmatrix} \int_{-\pi}^{\pi} \frac{\sin 2\phi \; d\phi}{1-e^{-2\phi/x}} & \frac{-}{+} 2\int_{-\pi}^{\pi} \frac{\cos^2\phi \; d\phi}{1+e^{2\phi/x}} \\ \pm 2\int_0^{\pi} \frac{\sin^2\phi \; d\phi}{1-e^{-2\phi/x}} & \int_{-\pi}^{\pi} \frac{\sin 2\phi \; d\phi}{1+e^{-2\phi/x}} \end{vmatrix}$$

for the region $y>0/y<0$.

The semi-classical calculation of the contribution to the electrical conductivity due

to the presence of a 180° domain wall has been calculated using the Chambers' solution for the classical Boltzmann equation. It has been shown that the additional conductivity is larger in close proximity to the domain wall than further away, and eventually dies away at a distance of twice the cyclotron radius. Also this contribution is scaled by a factor of χ, and hence is significant only in the clean limit, where the calculated corrections in this investigation were as high as $\Delta\sigma_{zz}/\sigma_{zz} \approx 4$. For the smaller values of χ, that are characteristic of real materials, the magnitude of the additional conductivity introduced by the new set of open trajectories is quite small in magnitude, on the order of 1×10^{-4} times smaller.

Similar quantitative results were found by Cabrera and Falicov (1974a; 1974b) for conductivity at the domain wall, and similar qualitative results arose from the treatment of the classical trajectories by Zakharov and Man'kov (1984). The latter investigation showed that for a single domain wall, the conductivity increased near the wall as was seen here, a phenomenon which was attributed to the increase in the number of electrons following the new open oribit across the domain wall. The non-monotonic behavior on the additional conductivity seen in that analysis was also observed here. The order of the effect of these new trajectories again agree well with the present results. The open orbits may increase the conductivity near the domain wall by as much as four times the homogeneous field value for very clean samples.

The domain wall effect calculated here can be experimentally measured if the discussion is expanded to include bulk conductivity. The current, j_i, is related to the conductivity through the relation

$$j_i(\mathbf{x}) = \sigma_{ij}(\mathbf{x})\, E_j(\mathbf{x})$$

where $i, j = x, y, z$ in bulk materials of large enough dimension so the inhomogenities that arise in the conductiviy are negligible. Depending on whether a voltage drop is applied in a direction parallel or perpendicular to the domain wall, the current reduces to an average over y of either the resistivity or the conductivity. The resistivity tensor has elements

$$\rho_{ij} = [\sigma^{-1}]_{ij}$$

and, based on the expressions found here for the elements of the conductivity tensor, the resistivity does not have a simple form unless the restrictive assumption of equal concetration of electrons and holes is made, as in the investigation by Zakharov and Man'kov. This assumption ignores the voltage perpendicular to the applied voltage, since over the average of all domains, it should vanish. The asymmetry of the additional cross conductivity curves (figures 1.5 and 1.6) indicated that this requirement is satisfied in the present treatment.

If the separation between domains exceeds $4r_c$, then the average becomes the sum of homogeneous domain contributions to the conductivity. For narrower domains, new classes of electron trajectories arise as the electron crosses in and out of more domains, in much the same way as for two domains. In the two domain wall case, for example, there arises an additional third group of closed classical trajectories crossing both walls. The application of an external field creates domain wall movement, and so an experimental measurement should involve both effects. As the walls move closer together, more trajectories arise that cross both walls until domains collapse, in which case the electrons describe their homogeneous field closed orbits. Measurement of the resistivity should indicate this behaviour, and give an upper limit on the size of the effect, which is a maximum when the domains have a width of $4r_c$.

Previous experimental investigations (Isin and Coleman, 1966; Taylor, Isin and Coleman, 1968; Shumate, Coleman and Fivaz, 1970) have seen that the scattering of electrons from the domain wall, as well as the formation of domains is insufficient to completely account for negative magnetoresistance which is strongest in the clean limit of large χ. It is in this limit that the classical trajectories are important.

The calculation has been fairly lengthly, and an equal amount of effort, if not more, was required to interpret the results. It remains to be seen how the quantum mechanical calculation is done, and what extra considerations arise. Although the quantum mechanical corrections will not be discussed in this report, for completeness, the energy levels of the domain wall system will be found. Once having this solution, all the steps in the derivation of the transport equation and its solution will have been established.

The Energy Levels of an Electron in the Presence of a Domain Wall of Bloch Type

It was demonstrated how a quantum mechanical master equation could be derived using the TFD formalism in the previous chapter. Following this derivation, it was shown how an explicit expression for the conductivity tensor could be calculated to leading order in the electric field. The relationship between the master equation and the semi-classical Boltzmann equation was then established. In this chapter, the Chambers solution to the Boltzmann equation was used to compute the conductivity tensor for a homogeneous field, and also for the field including a Bloch type domain wall. This investigation will be concluded with a discussion of the quantum mechanical approach to the Bloch wall problem. This would complete the steps needed to look at the quantum

effects of this type of rapid variation of the magnetic field, since these energy levels may then be used instead of the Landau levels in the evaluation of conductivity discussed in chapter II.

The problem is to find the energy levels of an electron in the presence of an infinitely thin 180° domain wall of Bloch wall at position $y=0$, by treating the system as two homogeneous magnetic fields. The energy levels will be found by matching the electronic wavefunctions at $y=0$. The potential in such a case will be of the form of a double oscillator potential, and the solution for the energy will follow the treatment of Merzbacher (1970).

The field will be homogeneous in the $y>0$ and the $y<0$ domains,

$$\mathbf{B} = -\text{sgn } y \quad B \, \hat{e}_z \tag{3.48}$$

and the choice of gauge will be the same as has been used throughout this investigation.

$$\mathbf{A} = -B \; y \; \hat{e}_x \tag{2.3.1}$$

The Shrödinger equation is

$$\frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2\psi = E \; \psi. \tag{3.49}$$

The wavefunction solutions will be the same as those given by (I.5) for the Landau levels, but matching the boundary conditions at the wall $y=0$ will give rise to a new energy spectrum. The Shrödinger equation can be written in the same form as (I.4)

$$\frac{1}{2m}\chi'' - \Big\{V(y) + E\Big\}\chi = 0 \tag{3.50}$$

$$\text{with} \quad V(y) = \frac{1}{2}\frac{e^2B^2}{mc^2}\left(\mid y \mid - \frac{p_z c}{eB} \right)^2. \tag{3.50.1}$$

Equation (3.50.1) is the potential for the double harmonic oscillator, and may be solved from Merzbacher's (1970) solution, using the substitution

$$\frac{\sqrt{2c}}{\sqrt{eB}}\left(y - \frac{p_z c}{eB}\right) = (\xi - \xi_0),$$

the solution for the wavefunction is in terms of the parabolic cylinder function

$$\psi(y) = \begin{cases} D_\nu(\xi - \xi_0), & \xi > 0 \\ D_\nu(\xi + \xi_0), & \xi < 0 \end{cases} \tag{3.51}$$

and the energies are given by

$$E = \frac{eB}{mc}\left(\nu + \frac{1}{2}\right) + \frac{p_z^2}{2m}. \tag{3.52}$$

The even values of ν are determined from

$$D'_\nu(-\xi_0) = D'_\nu\left(\sqrt{\frac{2\,c\,p_z}{eB}}\right) = 0,$$

and the odd, from the condition

$$D_\nu\left(\sqrt{\frac{2\,c\,p_z}{eB}}\right) = 0.$$

These are the energy levels and wavefunctions for an electron in the presence of a domain wall.

Explicit forms of the energy may be obtained only for the limiting values of ν, that is, for energies very near or much greater than that of the lowest energy state. Since at high energies, the double harmonic oscillator potential tends toward the single, simple harmonic oscillator, the energy levels just approach the landau levels. Only the low energy spectrum will differ significantly. For a given value of p_z, the lowest energy level may be obtained as

$$E^{(0)} \to \frac{p_z}{\sqrt{\pi} r_c m}\, e^{-(p_z r_c)^2} + \frac{r_c^2}{2m} + \frac{p_z^2}{2m}.$$

The energy levels very near the ground state have been derived for an electron in the presence of an infinitely thin Bloch wall. These may be used as the base, unper-

turbed states for a system including a perturbing electric field, and the conductivity may be found from the solution of the resulting transport equation. If any additional effects are to be investigated that can be absorbed as part of the potential, this is the point in the treatment where they should be introduced.

For example, if the effects of finite domain wall thickness are to be examined, the general form of the magnetic induction for a domain wall of width δ should be used instead of the discontinuous field defined by (3.48).

$$\mathbf{B} = B_x \hat{x} + B_y \hat{y} + B_z \hat{z}$$

$$\text{where} \begin{cases} B_x = \dfrac{B}{\cosh(\frac{y}{\delta})} \\ B_y = 0 \\ B_z = -B \tanh(\frac{y}{\delta}). \end{cases}$$

The choice of gauge is made to retain only a y-dependence.

$$\left\{ A_x = B\ \delta \ln[\cosh(\tfrac{y}{\delta})] A_y = 0 A_z = B\ \delta \tan^{-1}[\sinh(\tfrac{y}{\delta})] \right.$$

The method of solution used by Mints (1989) may be used to find the energy levels of electrons is this field. The result, for small domain wall thickness, at low energy, is

$$E^{(0)} \to \frac{1}{m}\left\{ \frac{p_z}{\sqrt{\pi} r_c} e^{-(p_z r_c + \delta \ln 2/r_c)^2} + \frac{r_c^2}{2} \right\} + \frac{\delta \ln 2}{\sqrt{\pi} r_c^2 m} e^{-(r_c/\lambda_c + \delta \ln 2/r_c)^2} + \frac{p_z^2}{2m}$$

The purposes of this chapter have been completed. By way of completing the correspondence between the quantum transport equation and the Boltzmann equation, the Chambers solution and subsequent evaluation of the conductivity tensor in a homogeneous magnetic field have been discussed. The conductivity was then found in the

presence of a 180° Bloch type domain wall using classical electron trajectories in an attempt to establish the treatment of this problem from a quantum mechanical approach, through the Boltzmann equation. The energy spectrum for the magnetic field including the domain wall was found, and hence using these instead of the Landau levels in the procedure of chapter II, the steps of the quantum mechanical evaluation of the conductivity have been completely outlined.

Chapter IV: Conclusions

The preceding extension of the work by Arimitsu and Umezawa (1985; 1987) and by Whitehead (1985), discussed the steps involved in the derivation of a transport equation for electrons, in crossed magnetic and electric fields, within the framework of NETFD. Gauge invariance was a primary consideration throughout the procedure, and this was initially manifested by the choice of the electric field as the perturbing field in the interaction representation. The quantization of the magnetic field was carefully treated, again because of the inherent gauge dependence of calculations involving magnetic fields. Once the creation and annihilation operators had been defined, the reservoir operators were introduced through the choice of the simple coupling of the electron system to the thermal reservoir, which was used to describe the solely thermal relaxation process. The mechanisms of NETFD were then used to derive a master equation for a thermal electron wavefunction.

The master equation was linearized, then solved, and the usual result for the homogeneous field conductivity was shown to emerge.

The master equation was then shown to correspond to the semi-classical Boltzmann equation by transforming from the Landau level-based space to momentum space, with an intermediary transformation to position space. A gauge dependence arose, requiring the definition of a density function to produce a gauge invariant equation. The major

assumption that arose from this consideration was that the correlation length between the thermal states are very small, thus particles only undergo very short range interactions. This amounts essentially to the "classical" assumption, and having made it, the Boltzmann equation associated with the derived transport equation was found.

The solution of the transport equation associated with the Boltzmann equation, and its application to the derivation of the electrical conductivity tensor were extensively studied. The standard Hall conductivities were briefly derived, to establish the method for the more interesting case of an abruptly discontinuous magnetic field. The presence of the discontinuity introduced a new class of classical trajectories, and their effects on the conductivity were investigated.

The conductivity was found to increase by a significant amount only in the limit of long relaxation times, or the "clean" limit. This is in agreement with a very similar study done by Zakharov and Man'kov (1984), where the increasing negative magnetoresistance was related to the increase of magnetic domains in response to an external field. The order of this effect is roughly comparable to the paramagnetic effects on the conductivity as found by Cabrera and Falicov (1974a), tending to be smaller.

The study concluded with finding the energy of the system of the inhomogeneous field, quantum mechanically, in order to furnish, together with the discussion of chapter II, all the steps in the procedure of the quantum mechanical calculation of the conductivity tensor. Using the new energy states to replace the Landau levels in the derivation of a master equation as outlined in chapter II, the equation can be linearized, and the solution to lowest ordering in the energy found, and hence the conductivity can be calculated. The purely quantum mechanical calculation of the conductivity tensor in the

presence of a Bloch type domain wall has been outlined.

Further Investigations

The first, immediate extension of this work is the actual quantum mechanical calculation of the conductivity tensor, now that the ground work has been set. The resistivity is calculated according to the method discussed in chapter II, using the energy state derived in chapter III. Although this approach is limited to two energy regimes, it will still indicate what effects a spatially inhomogeneous magnetic field would have on the electron transport. The only difficulty will arise in the treatment of the gauge dependence, since the complexity of the potential indicates a significant dependence on the form of the vector potential.

One of the shortcomings of this analysis is the neglect of other relaxation mechanism, especially scattering. Closely connected with this was the assumption of very short correlation lengths, thus if scattering were included in the interaction Hamiltonian, finite coherence lengths would also have to be considered. This problem of realistic scattering techniques in the derivation of quantum transport equations has been very recently addressed by Arimitsu (U. of Tsukuba pre-print), however not for a magnetic field. It would be interesting to see what corrections the introduction of scattering would produce.

The other major point that was not treated was the fact that rapid variations in the magnetic field such as the discontinuity discussed here, will surely give rise to quantum corrections to the conductivity. The scattering of electrons from the domain wall has been neglected in this work, but for such a rapid change in the potential, should

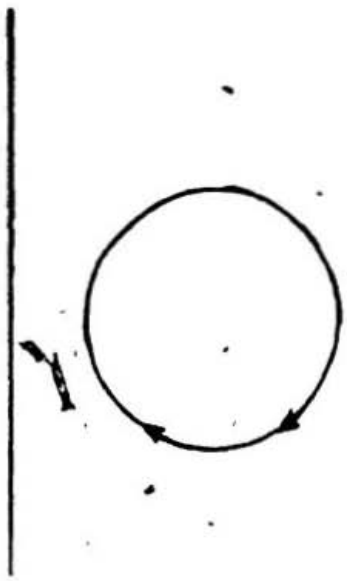
really be considered. The approach that was investigated for homogeneous fields can readily be extended to slowly varying fields with a little more general distribution kernel, but an extensive adjustment is required to account for rapid variations of the fields.

The same can be said for the determination of the energy levels. Inclusion of finite domain wall thickness in the quantum mechanical calculation of the energy levels would involve at least higher order expansions than those used in the last section of chapter III, and would not be in the context of the preceding work. Quite a bit of work is required to give a more complete analysis of the the Bloch wall effect on the electron conductivity.

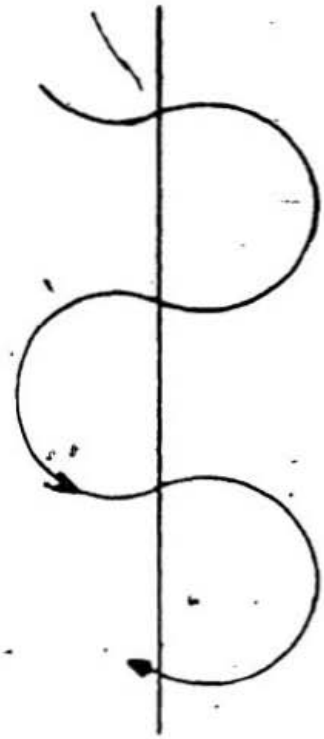
The derivation of quantum transport equations from the usual field theory (Mahan, 1987; Kreiger and Iafrate, 1987), and using Thermo Field Dynamics (Arimitsu, 1987) has been the subject of some recent work. A detailed comparison of these techniques remains to be carried out. This should establish an equivalence, or at least some sort of correspondence between the transport equations that emerge from a Green's function approach, and two different formulations of NETFD.

There still remain some considerations open to investigation in establishing the derivation of a transport equation including magnetic and electric fields within the framework of quantum field theory. Solutions of such a transport equation will provide a deeper insight into transport properties such as electrical conductivity. However, having found the connection between a quantum mechanically derived transport equation and the classical Boltzmann equation in this work, the superoperator formalism of NETFD which is inherently a more physically insightful theory than the traditional Greens' function-based field theory, has been established as a viable framework for calcu-

lations of this type.



Electron describes a closed circular orbit, unaffected by the wall.



Electron describes an open orbit along the positive x-direction.

Figure 1.1 Position space representations of possible electron trajectories.

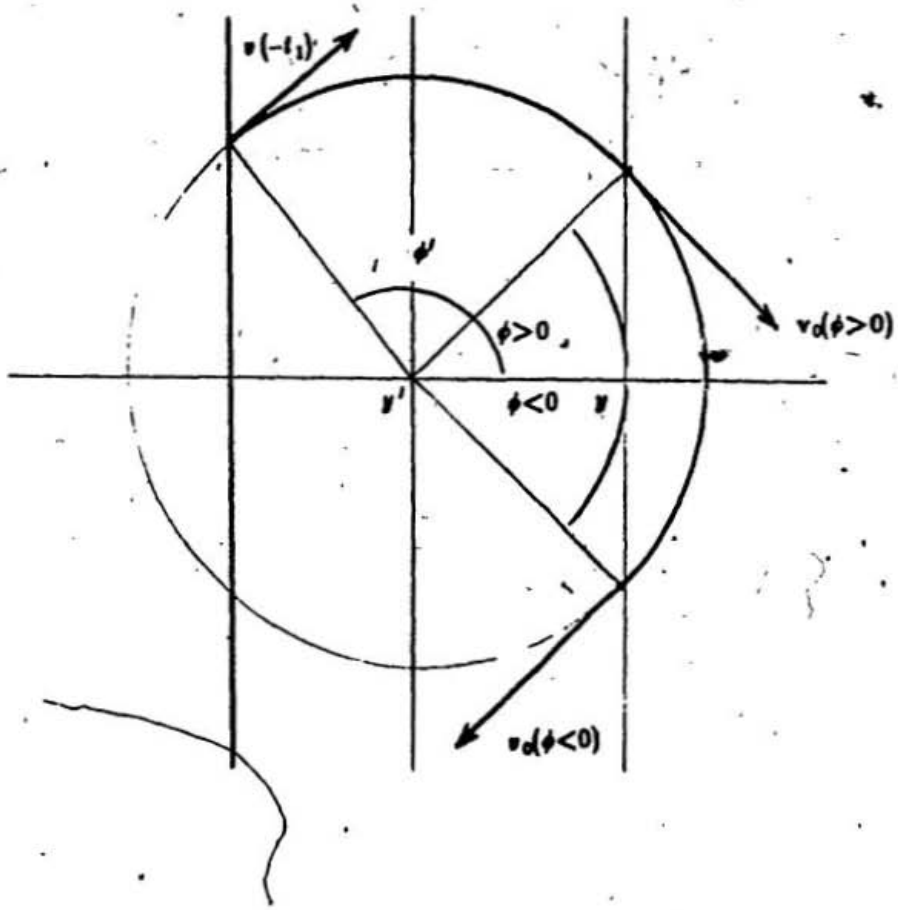


Figure 1.2 Geometric interpretation of the trajectory

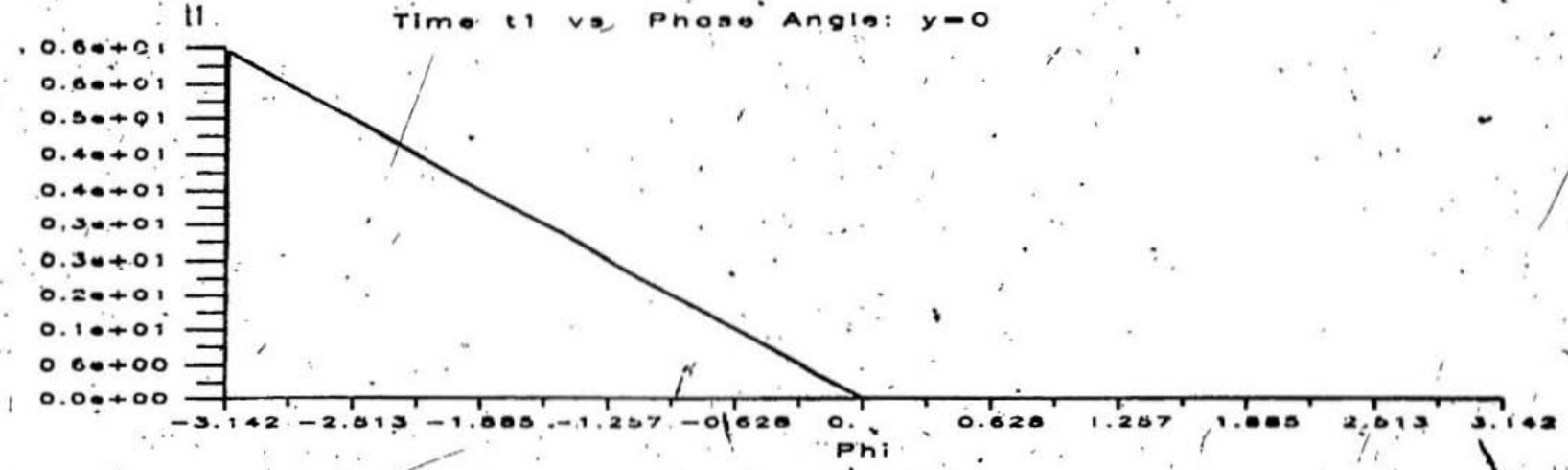


Figure 1.3.1

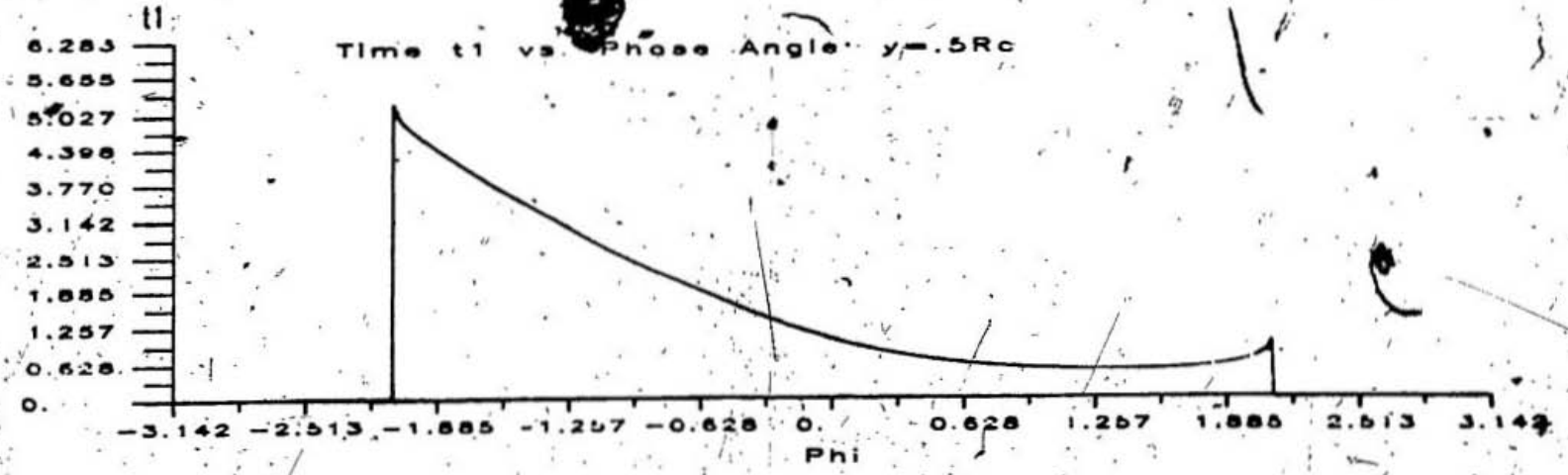
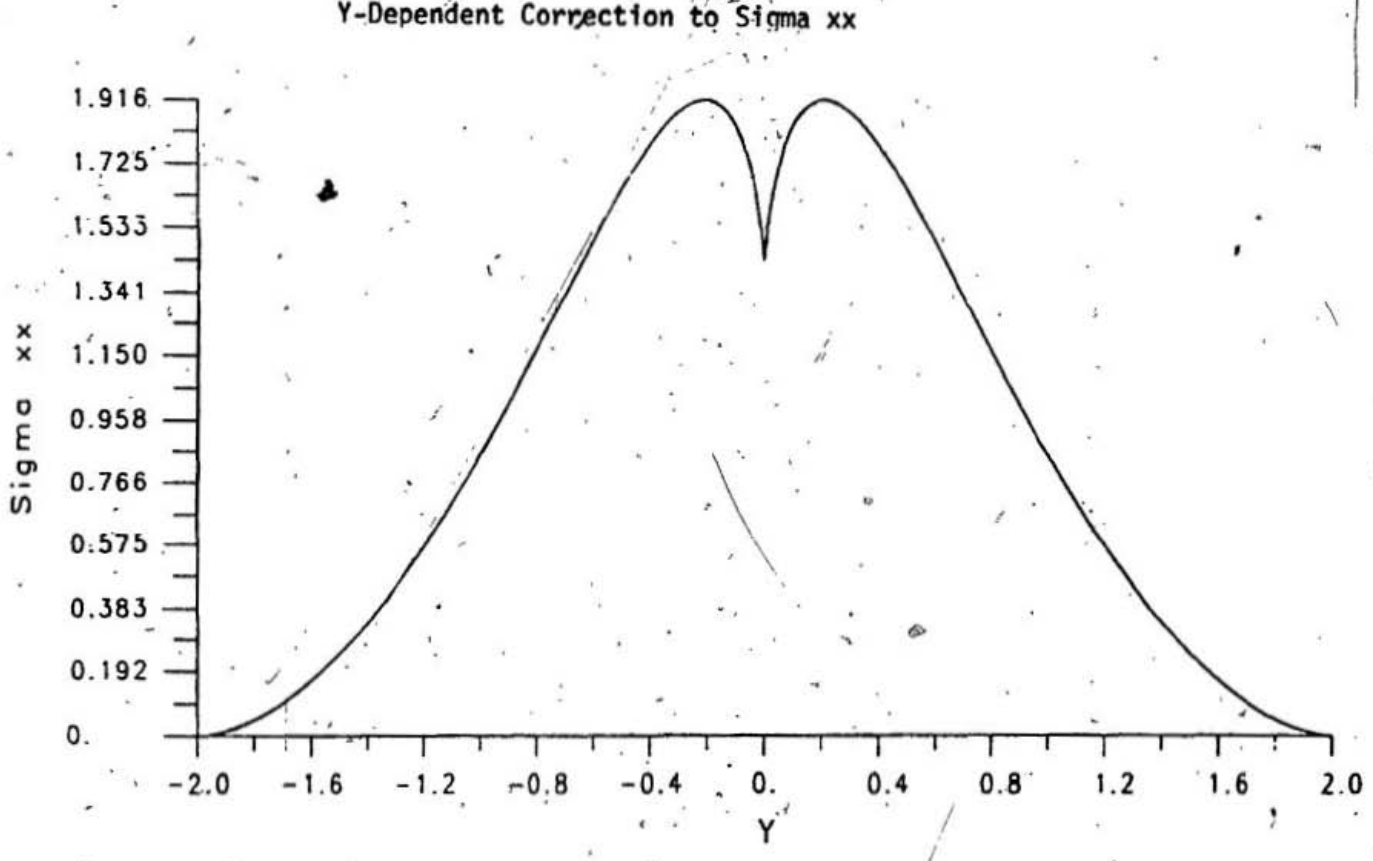


Figure 1.3.2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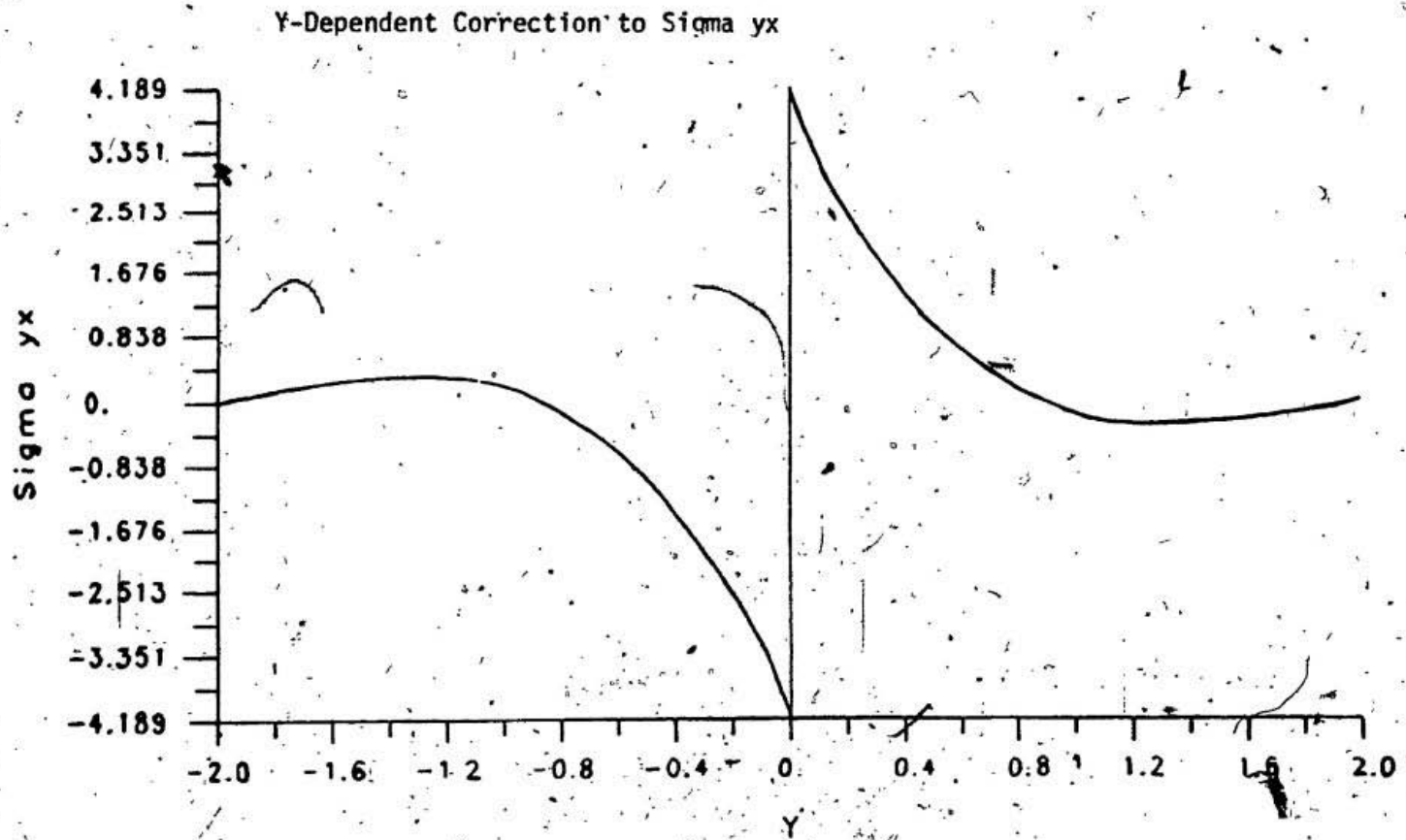
1.341
1.150
0.958
0.766
0.575
0.383
0.192
0.
-2.0
-1.6
-1.2
-0.8
-0.4
0.
0.4
0.8
1.2
1.6
2.0
Y

Figure 1.4


Y-Dependent Correction to Sigma yx
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0.838
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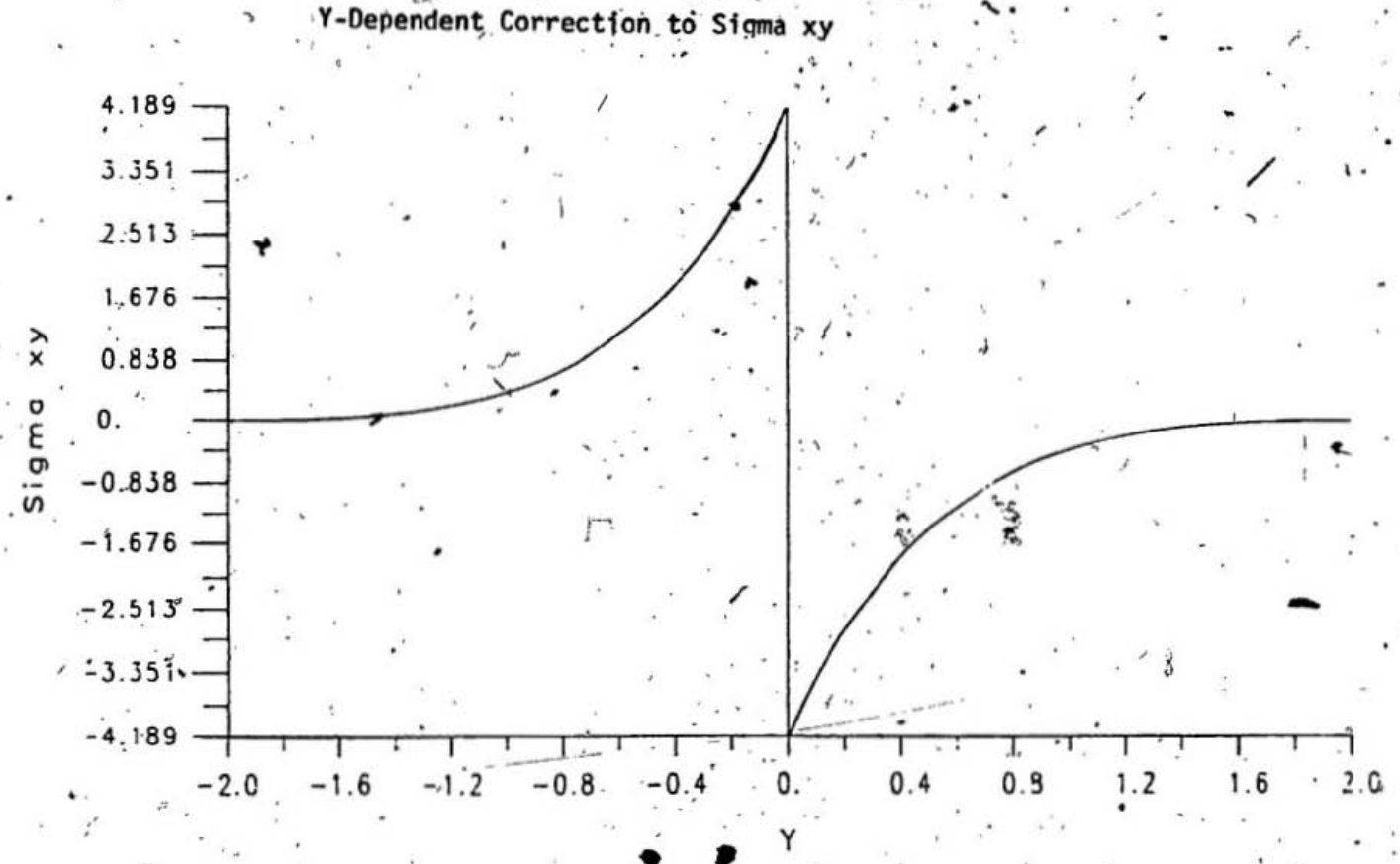
-1.676
-2.513
-3.351
-4.189
-2.0
-1.6
-1.2
-0.8
-0.4
0
0.4
0.8
1.2
1.6
2.0
Y

Figure 1.5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-2.0
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1.6
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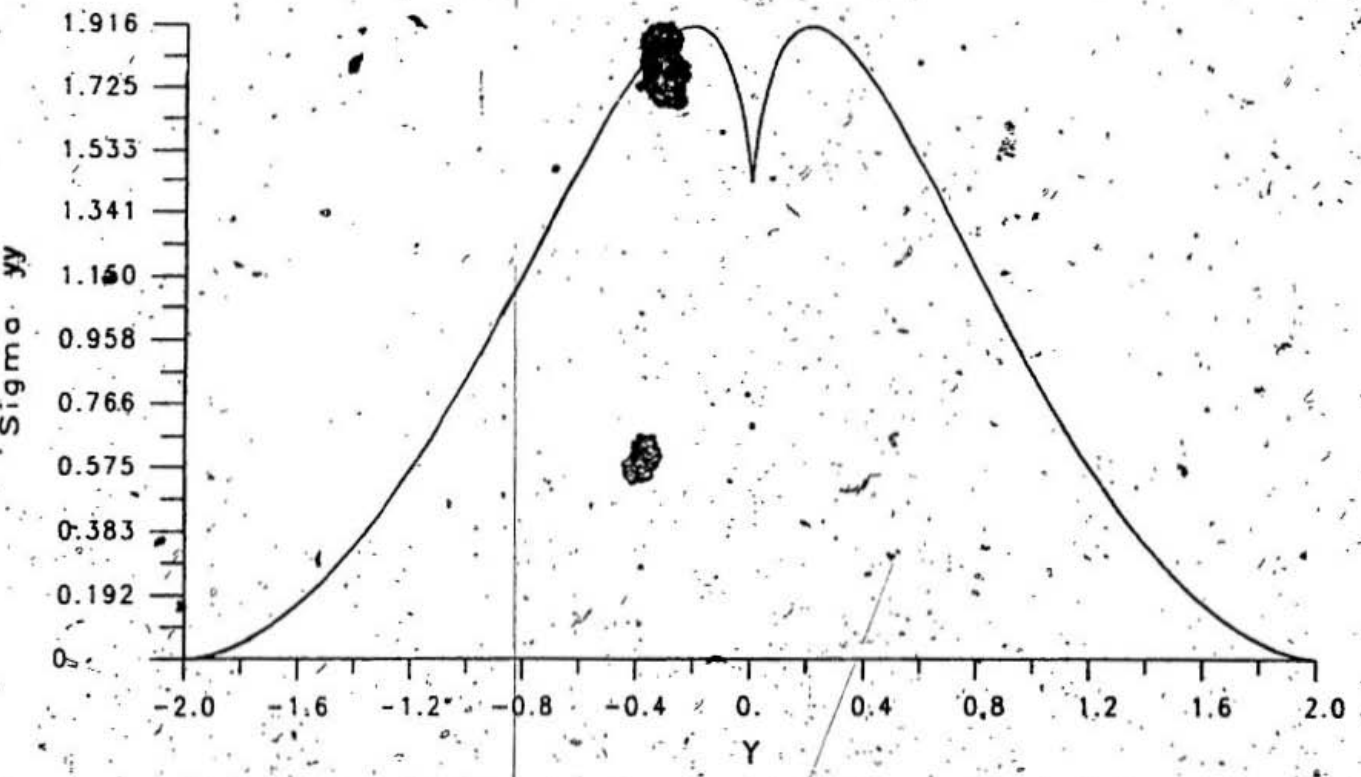
Y

Figure 1.6


Y-Dependent Correction to Sigma yy
Sigma yy
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1.533
1.341
1.150
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0.575
0.383
0.192
0
-2.0
-1.6
-1.2
-0.8
-0.4
0.
0.4
0.8
1.2
1.6
2.0
Y

Figure 1.7

Appendix I: The Landau Levels and Their Degeneracy

Landau (1965) quantized a system of interacting particles in a constant uniform magnetic field with vector potential $\mathbf{A}$. Assuming the particles have no spin, the Hamiltonian has the form

$$\hat{H} = \frac{(\hat{p} - \frac{e\mathbf{A}}{c})^2}{2m} \tag{I.1}$$

The field is taken to be in the z-axis direction, and the gauge is chosen so that

$$\begin{cases} A_x = -By \\ A_y = 0 \\ A_z = 0. \end{cases} \tag{I.2}$$

The Schrodinger equation, $\hat{H}\psi = E\psi$, using this potential, and assuming the form of ψ looks like

$$\psi = \exp\left[i(p_x x + p_z z)\right] \chi(y), \tag{I.3}$$

becomes the following differential equation.

$$\chi'' + 2m\left\{E - \frac{1}{2}m\omega^2(y - y_0)^2\right\}\chi = 0 \tag{I.4}$$

where $E = E - \frac{p_z^2}{2m}$,

$$\omega = \frac{eB}{mc},$$

$$y_0 = -\frac{cp_x}{eB},$$

following Landau and Lifshitz (1965). This is the equation for a simple harmonic oscillator for which the solutions are the wave functions

$$\psi = A e^{[i(p_x x + p_z z)]} e^{[-|e|B(y-y_0)^2/2c]} H_n\left[\sqrt{\frac{|e|B}{c}}(y - y_0)\right] \tag{I.5}$$

where A is the normalization constant and H_n are Hermite polynomials, and the energy levels are the so-called Landau levels

$$E_n = (n + \tfrac{1}{2})\,\omega + \frac{p_z^2}{2m} \tag{I.6}$$

where $\omega_c = |e|B/mc$ is the cyclotron frequency.

The degree of degeneracy of the Landau levels is finite if the motion of the electron is limited to a large but finite volume $L_x L_y L_z$. The number of possible values of p in any one direction is $L\,\Delta p$. In the x-y plane, for a given p_z, assuming $0 < y_0 < L_y$, then $\Delta p_x = eBL_x L_y/c$ which means that if the electron is constrained to move in two dimensions, the number of degenerate levels is

$$\frac{eBL_x L_y}{c} \tag{I.7}$$

So, if bound in all three dimensions, from equation (I.6) there are

$$\frac{eBL_x L_y}{c} L_z\,\Delta p_z \tag{I.8}$$

energy levels possible for one n.

Appendix II: Coarse Graining

The details of the derivation of the master equation are contained in the paper by Arimitsu and Umezawa (1987), and can be summarized in the following way.

The reservoir expectation value of equation (2.19) may be expanded according to theorem V, Kubo (1962), as follows:

$$<<1_R \mid T\ exp\left[-ig\int_{t_0}^{t} ds\ \hat{H}_I(s)\right] \mid W_R>> = \tag{II.1}$$

$$\sum_{n=1}^{\infty}(-ig)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-2}} dt_{n-1} <<1_R \mid \hat{H}_I(t)\hat{H}_I(t_1)\cdots\hat{H}_I(t_{n-1}) \mid W_R>>$$

From the definition of operator $\hat{Z}(t,t_0)$, the expression for the state in the interaction representation given by equation (2.17), and from the fact that $\hat{H}_I(t)$ has no effect on $<<1_R \mid$ and $\mid W_R>>$,

$$\ln <<1_R \mid \hat{Z}(t,\tau) \mid W_R>> = <<1_R \mid T\left[-ig\int_{\tau}^{t} ds\ \hat{H}_I(s)\right] \mid W_R>>.$$

The bra and ket vectors can be taken inside the integration as they are independent of time, so, substituting this into (II.1), we have:

$$<<1_R \mid T\exp[-ig\int_{t_0}^{t} ds\ \hat{H}_I(s)] \mid W_R>> =$$

$$= \mathcal{T}\sum_{n=1}^{\infty}(-ig)^n \left[<<1_R \mid \ln \hat{Z}(t,t_0) \mid W_R>>\right]\left[<<1_R \mid \ln \hat{Z}(t_1,t_0) \mid W_R>>\right]$$

$$\cdots \left[<<1_R \mid \ln \hat{Z}(t_{n-2},t_0) \mid W_R>>\right]$$

$$= \sum_{n=1}^{\infty}\left[\int_{t_0}^{t} ds\ \partial_t\, T\ln <<1_R \mid \hat{Z}(s,t_0) \mid W_R>>\right]^n$$

Note that upon taking T inside the integral, it became $\partial_t\, T$. Now summing over the index n, the exponential is regained. Define

$$\hat{K}_I(t) = \partial_t T \ln \langle\langle 1_R \mid \hat{Z}(t, t_0) \mid W_R(t_0)\rangle\rangle$$

so that we may write (2.19)

$$\mid W_S(t)\rangle\rangle_I = T \exp\left[\int_{t_0}^{t} ds \ \hat{K}_I(s)\right] \mid W_S(t_0)\rangle\rangle \qquad \text{(II.2)}$$

Finally, the master equation for $\mid W_S(t)\rangle\rangle$ is achieved by substituting (II.2) into the time derivative of the relation between Schrödinger and interaction states

$$\mid W_S(t)\rangle\rangle = e^{-i\hat{H}_S(t-t_0)} \mid W_S(t)\rangle\rangle_I . \qquad \text{(II.3)}$$

$$\partial_t \mid W_S(t)\rangle\rangle = -i\hat{H}_S \mid W_S(t)\rangle\rangle + e^{-i\hat{H}_S(t-t_0)}$$

$$\partial_t T \exp\left[\int \partial_t T \ln \langle\langle 1_R \mid \hat{Z}(t, t_0) \mid W_R\rangle\rangle\right] e^{i\hat{H}_S(t-t_0)} e^{-i\hat{H}_S(t-t_0)} \mid W_S(t)\rangle\rangle_I$$

$$= -i\left[\hat{H}_S + i\hat{K}(t)\right] \mid W_S(t)\rangle\rangle \qquad \text{(II.4)}$$

Appendix III: The Time Parameters

The analytic solution for the time parameters t_1 and Θ from the solutions for the equations of motion

$$\begin{cases} v_x(t) = A\cos\omega_c(t-t') + B\sin\omega_c(t-t') \\ v_y(t) = B\cos\omega_c(t-t') - A\sin\omega_c(t-t') \end{cases} \tag{3.24}$$

agree with the more intuitive geometrically argued solutions.

If $t'=0$ is chosen, then at time $t=0$, we have $A=v_x^0$, and $B=v_y^0$. Since we will eventually be integrating over a circular phase space, the spherical polar coordinates are introduced.

$$\begin{cases} v_x^0 = v_f\sin\theta\cos\phi \\ v_y^0 = v_f\sin\theta\sin\phi \end{cases}$$

Substituting this back into solution (3.26) at time $t=t_1$, the resulting equations

$$\begin{cases} v_x(-t_1) = v_f\sin\theta[\cos\phi\cos(-\omega_c t_1) + \sin\phi\sin(-\omega_c t_1)] = v_f\sin\theta\cos(\phi+\omega_c t_1) \\ v_y(-t_1) = v_f\sin\theta[\sin\phi\cos(-\omega_c t_1) + \cos\phi\sin(-\omega_c t_1)] = v_f\sin\theta\sin(\phi+\omega_c t_1) \end{cases}$$

may be solved to give an expression for the time t_1 in terms of the initial conditions, by dividing them and using the trigonometric identity.

$$\tan^{-1}\left[\frac{v_y}{v_x}\right] = \cos^{-1}\left[\frac{v_x}{\sqrt{v_x^2+v_y^2}}\right]$$

The resultant expression is the following.

$$\omega_c t_1 = \cos^{-1}\left[\cos\phi - \frac{\omega_c y}{v_f\sin\theta}\right] - \phi \tag{III.1}$$

This expression is the same as that given in (3.27).

Following the same method as for deriving t_1, equations (3.24) can be used to find Θ, by setting $t'=-t_1-(n-1)\Theta$, and solving the equations for time, at time

$t = -t_1 - n\Theta.$

$$\begin{cases} v_x(-t_1 - n\Theta) = v_f \sin\theta[\cos\phi\cos(-\omega_c\Theta) + \sin\phi\sin(-\omega_c t_1)] = v_f \sin\theta\cos(\phi+\omega_c t_1) \\ v_y(-t_1 - n\Theta) = v_f \sin\theta[\sin\phi\cos(-\omega_c\Theta) + \cos\phi\sin(-\omega_c t_1)] = v_f \sin\theta\sin(\phi+\omega_c t_1) \end{cases} \quad \text{(III.2)}$$

Now to reduce the $(t_1+n\Theta)$ dependence of the velocity in these expressions to just Θ dependence, consider the actual motion of the particle. The electron encounters the wall at times $-(t_1+n\Theta)$,

$$y(-[t_1+n\Theta]) = 0,$$

and from the equation (1.10) giving the constants of motion,

$$v_x(-[t_1+(n-1)\Theta]) = v_x(-[t_1+n\Theta]) = v_x(-t_1) \quad \text{(III.3)}$$

Intuitively, because the electron crosses the domain wall, and re-crosses in the opposite y-direction, it is also true that

$$v_y(-[t_1+(n-1)\Theta]) = -v_y(-[t_1+n\Theta]) = (-1)^{(n-1)} v_x(-t_1) \quad \text{(III.4)}$$

From the expressions for $v_i(-t_1-n\Theta)$ where $i=x,y$, (III.3) and (III.4), comes the relation

$$v_x(-t_1-n\Theta) = v_x{}^0 - \omega_c y_0 = v_f \sin\theta\cos\Gamma \quad \text{(III.5)}$$

where $\Gamma \equiv \cos^{-1}[\cos\phi - \omega_c y_0/v_f \sin\theta]$. Making use of the inverse trigonometric identities with this definition of Γ, this means that

$$v_y(-t_1-n\Theta) = v_f \sin\theta \sin\Gamma.$$

The result from substituting the above into (III.2), dividing the equations and equating the arguments of the tangents (or cotangents) is

$$\omega_c\Theta = 2\cos^{-1}\left[\cos\phi - \frac{\omega_c y}{v_f \sin\theta}\right] \quad \text{(III.6)}$$

which agrees with the expression (3.28).

Appendix IV: Additional Longitudinal Conductivity at the Domain Wall

The numerically derived curve shown in figure 1.4 represents the behaviour of the contribution to the conductivity that arises from the presence of the infinitely thin domain wall. The dependence on the distance from the wall can be seen to be non-monotonic. The behaviour may be justified analytically by considering the limiting case of $y \to 0$, where the expression for the longitudinal conductivity contribution given in equation (3.34) greatly simplifies.

According to the definition of ϕ' given in equation (3.26), at $y=0$, $\phi' = |\phi|$. This means that the ranges $-\pi \leq \phi \leq 0$ and $0 \leq \phi \leq \pi$ must be looked at separately, since for $\phi < 0$, $|\phi| = -\phi$, and $|\phi| = \phi$ for positive values. Dividing the integration over ϕ appropriately, and performing the integration over θ, equation (3.34) may be rewritten.

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y \to 0^+) = \frac{4\chi}{3}\{\int_0^{\pi} \sin\phi \left[1+\coth\frac{\phi}{\chi}\right] + \int_{-\pi}^{0} e^{-(-2\phi)/\chi}\sin(-\phi)\left[1+\coth\frac{-\phi}{\chi}\right]\}\cos\phi \, d\phi$$

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y \to 0^+) = \frac{4\chi}{3}\{\int_0^{\pi} \frac{2\, e^{\phi/\chi}}{e^{\phi/\chi} - e^{-\phi/\chi}} - \int_{-\pi}^{0} e^{2\phi/\chi}\frac{2\, e^{-\phi/\chi}}{e^{-\phi/\chi} - e^{\phi/\chi}}\}\cos\phi \sin\phi \, d\phi$$

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y \to 0^+) = \frac{4\chi}{3}\int_{-\pi}^{\pi} \frac{2\, e^{\phi/\chi}}{e^{\phi/\chi} - e^{-\phi/\chi}} \sin 2\phi \, d\phi$$

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y \to 0^+) = \frac{4\chi}{3}\int_{-\pi}^{\pi} \frac{\sin 2\phi \, d\phi}{1 - e^{-2\phi/\chi}} \qquad \text{(IV.1)}$$

The integrand will always be positive. The numerical result is the following;

$$\frac{4}{3}\int_{-\pi}^{\pi} \frac{\sin 2\phi \, d\phi}{e^{2\phi/\chi} - 1} = 1.43$$

which matches the result at $y=0$ found from the numerical integration of the full expression.

In the other domain, $y<0$, because the angles are defined in the opposite sense to those in the $y>0$ domain, the transformation $\phi \rightarrow -\phi$ will have to be made before the results may be compared with equation (IV.1). The main consequence of this definition of the angle in the second domain is that,

$$|\phi|_{y<0} = -|\phi|_{y>0} \tag{IV.2}$$

Hence the integral over ϕ in the expression for the domain wall conductivity contribution in the $y<0$ domain can be divided in a similar fashion as that in the positive y domain.

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y\rightarrow 0^-) = -\frac{4\chi}{3}\{\int_0^{\pi} e^{-2\phi/\chi}[-\sin\phi]\left[1+\coth\frac{\phi}{\chi}\right] + \int_{-\pi}^{0}[-\sin(-\phi)]\left[1+\coth\frac{-\phi}{\chi}\right]\}\cos\phi\, d\phi$$

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y\rightarrow 0^-) = \frac{4\chi}{3}\int_{-\pi}^{\pi}\frac{\sin 2\phi\, d\phi}{e^{2\phi/\chi}-1} \tag{IV.3}$$

Under the transformation $\phi \rightarrow -\phi$, it can be seen that these two expressions are the same.

$$\frac{\Delta\sigma_{zz}}{\sigma_0}(y\rightarrow 0^-) \rightarrow \frac{4\chi}{3}\int_{-\pi}^{\pi}\frac{\sin(-2\phi)\, d\phi}{e^{-2\phi/\chi}-1}$$

$$= \frac{4\chi}{3}\int_{-\pi}^{\pi}\frac{\sin 2\phi\, d\phi}{1-e^{-2\phi/\chi}}$$

$$= \frac{\Delta\sigma_{zz}}{\sigma_0}(y\rightarrow 0^+)$$

Appendix V: Slope of Longitudinal Conductivity Contribution

Equation (3.34), the contribution to the longitudinal conductivity due to the presence of an infinitely thin domain wall, has three y-dependent terms. Once $\frac{d\phi'}{dy}$ is known the slope of the curve can be determined using the product rule for differentiation. In the positive y domain, if the center of curvature of the electron trajectory moves away from the domain wall, the angular distance, measured from the positive y-axis, which the electron must cover to reach the wall, will increase. This explains the result found from (3.26) that

$$\frac{d\phi'}{dy} = \frac{\omega_c}{v_f \sin\theta \sin\phi'}, \quad y > 0$$

In the negative y domain, movement of the center of curvature in the positive y-direction will decrease the angular distance the electron travels to the wall. Again this geometric argument holds true when the derivative of equation (3.30) is taken.

$$\frac{d\phi'}{dy} = \frac{-\omega_c}{v_f \sin\theta \sin\phi'}, \quad y < 0$$

The three y-dependent terms can now be differentiated, giving the following results in the $y > 0 / y < 0$ domains.

$$\frac{d}{dy}[\pm \sin\phi'] = \frac{\omega_c \cot\phi'}{v_f \sin\theta}$$

$$\frac{d}{dy} e^{-(\phi' - +\phi)/\chi} = -+\frac{\omega_c \; e^{-(\phi' \pm \phi)/\chi}}{\chi v_f \sin\theta \sin\phi'}$$

$$\frac{d}{dy}[1 + \coth\frac{\phi'}{\chi}] = -+\frac{\omega_c}{\chi v_f \sin\theta \sin\phi \sinh^2\frac{\phi}{\chi}}$$

Finally, combining terms, the general expression for the slope of the domain wall contribution to the conductivity curve is as follows.

$$\frac{d\,\Delta\sigma_{zz}}{dy}(y>/<0) = \pm\chi\sigma_0 \int\int d\theta\; d\phi\; \sin^3\theta\; \cos\phi\; e^{-(\phi'-+\phi)/\chi}$$

$$\left\{ [1 + \coth\frac{\phi'}{\chi}][\cot\phi' - \frac{1}{\chi}] - \frac{1}{\chi \sinh^2\frac{\phi}{\chi}} \right\}$$

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