QUANTUM LIMIT MAGNETOCONDUCTIVITY IN THE DILUTE IMPURITY REGIME

by

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Semiclassical calculation shows that in the limit of high magnetic fields, the Hall conductivity is independent of any scattering mechanism (for closed orbits of the carriers). That this result is not true quantum mechanically for impurity scattering was recently shown by Nozieres and collaborators. However, these workers used an oversimplified model for the impurity scattering and their calculation contains some logical inconsistencies.

In the present work, a system containing a low concentration of impurities with short-ranged potentials in the presence of a very strong magnetic field is investigated. Here, fairly realistic potential models, such as the Thomas-Fermi potential are considered. These potential models are approximated in a systematic fashion to obtain a potential model for which there is an exact expression for the single-site t-matrix. The single-site t-matrix is then inserted into a general expression for the static magnetoconductivity tensor. The potential models used are

all non-local and their non-locality alters the velocity operator which in turn changes the transport properties of the system. This aspect of the theory is very important and is correctly taken care of in this work.

A generalization of the Nozieres result is obtained for the Hall conductivity o_{xy} plus a correction term which is very important in the case of strong potential scattering. Thus the Hall conductivity obtained in this work can differ greatly from the usual semiclassical expression for strong scattering. The result obtained for o_{xx} in the present work is, however, similar to Nozieres' except that the inconsistency in the potential model leads to a different numerical result.

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CHAPTER I

INTRODUCTION

When a material is placed in a strong magnetic field, the motion of the conduction electrons become quantized. Classically a free electron in a magnetic field moves in a circular orbit in the plane perpendicular to the field while the motion along the field direction remains that of a free particle. The quantization of the electronic motion is manifest in the oscillatory character of the various galvanomagnetic phenomena, such as the Shubnikov-deHaas effect, the deHaas-vanAlphen effect and in many other electronic properties.

Suppose an electric field is applied to a wire extending in the x-direction and a current density flows in the wire. If we now apply a magnetic field along the z-direction, electrons will be deflected in the negative y-direction by the Lorentz force (Fig. 1)

$$\vec{F} = -(e/c)\ [\vec{v} \times \vec{B}] \qquad \text{I.1}$$

Here the charge of an electron is -e, i.e. e > 0. As a result, electrons accumulate on the sides of the wire and consequently build up an electric field in the y-direction which opposes further accumulation of the electrons. This transverse electric field is referred to as the Hall field and in equilibrium balances the Lorentz force, so that current would flow only in the x-direction. Quantities of experimental interest include the resistance of the wire along the direction of the applied electric field E_x and the size of the Hall field E_y. According to

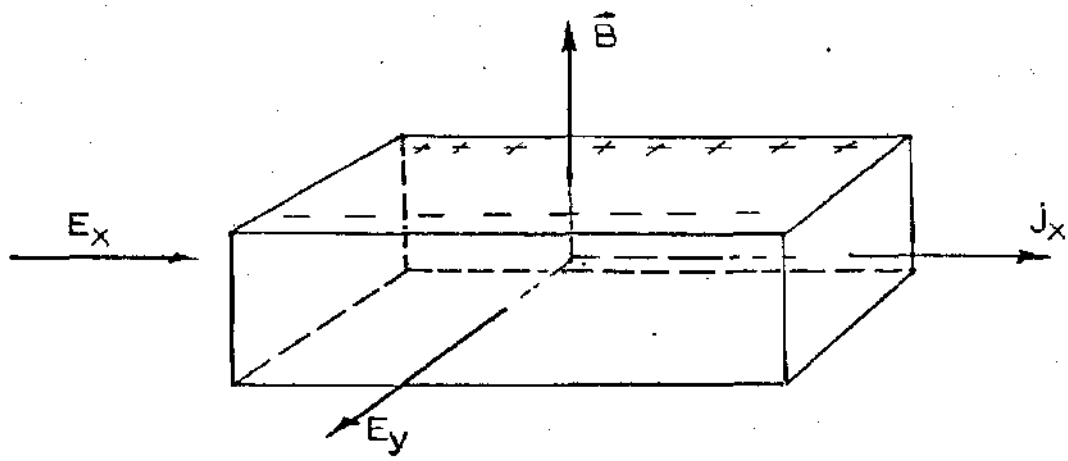


Fig. 1. A schematic view of Hall's experiment, with the magnetic field $\vec{B}$ in the z-direction, the applied electric field, E_x in the x-direction and Hall field E_y in the y-direction.

Ohm's law

$$E_x = \rho j_x \qquad \text{I.2}$$

but in general ρ is a second rank tensor, for which the Ohm's law could be generalized as

$$\vec{E} = \hat{\rho}\vec{j} \quad \text{or} \quad \vec{j} = \hat{\sigma}\vec{E} \qquad \text{I.3}$$

where $\hat{\sigma} = \hat{\rho}^{-1}$ is the conductivity tensor. Hence, for isotropic materials, we can write down the various components of the conductivity tensor

$$j_x = \sigma_{xx}E_x + \sigma_{xy}E_y \qquad \text{I.4}$$

$$j_y = \sigma_{yy}E_y + \sigma_{yx}E_x \quad . \qquad \text{I.5}$$

Since $j_y = 0$, and $\sigma_{xx} = \sigma_{yy}$ from symmetry and $\sigma_{xy} = -\sigma_{yx}$ from the Onsager relations, we therefore have that

$$E_y/E_x = \sigma_{xy}/\sigma_{xx} \quad . \qquad \text{I.6}$$

A quantity characterizing the size of the Hall field is defined by

$$R_H = E_y/j_xB \qquad \text{I.7}$$

and is called the Hall coefficient. The sign of the Hall field (or equivalently of the Hall coefficient) determines the sign of the charge carriers. Combining Eqs. I.4 and I.5 we can finally rewrite these two quantities as

$$\rho_{xx} = \rho_{\perp} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} \qquad \text{I.8}$$

and

$$BR_H = \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2} \quad . \qquad \text{I.9}$$

According to the classical transport theory for the free electron, where one assumes an isotropic mass, M, for the carrier and an isotropic

relaxation time, τ, the two transverse components of the conductivity tensor can be written as

$$\sigma_{xx} = \frac{\sigma_o}{1 + (\omega_c \tau)^2} \qquad \text{I.10}$$

and

$$\sigma_{xy} = \frac{-\sigma_o \omega\tau}{1 + (\omega_c \tau)^2} \qquad \text{I.11}$$

where σ_o is the Drude model DC conductivity in the absence of a magnetic field and is given by

$$\sigma_o = \frac{ne^2\tau}{M} \qquad \text{I.12}$$

where n is the density of carriers,

c is the velocity of light,

ω_c is the cyclotron frequency defined by $\omega_c = eB/Mc$,

and B is the magnetic field strength.

Substituting for σ_{xx} and σ_{xy} in the expression for R_H and we thus finally have

$$R_H = -1/nec \qquad \text{I.13}$$

which is a measure of the density and type of carriers.

The dimensionless quantity $\omega\tau$ is a measure of the strength of the magnetic field. Thus a weak magnetic field slightly deforms the electronic orbit, but when $\omega\tau$ is comparable or larger than unity, then the effect of the field on the electronic orbits needs to be treated at least quasi classically.

In the limit of high magnetic field, the classical theory gives

$$\sigma_{xx} \to \frac{nmc^2}{\tau B^2} \qquad \text{I.14}$$

and

$$\lim_{B \to \infty} \sigma_{xy} \to \frac{-nec}{B} \qquad \text{I.15}$$

Eq. I.15 is more general than Eq. I.13 which also requires that $|\sigma_{xy}/\sigma_{xx}| << 1$. This result is in good agreement with the semiclassical treatment of the problem (Lishitz 1957, 1958). In the case of a two carrier system where there are positively and negatively charged carriers, the expression for the Hall conductivity at large field becomes,

$$\sigma_{xy} \to \frac{ec}{B}(p-n), \quad B \to \infty \qquad \text{I.16}$$

where p is the number of positively charged carriers (holes) per unit volume, and n is again the number of negatively charged carriers (electrons) per unit volume. In the semiclassical theory, this result is good for any energy band structure and any scattering mechanism (if there are no open orbits) (Swanson 1955). This rule has been used to determine the difference of carrier densities (p-n) from the experimentally measured σ_{xy} (McClure 1958, Dillon 1978).

For the constant effective mass case, the semiclassical result Eq. I.15 is valid quantum mechanically in the absence of scatterers, and also in the case of phonon scattering (Argyres 1959). The effect of impurity scattering on the Hall conductivity was conjectured by Kubo et al (1965) and by Abrikosov (1969) to be just the addition of higher order terms in inverse magnetic field and consequently, is of little significance in the high field limit. But Nozieres and collaborators

(Bastin 1971) showed, on the contrary, that there is actually a non-trivial change in the Hall conductivity which is proportional to the real part of the t-matrix. Due to the singular behavior of the t-matrix, its real part cannot be considered just as a renormalization of the chemical potential, which violates the assumption of Abrikosov (1969).

In the present work, it is shown that the calculation by Nozieres has some logical inconsistencies emanating from the Dirac delta function potential model used. Starting with a fairly realistic potential model (such as the Thomas-Fermi potential) and making series of systematic approximations, we produced a more accurate potential model having a separable form, for which there is a simple exact t-matrix (Lifshitz 1964). Using this t-matrix expression, we calculated the transverse components of the magnetoconductivity tensor. In this calculation, we made the following assumptions:

a) that the magnetic field is extremely strong, i.e. $\hbar\omega_c \tilde{>} \epsilon_F$ for a degenerate electron gas, ϵ_F is the Fermi energy

b) that the impurity system is dilute, i.e. $n_I << 1/\lambda_B^2\lambda_z$ where n_I is the number of impurities per unit volume, λ_B is the deBroglie wave length in the plane perpendicular to the magnetic field and given for each Landau quantum number, n as $\lambda_B = \ell/\sqrt{2n+1}$, ℓ is the radius of the Landau ground state orbit and is given by $\ell = \sqrt{\hbar c/eB}$. λ_z is the deBroglie wave length in the direction of the magnetic field. This assumption implies that the diameter of a wave packet is much smaller

than the mean distance between the impurities. Hence, one can consider each collision separately.

c) and finally, that the scattering potential is short ranged, i.e. $a \ll \ell$ and $a \ll \lambda_z$ where a is the range of the potential and ℓ is again the radius of the Landau ground state orbit.

Short-ranged potential models have been considered by previous workers, their results are however, inconsistent. The inconsistency of their results arises from the zero range of the Dirac delta function potential they used. The case of high impurity concentration considered by Fukuyama and collaborators (Shiba 1971) and by Hasegawa (1969) has this problem, just as the case of the low impurity concentration considered by Nozieres and collaborators (Bastin 1971). Using the Dirac delta function potential model, one runs into some unphysical divergencies arising from the constant coupling between all Landau levels, even when the magnetic field is extremely strong (Barnes 1967). This results in the divergence of a sum over the Landau levels in the denominator of the scattering matrix, thus making the latter identically zero. This implies that, the presence of impurities in the system does not affect conduction, which is not physically correct. There were attempts by previous workers to redeem the model by introducing a cut-off Landau number (Skobov 1960), but in an arbitrary and inconsistent fashion.

A physically reasonable cut-off which removes the unphysical aspect of the delta function model in a consistent manner was suggested by McClure and Doar (1972) as the index of the Landau level for which the deBroglie wavelength λ_B is just equal to the range of the potential.

Thus, we have the cut-off delta potential model which will be discussed in greater detail in Chapter IV. In the general case of a short-ranged potential, we established that, for the potential model to have a simple form with a finite scattering matrix, it has to be non-local. The non-locality of the potential alters the velocity operator which in turn changes the transport coefficients of the system. We reproduced the result of Nozieres (Bastin 1971) for σ_{xy} and also obtained a new importnat contribution to the Hall conductivity, which is dominant in the case of strong scattering. We also obtained a general expression for the diagonal element of the transverse magnetoconductivity tensor, σ_{xx}. Finally, we note that using the single-site t-matrix obtained in this work, one can improve the results obtained by Fukuyama and collaborators (Shiba 1971) without the need for any "automatic inclusion of collision broadening effects", to get rid of the unphysical divergencies.

CHAPTER II

REDUCTION OF THE KUBO LINEAR RESPONSE FORMULA

In the regime of strong magnetic field, which is the case of interest in the present work, quantum effects are dominant. Therefore, only quantum theory can best explain the properties of such a system. This was clearly pointed out by Kubo et al. (Kubo 1965) that for extremely strong magnetic fields, the Boltzman equation becomes inadequate for the calculation of the transport coefficients of the system. Hence, we make Kubo's formula our starting point in the present work. According to this formula, the electric conductivity tensor of a system of electrons perturbed by a weak electrical field is given by

$$\sigma_{\mu\nu}(\omega) = V^{-1} \int_0^\infty dt\, e^{i\omega t} \int_0^\beta d\lambda \, \langle \hat{j}_\nu(-i\hbar\lambda)\hat{j}_\mu(t)\rangle, \qquad \text{II.1}$$

where

$$J_\mu(\omega) = \sigma_{\mu\nu}(\omega)E_\nu \ , \qquad \text{II.2}$$

In the above ω is the frequency of the applied electric field,

$$\beta = \frac{1}{kT} \ ,$$

$$J_\mu = \int_V \hat{\psi}^+(r) j_\mu \hat{\psi}(\vec{r}\,)d\vec{r} \ , \qquad \text{II.3}$$

is the current along the μ-direction in the volume V, and

$j_\mu = -ev_\mu$ is the one-electron current operator. In general $\psi(\vec{r}\,)$ is the second quantized, one-particle creation operator, but in the case of the independent electron approximation, this is just

the electron wave function normalized in the volume V. The hat "^" is a symbol for operator.

The equilibrium average is defined as

$$\langle\hat{A}\rangle = \mathrm{Tr}\{\hat{\rho}\hat{A}\}, \qquad \text{II.4}$$

In the grand canonical ensemble the density operator, $\hat{\rho}$ is given by

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}-\mu\hat{N})}, \qquad \text{II.5}$$

with μ the chemical potential and $\hat{N}$ the particle number operator. The chemical potential μ is determined from the fact that the expectation value of $\hat{N}$ remains fixed.

Finally,

$$Z = \mathrm{Tr}(\hat{\rho}) = \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} \qquad \text{II.6}$$

is the normalization constant and

$$\hat{j}(t) = e^{(i/\hbar)\hat{H}t}\hat{j}(0)e^{-(i/\hbar)\hat{H}t}, \qquad \text{II.7}$$

where $\hat{H}$ is the Hamiltonian of the system. Eq. II.1 for $\sigma_{\mu\nu}$ can thus be rewritten as

$$\sigma_{\mu\nu}(\omega) = V^{-1}\int_0^\infty dt\, e^{i\omega t}\int_0^\beta d\lambda\langle j_\nu(-i\hbar\lambda)j_\mu(t)\rangle$$

$$= V^{-1}\int_{-\infty}^{\infty} dt\ \theta(t)e^{i\omega t}\int_0^\beta d\lambda\langle j_\nu(0)j_\mu(t + i\hbar\lambda)\rangle. \qquad \text{II.8}$$

where $\theta(t)$ is the Heaviside step function defined by

$$\theta(t) = \begin{cases} 1 & , \quad t > 0 \\ 0 & , \quad t < 0 \end{cases} = \frac{i}{2\pi}\int_{-\infty}^{\infty} dz\, \frac{e^{-izt}}{z+i\delta} \quad \text{and } \delta \to +0.$$

Hence, we have

$$\sigma_{\mu\nu} = \frac{i}{2\pi V}\int_{-\infty}^{\infty} dt\int_{-\infty}^{\infty} dz\ \frac{e^{-izt}}{z+i\delta}\ e^{i\omega t}\int_0^\beta d\lambda\langle j_\nu(0)j_\mu(t + i\hbar\lambda)\rangle.$$

According to the independent electron formalism

$$\langle j_\nu(0) j_\mu(t + i\hbar\lambda)\rangle = \frac{1}{Z}\,\mathrm{Tr}\{e^{-\beta(\hat{H}-\mu)} j_\nu(0)\; e^{(i/\hbar)\hat{H}(t+i\hbar\lambda)} \times\; j(0) e^{-(i/\hbar)\hat{H}(t+i\hbar\lambda)}\}$$

$$= \sum_{nm} \rho_n j^{\nu}_{nm} j^{\mu}_{mn} e^{(i/\hbar)(t+i\hbar\lambda)(E_m-E_n)}, \qquad \text{II.9}$$

where

$$\hat{H}|n\rangle = E_n|n\rangle,$$

$$\rho_n = \rho_{nn} \equiv \langle n|\hat{\rho}|n\rangle,$$

and $|n\rangle$ is a 1-particle state.

Hence we can write

$$\sigma_{\mu\nu}(\omega) = \frac{i}{2\pi V} \sum_{n,m} \rho_n\, j^{\nu}_{nm} j^{\mu}_{mn} \int_{-\infty}^{\infty} \frac{dz}{z+i\delta} \int_{-\infty}^{\infty} dt\; e^{it[\omega - z + \frac{E_m - E_n}{\hbar}]} \times \int_0^{\beta} d\lambda e^{-\lambda(E_m-E_n)} \qquad \text{II.10}$$

or

$$\sigma_{\mu\nu}(\omega) = \frac{i}{2\pi V} \sum_{n,m} \rho_n j^{\nu}_{nm} j^{\mu}_{mn} \int_{\infty}^{\infty} \frac{dz}{z+i\delta} \left[2\pi S[\omega - z + \frac{E_m-E_n}{\hbar}]\right]\left[\frac{1-e^{-\beta(E_m-E_n)}}{E_m-E_n}\right]$$

$$= \frac{i\hbar}{V} \sum_{n,m} \rho_n j^{\nu}_{nm} j^{\mu}_{mn} \frac{[1-e^{-\beta(E_m-E_n)}]}{[E_m-E_n+h(\omega+i\delta)][E_m-E_n]}\,. \qquad \text{II.11}$$

But

$$\rho_n[1-e^{-\beta(E_m-E_n)}] = \rho_n - \rho_m\,.$$

Hence II.12

$$\sigma_{\mu\nu}(\omega) = \frac{i\hbar}{V} \sum_{n,m} \frac{(\rho_n-\rho_m) j^{\nu}_{nm} j^{\mu}_{mn}}{[E_m-E_n+\hbar(\omega+i\delta)][E_m-E_n]} = \frac{i}{V(\omega+i\delta)} \{F_{\mu\nu}(\omega)-F_{\mu\nu}(0)\}$$

$$= \frac{-i}{V(\omega+i\delta)} \sum_{n,m} (\rho_n-\rho_m) j^{\nu}_{nm} j^{\mu}_{mn} \{\frac{1}{E_m-E_m+\hbar(\omega+i\delta)} - \frac{1}{E_m-E_n}\} ,$$

where we have defined

$$F_{\mu\nu}(\omega) = \frac{1}{V} \sum_{n,m} \frac{(\rho_n-\rho_m) j^{\nu}_{nm} j^{\mu}_{mn}}{E_n-E_m-\hbar(\omega+i\delta)} . \qquad \text{II.13}$$

Using the identity

$$\delta(Z) = \frac{1}{2\pi i} [G^A(Z) - G^R(Z)] = -\frac{1}{\pi} \text{Im } G(Z) ,$$

we can further simplify $F_{\mu\nu}(\omega)$. Here $G^R(E)$ is the retarded or causal Green's function, analytic in the upper half plane while $G^A(E)$ is the advanced or anticausal Green's function, analytic in the lower half plane, and are given by

$$G^{R,A}_{nn'}(E) = \langle n|(E-\hat{H}\pm i\delta)^{-1}|n'\rangle . \qquad \text{II.14}$$

The Green's function method is discussed in standard references (Abrikosov 1963). Im G(E) is the discontinuity of the two functions along the Im E=0 axis. On the other hand,

$$\rho_n = \rho(E_n) = \int_{-\infty}^{\infty} dE \rho(E) \delta(E-E_n) = \int_{-\infty}^{\infty} dE f(E) \delta(E-E_n)$$

where f(E) is the Fermi distribution function.

Thus

$$F_{\mu\nu}(\omega) = \frac{1}{2\pi iV} \int_{-\infty}^{\infty} dE\ f(E) \sum_{n,m} \{[G_n^A(E)-G_n^R(E)]G_m^A(E-\hbar\omega) +$$

$$+ [G_m^A(E)-G_m^R(E)]G_n^R(E+\hbar\omega)\} j^{\nu}_{nm} j^{\mu}_{mn}$$

$$= \frac{1}{2\pi iV} \int_{-\infty}^{\infty} dE\ f(E)\ \mathrm{Tr}\{j^{\nu}G^A(E)j^{\mu}G^R(E+\hbar\omega) - j^{\nu}G^A(E-\hbar\omega)j^{\mu}G^R(E) +$$

$$+ j^{\nu}G^A(E-\hbar\omega)j^{\mu}G^A(E) - j^{\nu}G^R(E)j^{\mu}G^R(E+\hbar\omega)\} . \qquad \text{II.15}$$

In the present work, we are interested in the static conductivity; hence one can expand $F_{\mu\nu}(\omega)$ in powers of ω.

i.e.

$$F_{\mu\nu}(\omega) = F_{\mu\nu}(0) + \frac{\omega \partial F_{\mu\nu}(\omega)}{\partial\omega}\bigg|_{\omega\nu} + \ldots , \qquad \text{II.16}$$

with

$$\frac{\partial F_{\mu\nu}(\omega)}{\partial\omega}\bigg|_{\omega\to 0} = \frac{\hbar}{2\pi iV} \int_{-\infty}^{\infty} dE\ f(E)\ \mathrm{Tr}\{j^{\nu}G^A(E)\ \frac{j^{\mu}dG^R(E)}{dE} +$$

$$+ \frac{j^{\nu}dG^A(E)}{dE}\ j^{\mu}G^R(E) - \frac{j^{\nu}dG^A(E)}{dE}\ j^{\mu}G^A(E) -$$

$$- j^{\nu}G^R(E)\ \frac{j^{\mu}dG^R(E)}{dE}\ \}, \qquad \text{II.17}$$

or

$$\frac{\partial F_{\mu\nu}(\omega)}{\partial\omega}\Big|_{\omega\to 0} = \frac{-\hbar}{\pi V}\int_{-\infty}^{\infty} dE\ f(E)\ \mathrm{Tr}\{j^{\nu}\mathrm{Im}G(E)j^{\mu}\frac{dG^{R}(E)}{dE} -$$

$$- j^{\nu}\frac{dG^{A}(t)}{dE}\ j^{\mu}\mathrm{Im}G(E)\}\ , \qquad \text{II.17a}$$

so that

$$\sigma_{\mu\nu}(0) = \lim_{\substack{\omega\to 0\\ \delta\to 0}} \frac{i}{\omega+i\delta}\ \{F_{\mu\nu}(\omega)-F_{\mu\nu}(0)\} = \frac{i\omega}{\omega+i\delta}\ \frac{\partial F_{\mu\nu}(0)}{\partial\omega}\ ,$$

and finally

$$\sigma_{\mu\nu}(0) = \frac{i\hbar}{\pi V}\int_{-\infty}^{\infty} dE\ f(E)\ \mathrm{Tr}\{j_{\mu}\mathrm{Im}G(E)j_{\nu}\frac{dG^{A}(E)}{dE} - j_{\mu}\frac{dG^{R}(E)}{dE}\ j_{\nu}\mathrm{Im}G(E)\}. \qquad \text{II.18}$$

A similar expression was obtained by Nozieres and co-workers (Bastin 1971) in a different fashion except for a sign error. This result simplifies in the case of the diagonal elements:

$$\sigma_{\mu\mu}(0) = \frac{i\hbar}{V}\int_{-\infty}^{\infty} dE\ f(E)\mathrm{Tr}\{j_{\mu}\mathrm{Im}G(E)j_{\mu}\frac{dG^{A}(E)}{dE} - j_{\mu}\frac{dG^{R}(E)}{dE}\ j_{\mu}\ \mathrm{Im}G(E)\}$$

$$= \frac{2\hbar}{\pi V}\int_{-\infty}^{\infty} dE\ f(E)\mathrm{Tr}\{j_{\mu}\mathrm{Im}G(E)j_{\mu}\frac{d}{dE}\ \mathrm{Im}G(E)\}$$

$$= -\frac{\hbar}{\pi V}\int_{-\infty}^{\infty} dE\ \frac{\partial f}{\partial E}\ \mathrm{Tr}\ \{j_{\mu}\mathrm{Im}G(E)j_{\mu}\mathrm{Im}G(E)\}\ , \qquad \text{II.19}$$

or at T = 0

$$-\frac{\partial f}{\partial E} = \delta(E-\varepsilon_{F}),$$

$$\sigma_{\mu\mu}(0) = \frac{\hbar}{\pi V}\ \mathrm{Tr}\ \{j_{\mu}\mathrm{Im}G(\varepsilon_{F})j_{\mu}\mathrm{Im}G(\varepsilon_{F})\}\ . \qquad \text{II.20}$$

CHAPTER III

REDUCTION OF THE SCHROEDINGER EQUATION

As a model for this problem, we consider a system of a non interacting electron gas with randomly distributed impurities, in an external uniform magnetic field. The impurity concentration is sufficiently low that each collision can be treated separately. Furthermore, each impurity potential has rotational symmetry about the direction of the magnetic field, which is chosen as the z-axis. It is also assumed that the potential is short-ranged and that the electronic mass is isotropic. Such a system can be described by a Hamiltonian

$$H = H_o + V(r), \qquad \text{III.1}$$

where

$$H_o = \frac{1}{2M}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 \qquad \text{III.2}$$

is the unperturbed Hamiltonian for an electron in a magnetic field,

-e is the electronic charge, i.e. e > 0

$$\vec{A} = \left(-\frac{By}{2}, \frac{Bx}{2}, 0\right) \qquad \text{III.3}$$

is the vector potential chosen in the symmetric gauge, and

$$V(r) = \sum_{j=1}^{N_j} v(\vec{r} - \vec{R}_j) \qquad \text{III.4}$$

is the scattering potential due to the various impurity centers. The solution of the unperturbed Schroedinger equation

$$H_o \psi_{nkm}(\vec{r}) = \varepsilon_n(k)\psi_{nmk}(\vec{r}) \qquad \text{III.5}$$

leads to the quantization of the motion in the xy plane.

The Landau energy levels are

$$\varepsilon_n(k) = \hbar\omega(n + \tfrac{1}{2}) + \frac{\hbar^2 k^2}{2M} , \qquad \text{III.6}$$

where

n is the principal quantum number,

m is the magnetic quantum number,

and k is the z-component of the linear momentum. The functions

$$\psi_{nmk}(\vec{r}) = \chi_{nm}(\rho) \frac{e^{im\phi}}{\sqrt{2\pi}} \frac{e^{ikz}}{\sqrt{2\pi}} \equiv \phi_{nm}(\rho,\phi) \frac{e^{ikz}}{\sqrt{2\pi}} \qquad \text{III.7}$$

are the eigenfunctions of the unperturbed Hamiltonian H_o in cylindrical coordinates (ρ,ϕ,z). The function (Dingle 1952)

$$\chi_{n,m}(\rho) = \left(\frac{\alpha N!}{(N+|m|)!}\right)^{\frac{1}{2}} e^{-\alpha\rho^2/4} \left(\frac{\alpha\rho^2}{2}\right)^{\frac{|m|}{2}} L_N^{|m|}\left(\frac{\alpha\rho^2}{2}\right) \qquad \text{III.8}$$

is the radial part of the eigenfunction expressed in terms of the normalized Laguerre function, and

$$N = n - \frac{(m+|m|)}{2} , \quad -\infty < m \leq n, \qquad \text{III.9}$$

$$\alpha = \frac{eB}{\hbar c} = \frac{1}{\ell^2} . \qquad \text{III.10}$$

Here ℓ is the classical radius of the ground state Landau orbit and its given from (III.10) by

$$\ell = \sqrt{\hbar c/eB} .$$

The radial wave functions, $\chi_{nm}(\rho)$ are orthonormal,

$$\int_0^\infty \rho d\rho \; \chi_{nm}(\rho) \, \chi_{n'm}(\rho) = \delta_{n'n} . \qquad \text{III.11}$$

In the dilute impurity limit, it is sufficient to consider first the effect of one impurity located at the origin. Thus

$$H_1 = H_o + v(\vec{r}) \qquad \text{III.12}$$

where $v(\vec{r})$ is the potential due to one impurity located at the origin and has a rotational symmetry about the z-axis, so that the magnetic quantum number m is still conserved. This Hamiltonian, H_1, is however, not diagonal in the Hilbert space spanned by the eigenstates of H_o. Hence any wave function ψ, of the system can be expressed as a linear combination of the $\phi_{nm}(\rho,\phi)$,

$$\psi(\rho,\phi,z) = \sum_n \phi_{nm}(\rho,\phi)\, f_n^m(z) \qquad \text{III.13}$$

after Yafet, Keyes, and Adams (Yafet 1956). Substituting Eq. III.13 into the Schroedinger equation for one impurity

$$H_1\psi = E\psi \qquad \text{III.14}$$

and using the fact that $\phi_{nm}(\rho,\phi)$ form an orthonormal set, Eq. III.14 can be reduced to a one dimensional Schroedinger equation:

$$-\frac{\hbar^2}{2M}\frac{d^2 f_n^m(z)}{dz^2} + \sum_{n'=0}^{\infty} v_{nn'}^m(z)\, f_{n'}^m(z) = \epsilon_n f_n^m(z) \qquad \text{III.15}$$

where

$$v_{nn'}^m(z) = \int_o^\infty \rho d\rho\, \chi_{nm}^*(\rho)\, \chi_{n'm}(\rho)\, v(\rho,|z|) \qquad \text{III.16}$$

and

$$\epsilon_n = E - \hbar\omega_c(n + \tfrac{1}{2}) \ . \qquad \text{III.17}$$

Eq. III.15 is an infinite set of coupled linear, second order differential equations, for each value of the azimuthal quantum number, m. Analytical solution of this equation is generally difficult to obtain in a non-perturbative manner, and so will not be considered in the present work.

Barnes (Barnes 1967) solved Eq. III.15 numerically for certain cases in terms of the phase shift and for general potential strength values. In the present case, however, we assume that the scattering potential is also short ranged in the z-direction, so that the calculations can be done more easily in the wave number (k) space. We are also interested in the scattering potentials of arbitrary strength, hence we need to go beyond the Born approximation and we therefore invoke a full scattering theory for the calculation of the magneto-conductivity tensor, using the eigenstates of the unperturbed Hamiltonian H_o, as the basis set.

CHAPTER IV

MATRIX ELEMENTS FOR THE VARIOUS IMPURITY POTENTIAL MODELS

The various physical quantities of interest are all expressed in terms of the single site t-matrix which in turn is related to the single site scattering potential by the Lippmann-Schwinger equation. Hence, we need to consider some concrete potential models in order to carry out a numerical evaluation of these physical quantities. The fact that the range of the potential is very short but finite suggests the existence of some cut-off parameter in the theory.

The matrix elements for the potential models are evaluated using the basis set $\psi_{nmk}(\vec{r})$ given by Eqs. III.7-III.10

$$\psi_{nmk}(\vec{r}) = \phi_{nm}(\rho,\phi)\,\frac{e^{ikz}}{\sqrt{2\pi}}\quad , \tag{III.7}$$

and

$$\phi_{nm}(\rho,\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}\left(\frac{\alpha N!}{(N+|m|)!}\right)^{\frac{1}{2}} e^{-\frac{\alpha\rho^2}{4}}\left(\frac{\alpha\rho^2}{2}\right)^{\frac{|m|}{2}} L_N^{|m|}\left(\frac{\alpha\rho^2}{2}\right) \tag{III.8}$$

where again

$$N = n - \frac{(m+|m|)}{2}\quad , \quad -\infty<m\leq n \tag{III.9}$$

and

$$\alpha = \frac{eB}{\hbar c} = \frac{1}{\ell^2}\quad . \tag{III.10}$$

A. The Cut-Off Delta Function Model Potential.

This constitutes the most mathematically simple of all the models and has therefore been considered by many authors
However, a self consistent approach to this model was considered only by Doar (Doar 1972), and we shall briefly discuss his argument here. The impurity potential is represented by a Dirac delta function located at the origin

$$V_1(\vec{r}\,) = V_1\delta(\vec{r}) = \frac{2\pi\hbar^2}{M} f_1\ \delta(\vec{r}) \qquad \text{IV.1}$$

where f_1 is the scattering amplitude for a zero energy electron due to this potential in the absence of the magnetic field. In this case only the m = 0 states will contribute since they are the only ones that do not vanish at the origin, hence

$$V^{(m)}_{nk,n'k'} = \frac{\alpha}{2\pi} V_1 \delta_{m,0} \qquad \text{IV.2}$$

which is independent of the indices. This leads to some divergent results, which, as pointed out by Bychkov (Bychkov 1961), are due to the zero range of the potential as for any finite range potential the Born series would converge. An attempt to save the situation was suggested by McClure and Doar (Doar 1972). This prescription assumes that the potential has a finite but short range such that if the de Broglie wavelength is greater than the range of the potential, then the delta function potential is valid. Conversely, when the de Broglie wavelength is less than the potential range, the impurity potential varies slowly compared to the electron wave function and is neglected.

Hence the value of λ_{N_T} equal to the range (a) constitutes the limit for which the approximation is valid, i.e.

$$a = \frac{\ell}{\sqrt{2N_T+1}} , \qquad \text{IV.3}$$

or

$$N_T \cong \tfrac{1}{2}\left(\frac{\ell}{a}\right)^2 , \qquad \text{IV.4}$$

so that

$$V_{nn'}^{(m)} = \begin{cases} \frac{\alpha}{2\pi} V_1 \delta_{m,0} , & n,n' \leq N_T \\ 0 , & \text{otherwise} \end{cases} . \qquad \text{IV.5}$$

This distinguishes our result for the t-matrix from that obtained by Bastin (Bastin 1971) in which the model was not used consistently, as will be shown in greater detail in the next chapter.

B. More General Potential Models.

For the other potential models that will be considered in the present work, it is convenient and more efficient to introduce a general technique for the evaluation of the matrix elements. This is very similar to the method used by Barnes (Barnes 1967) except for some error in his Eq. VI.11 arising from an eroneous expression in the integral table used (Gradshteyn 1965).

In this regard, the matrix elements for any arbitrary potential model is given by

$$V_{nk,n'k'}^{m} = \int d\vec{r} \quad V(\rho,z)\psi_{nmk}^{*}(\vec{r}\,)\,\psi_{n'mk'}(\vec{r}\,) . \qquad \text{IV.6}$$

Expressing $V(\rho,z)$ in terms of its Fourier components, we have

$$V(\rho,z) = \frac{1}{(2\pi)^3}\int d\vec{q}\ e^{i\vec{q}\,\vec{r}}\ V(\vec{q}\,) \quad . \qquad \text{IV.7}$$

So that

$$V^m_{nk;n'k'} = \frac{1}{(2\pi)^3}\int d\vec{r}\ \psi^*_{nmk}(\vec{r}\,)\psi_{n'mk'}(\vec{r}\,)\int d\vec{q}\ e^{i\vec{q}\,\vec{r}}\ V(\vec{q}\,)$$

$$= \frac{1}{(2\pi)^3}\int d\vec{q}\ V(\vec{q}\,)Q^m_{nn'}(\vec{q}_i,k,k'), \qquad \text{IV.8}$$

where $Q^m_{nn'}(\vec{q}\,,k,k')$ is independent of the potential model and thus need be evaluated only once. It is given by

$$Q^m_{nn'}(\vec{q}\,;k,k') = \int_0^\infty \rho d\rho\ \chi_{nm}(\rho)\chi_{n'm}(\rho)\int_0^{2\pi}\frac{d\phi}{2\pi}\int_{-\infty}^{\infty}\frac{dz}{2\pi}$$

$$\times\ e^{i(q_\perp\rho\cos\theta+q_z z)}e^{i(k'-k)z} \quad . \qquad \text{IV.9}$$

Integrating over z gives a Dirac delta function, and

$$\vec{q} \equiv (q_\perp,\theta,q_z)$$

so that

$$V^m_{nk,n'k'} = \frac{1}{(2\pi)^3}\int_{-\pi}^{\pi}d\theta\int_{-\infty}^{\infty}dq_z\int_0^\infty q_\perp dq_\perp V(\vec{q}\,)\delta(q_z+k'-k)$$

$$\times\int \rho d\rho e^{iq_\perp\rho\cos\theta}\chi_{nm}(\rho)\ \chi_{n'm}(\rho). \qquad \text{IV.10}$$

From the tables of integral (Erdelyi 1954), we have

$$\int_0^\pi e^{iq_\perp\rho\cos\theta}d\theta = \pi J_0(q_\perp\rho) \qquad \text{IV.11}$$

where $J_o(x)$ is the zero-order Bessel function of the first kind.

Hence we obtain

$$V^m_{nk,n'k'} = \frac{1}{(2\pi)^2} \int_o^\infty q_\perp dq_\perp v(q_\perp, k-k') \quad I^m_{nn'}(q_\perp) \qquad \text{IV.12}$$

where

$$I^m_{nn'}(q_\perp) = \int_o^\infty \rho d\rho \; \chi_{nm}(\rho)\chi_{n'm}(\rho) \; J_o \; (q_\perp \rho)$$

$$= K_{NN'} \int_o^\infty \alpha\rho d\rho \; e^{-(\alpha\rho^2/2)} \quad (\frac{\alpha\rho^2}{2})^{|m|} L_N^{|m|} (\frac{\alpha\rho^2}{2})$$

$$\times L_{N'}^{|m|} (\frac{\alpha\rho^2}{2}) \; J_o \; (q_\perp \rho) \qquad \text{IV.13}$$

with

$$K_{NN'} = \left[\frac{N!N'!}{(N+|m|)!(N'+|m|)!}\right]^{\frac{1}{2}} . \qquad \text{IV.14}$$

Changing the variable of integration to

$$x = \rho \sqrt{\alpha/2}$$

and making the substitution $y = (q_\perp^2)/(2\alpha)$,

Eq. IV.33 can be rewritten as

$$I^m_{nn'}(q_\perp) = 2K_{NN'} \int_o^\infty e^{-x^2} x^{2|m|+1} \; L_N^{|m|}(x^2) L_{N'}^{|m|}(x^2) \; J_o(2x\sqrt{y}\,)dx . \qquad \text{IV.15}$$

To evaluate this integral, first consider the expansion

$$t^m L_N^m(t) L_{N'}^m(t) = \sum_{k=m}^{N+N'} D_k^{NN'}(m) \; L_k(t) \qquad \text{IV.16}$$

in terms of the m=0 Laguerre polynomials. Substituting the expansion into Eq. IV.15 we obtain

$$I^{m}_{nn'}(y) = 2K_{NN'} \sum_{k=m}^{N+N'} D_k^{NN'}(m) \int_0^\infty e^{-x^2} x\, L_k(x^2) J_o(2x\sqrt{y})dx. \quad \text{IV.17}$$

Using a tabulated integral expression (Gradshteyn 1965) we have

$$\int_0^\infty dx\, e^{-x^2} x\, L_k(x)\, J_o(2x\sqrt{y}) = \frac{e^{-y}}{2} \frac{y^k}{k!} \quad . \quad \text{IV.18}$$

So that the problem of evaluating $I^{m}_{nn'}$, is reduced to determining the coefficients

$D_k^{NN'}(m)$, which are given by

$$D_k^{NN'}(m) = \int_0^\infty dt\, e^{-t} t^m L^m_{N'}(t)\, L^m_N(t) L_k(t) \quad . \quad \text{IV.19}$$

In the above expression, we have used the notation

$$L_k(t) = L^o_k(t) \quad .$$

Any product of two Laguerre polynomials can be expressed as a linear combination of Laguerre polynomials:

$$L^m_N(t) L^m_N(t) = \sum_{\ell=0}^{N+N'} C_\ell^{NN'}(m) L^m_\ell(t) \quad \text{IV.20}$$

where the coefficients $C_k^{NN'}(m)$ are totally symmetric with regards to k,N and N' and are given (Powell) by:

$$C_k^{NN'}(m) = \sum_s \frac{(-2)^{2s-p}(m+p-s)!}{(N+N'-s)!(N'+k-s)!(k+N-s)!(2s-p)!} \quad . \quad \text{IV.21}$$

The indices k,N and N' form a triangle with the perimeter

$$p = k+N+N'$$

and the summation in Eq. IV.21 goes from

$$p/2 \leq s \leq \min \left\{ \begin{matrix} k+N \\ N+N' \\ N'+k \end{matrix} \right\} .$$

It is instructive to note that

$$\left. \begin{aligned} C_0^{NN'}(m) &= \delta_{NN'} \\ C_k^{ON'}(m) &= \delta_{kN'} \\ C_k^{NO}(m) &= \delta_{kN} \end{aligned} \right\} \qquad \text{IV.22}$$

and also that for m=0

$$D_k^{NN'}(0) = C_k^{NN'}(0) . \qquad \text{IV.23}$$

To treat the case that m is not zero, it is useful to note that

$$L_k^o(t) = \sum_{r=0}^{m} \frac{m!}{r!(m-r)!} L_{k-r}^m(t) . \qquad \text{IV.24}$$

So that, on substituting Eq. IV.20 and Eq. IV.24 into Eq. IV.19, we have

$$D_k^{NN'}(m) = \int_o^\infty dt\, e^{-t} t^m \sum_{\ell=0}^{N+N'} C_\ell^{NN'}(m) \sum_{r=0}^{m} \frac{m!}{r!(m-r)!} L_\ell^m(t) L_{k-r}^m(t), \qquad \text{IV.25}$$

and from the orthogonality of the Laguerre polynomials, we finally obtain

$$D_k^{NN'}(m) = m! \sum_{\ell=0}^{N+N'} \frac{(\ell+m)!}{\ell!(k-\ell)!(m+\ell-k)!} C_\ell^{NN'}(m) \quad . \qquad \text{IV.26}$$

These summations were carried out numerically and used for different potential models. Numerical values for the coefficients $D_k^{NN'}(m)$ are given in Table 1 for values of m = 0 and m = 1.

Thus, we have after a simple arithmetic

$$I^m_{nn'}(y) = K_{NN'} \sum_{k=m}^{N+N'} D_k^{NN'}(m)\, e^{-y} \frac{y^k}{k!} \quad . \qquad \text{IV.27}$$

For the potential matrix elements we have

IV.28

$$V^m_{nk,n'k'} \equiv V^m_{nn'}(q_z) = \frac{K_{NN'}}{(2\pi)^2} \sum_{r=m}^{N+N'} D_r^{NN'}(m)\, 2\alpha \int_0^\infty dy\, \frac{e^{-y} y^r}{r!}\, v(\sqrt{2\alpha y}\,, q_z)$$

TABLE 1. Values of $D_K^{NN'}$ (m).

D(0)	N	N'	K	D(1)
1.0	0	0	0	1.0
0.0	1	0	0	0.0
1.0	1	1	0	1.0
-2.0	1	1	1	-3.0
2.0	1	1	2	5.0
0.0	2	0	0	0.0
0.0	2	0	1	0.0
1.0	2	0	2	1.7321
0.0	2	1	0	0.0
2.0	2	1	1	2.4495
-4.0	2	1	2	-7.3485
3.0	2	1	3	9.7980
1.0	2	2	0	1.0
-4.0	2	2	1	-5.0
10.0	2	2	2	16.0
-12.0	2	2	3	-28.0
6.0	2	2	4	26.0
0.0	3	0	0	0.0
0.0	3	0	1	0.0
0.0	3	0	2	0.0
1.0	3	0	3	2.0
0.0	3	1	0	0.0
0.0	3	1	1	0.0
3.0	3	1	2	4.2426
-6.0	3	1	3	-12.7279
4.0	3	1	4	15.0
0.0	3	2	0	0.0
3.0	3	2	1	3.4641
-12.0	3	2	2	-17.3205
24.0	3	2	3	45.0333
-24.0	3	2	4	-65.8179
10.0	3	2	5	51.9615
1.0	3	3	0	1.0
-6.0	3	3	1	-7.0
24.0	3	3	2	33.0
-56.0	3	3	3	-95.0
78.0	3	3	4	173.0
-60.0	3	3	5	-195.0
20.0	3	3	6	125.0

where $v(q_\perp, q_z)$ is the Fourier transform of $V(\rho,z)$

and $q_z = k-k'$.

Since $D_r^{NO}(0) = \delta_{rN}$, it is obvious that

$$V_{no}^{0}(q_z) = \frac{1}{(2\pi)^2} \; 2\alpha \int_0^\infty dy \; e^{-y} \frac{y^n}{n!} \; v(\sqrt{2\alpha y}, \; q_z), \qquad \text{IV.29}$$

so that a general matrix element is just a linear combination of the V_{ro}^{0} matrix elements which are much easier to calculate. Thus we have

$$V_{nn'}^{m}(q_z) = K_{NN'} \sum_{r=m}^{N+N'} D_r^{NN'}(m) \; V_{ro}^{0}(q_z). \qquad \text{IV.30}$$

At this juncture we consider some concrete potential models which are more realistic than the cut-off delta function model. In this regard, the screened Coulomb potential would be a better approximation to a short-ranged impurity potential, and it is given by

$$V(\rho,z) = V_2 \; \frac{e^{-(1/a)\sqrt{\rho^2+z^2}}}{\sqrt{\rho^2+z^2}} \qquad \text{IV.31}$$

where a is the range of potential. This expression is obtained from the linearized Thomas-Fermi theory in which case V_2 is given by

$$V_2 = \frac{-e^2}{\epsilon_b} \Delta Z, \qquad \text{IV.32}$$

where ϵ_b is the low frequency dielectric constant and ΔZ is the difference of the valence of the impurity and that of the host. The range a, is given by the Thomas-Fermi screening length (Ziman 1972)

$$a = \left(\frac{\epsilon_b}{4\pi e^2 \rho(\epsilon_F)} \right)^{\frac{1}{2}} \qquad \text{IV.33}$$

where $\rho(\epsilon_F)$ is the electron density of states (McClure 1968) evaluated at the Fermi energy ϵ_F. In the case of a free electron gas with no magnetic field, the density of states can be written as (neglecting spin degeneracy)

$$\rho(E) = \frac{1}{2\pi^2} \left(\frac{2M}{\hbar^2}\right)^{3/2} E^{\frac{1}{2}} \quad . \qquad \text{IV.34}$$

Starting with the above fairly realistic potential model, one can make a series of approximation for the t-matrix calculation, which are much better than any of those used previously. Moreover, the results obtained from this potential model can serve as a benchmark to compare and contrast the reasonableness of the other potential models.

The Fourier transform of the Thomas-Fermi potential model is given by (setting $\Delta Z = 1$ hereafter)

$$v_{TF}(q_\perp, q_z) = \frac{-4\pi e^2}{\epsilon_b (q_\perp^2 + q_z^2 + (1/a^2))} \quad . \qquad \text{IV.35}$$

So that

$$V^{o}_{ro}(q_z) = \frac{2\alpha}{(2\pi)^2} \int_0^\infty dy \, \frac{e^{-y} y^r}{r!} \, \frac{(-4\pi e^2)}{\varepsilon_b (2\alpha y + q_z^2 + (1/a^2))} \quad . \qquad \text{IV.36}$$

Using the fact that $N_T = \frac{1}{2}(\frac{\ell^2}{a^2})$ and denoting by

$$\gamma = \tfrac{1}{2}\ell^2 q_z^2 = \tfrac{1}{2}\ell^2 (k-k')^2$$

we obtain

$$V^{o}_{ro}(\gamma) = \frac{-e^2}{\pi\varepsilon_b} \int_0^\infty dy \, \frac{e^{-y}}{r!} \, \frac{y^r}{y+\gamma+N_T}$$

$$\equiv -\frac{e^2}{\pi\varepsilon_b} \, S^{TF}_r(\gamma, N_T) \quad . \qquad \text{IV.37}$$

So that the effect of k,k' in the matrix elements is only to define a new N_T parameter in the function

$$S^{TF}_r(\gamma, N_T) = \int_0^\infty dy \, \frac{e^{-y}}{y+N_T+\gamma} \, \frac{y^r}{r!} \qquad \text{IV.38}$$

and on using a table of integrals (Gradshteyn 1965) we finally have

$$S^{TF}_r(N_T) = \frac{\ell}{r!} \{(-1)^{r-1} N_T^r e^{N_T} E_i(-N_T) + \sum_{\ell=1}^{r} (\ell-1)!(-N_T)^{r-\ell}\} \qquad \text{IV.39}$$

where Ei(-x) is the exponential integral given by

$$Ei(-N_T) \equiv -\int_{N_T}^\infty \frac{e^{-t}}{t} \, dt \quad . \qquad \text{IV.40}$$

It is useful to note that

$$S_{r+1}(N_T) = [1-N_T S_r(N_T)]/(r+1) \ . \qquad \text{IV.41}$$

The function $S_r^{TF}(N_T)$ is a positive, monotonically decreasing function of r, so that all the $V^o_{no'}(\gamma)$ have the same sign and are monotonically decreasing function of n. It will be shown later, that the matrix elements corresponding to $m\neq 0$ are much smaller than their m=0 counterparts thereby justifying our approximation.

By method of steepest descent the expression for $S_n^{TF}(N_T)$ can be approximated by a polynomial in inverse $(n+N_T+1)$, hence in the first order approximation, we consider

$$S_n^{TF}(N_T) \simeq S_n^1 = \frac{1}{N_T+n+1} \qquad \text{IV.42}$$

which is then later compared with a second order approximation given by

$$S_n^2 = \frac{1}{N_T+n+1}\left[1 + \frac{n+1}{(N_T+n+1)^2}\right] . \qquad \text{IV.43}$$

In a detailed calculation, it was shown that for N_T=5 the maximum error in using S_n^1 is about 4.6% (corresponding to n=5), while the maximum error due to S_n^2 is only about .54% (for n=1). For the sake of comparison, N_T is set equal to 10 and the corresponding errors due to S_n^1 and S_n^2 are just 2.5% (for n=10) and .14% (for n=1) respectively.

Thus, the maximum fractional error for S_n^1 is equal to $1/4N_T$, coming at $n=N_T-1$ whereas the maximum error in S_n^2 is equal to $3/N_T^2$, corresponding to $n \simeq (N_T/2)-1$.

One concludes that S_n^1 is good to 1% for all n if $N_T \geq 25$, while S_n^2 is a better approximation for all n if $N_T > 10$.

If we take the limit $a \to \infty$ or $N_T \to 0$ in Eqs. IV.31-IV.38, we obtain the case of bare Coulomb potential model, which of course is not short ranged and so the result of such a limiting procedure.

Another non trivial potential model of interest is the Gaussian potential, given by

$$V(\rho,z) = V_3 \; e^{-((\rho^2+z^2)/a^2)} \qquad \text{IV.44}$$

and has a Fourier transform

$$V_G(q_\perp,q_z) = V_3 \; e^{-(a^2/4)(q_\perp^2+q_z^2)} \; . \qquad \text{IV.45}$$

So that for this model, we have

$$S_r^G(\gamma,N_T) = \frac{e^{-(\gamma/4N_T)}}{(1+\frac{1}{4N_T})^{r+1}} \; . \qquad \text{IV.46}$$

In this case also S_r is positive and monotonically decreasing function of r. The results for the various potential models can be cast into a short-hand form as

$$V^m_{nn'}(\gamma) = \hbar\omega_c \; K_{NN'} \; \frac{P}{\pi} \sum_{r=m}^{N+N'} D_r^{NN'}(m) \; S_r^V(\gamma,N_T) \qquad \text{IV.47}$$

where P is the dimensionless potential strength given by

$$P = \frac{f}{\ell\sqrt{2}} \qquad \text{IV.48}$$

and f is the scattering amplitude of a zero energy electron in the absence of the magnetic field.

Expressions for the potential matrix elements can further be simplified by invoking the Lifshitz ansatz, which assumes a separable form for these matrix elements, i.e.

$$V^{m}_{nn'}(\gamma) = V_o g_n g_{n'} \delta_{mo} \quad . \qquad \text{IV.49}$$

This approximation is exact for the cut-off delta function potential model. In other cases this is an approximation which is still better than the delta function model. This approximation enables one to calculate the t-matrix exactly.

To derive an expression for the g_n,s we compare the matrix elements $V^{o}_{no}(\gamma)$ obtained from Eqs. IV.47 and IV.49. Normalizing the g_n,s for each potential model, such that g_o=1, we obtain for the Lifshitz factors

$$g_n = \begin{cases} = \begin{cases} 1 & , \ n \leq N_T \\ 0 & , \ n > N_T \end{cases} & \text{Cut-off delta function model} \\ \dfrac{S^{TF}_n(N_T)}{S^{TF}_o(N_T)} \simeq \dfrac{N_T+1}{N_T+n+1} & , \ \text{TF model} \\ \dfrac{1}{(1+(1/4N_T))^n} & , \ \text{Gaussian model} \end{cases} \qquad \text{IV.50}$$

This approximation also implies that the potential is short ranged in the z-direction (by neglecting $\gamma << N_T$) which is not true for most systems. In fact, such an approximation would be valid in the case of graphite with the magnetic field perpendicular to the c-axis. The approximation would also be true in the case of the super lattice systems, which is not considered in the present work.

The Lifshitz formula gives exact results for V^{o}_{no} and is poorest for the diagonal elements. A comparison of the Lifshitz factors for the various potential models is plotted in Fig. 2. In the case of

Fig. 2. The Lifshitz factors for the potential models discussed in the text for $N_T = 50$:

I - Cut-off delta function model.

II - Gaussian model.

III - Thomas-Fermi model.

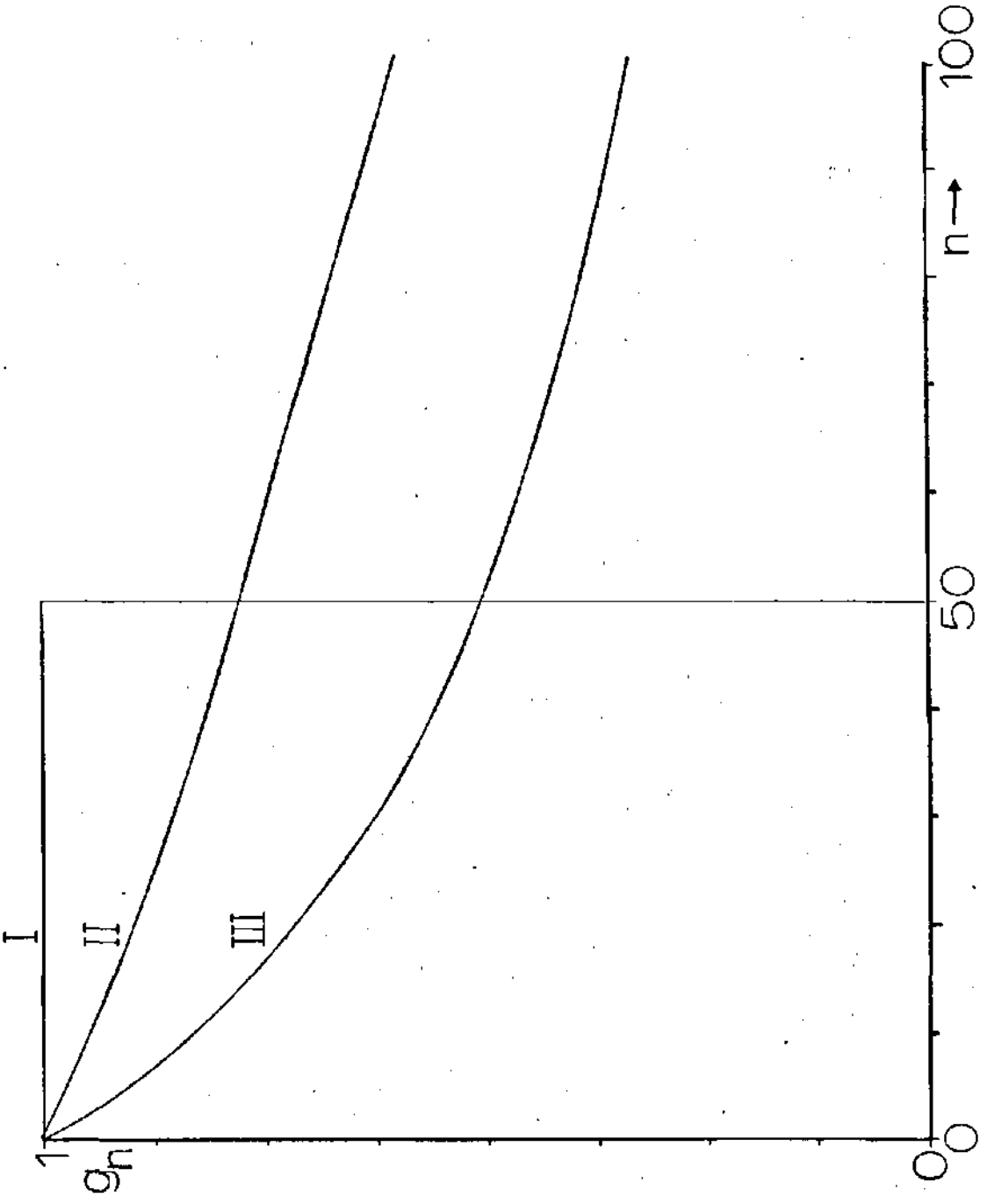


Fig. 2.

the TF model, the separable potential approximation is good to about 60% for any $n \leq N_T$ using S_n^1 and S_n^2 given by Eqs. IV.42 and IV.43, respectively. Fig. 3 shows the area of reliability of such an approximation. But in view of the fact that all the physical quantities of interest (as will be shown in the next two chapters) involve the diagonal elements of the t-matrix (and consequently the diagonal elements of the potential), an approximate potential model is proposed here (the consequence of which will be reported somewhere else) as an improvement to the one given by Eq. IV.49). The idea of such a model is to add a term to Eq. IV.49 that would compensate for the failure of the latter along the diagonal, but vanish along the edges of the matrix.

Thus we have

$$V^o_{nn'} = V_o \left[g_n g_{n'} + f_n f_{n'}\right] \qquad \text{IV.51}$$

such that $f_o = 0$. A model expression for f_n was constructed and used in Eq. IV.51 to compare with Eq. IV.49. The result of such a comparison shows that the new model given by Eq. IV.51 is a better fit to the true potential and this is clearly displayed in Fig. 3. Despite this improvement, along the diagonal, this model still gives a simple expression for the t-matrix. Here we used for f_n, a model expression given by

$$f_n = \left(\frac{N_T+1}{N_T+1+n}\right) \frac{n}{\sqrt{N_T(n+\beta N_T)}} \quad . \qquad \text{IV.52}$$

Fig. 3. The ratio of the diagonal elements, R_V, of the separable potential and the true potential, using the Thomas-Fermi model for different values of N_T:

I - N_T = 5

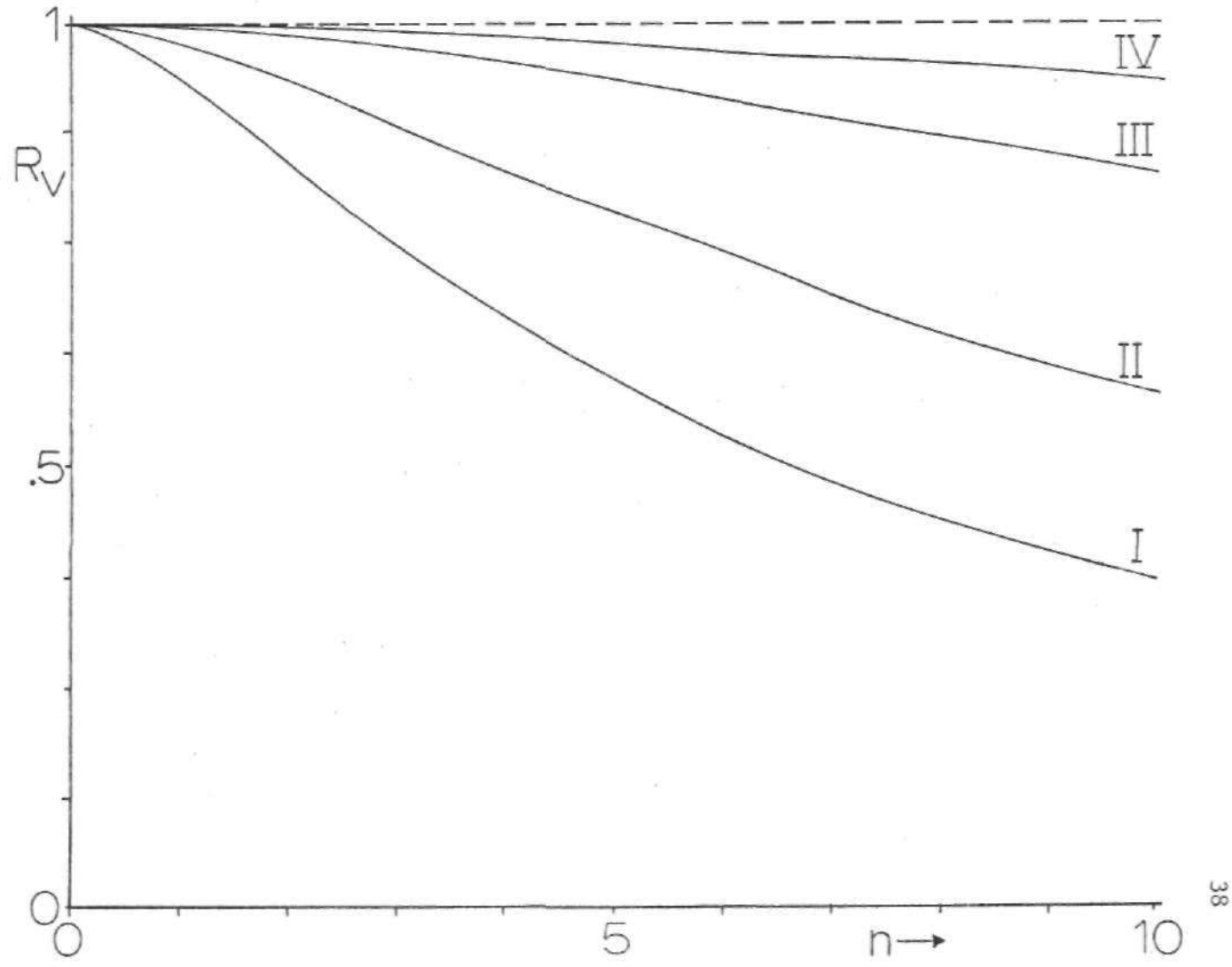
II - N_T = 10

III - N_T = 25

IV - N_T = 50 .

The dashed curve corresponds to the same ratio but using the improved potential for N_T = 5.

Fig. 3.



CHAPTER V

NON-BORN SCATTERING

In the present work we consider only impurity scattering and this is assumed to be elastic. Following Luttinger and Kohn (Kohn 1957), we introduce the scattering operator defined by

$$\hat{T}(z) = \hat{V} + \hat{V}\hat{G}(z)\hat{V} \qquad V.1$$

where z is the complex energy,

$\hat{V}$ is the scattering potential,

$\hat{G}(z)$ is the Green's function for the total Hamiltonian,

$$\hat{H} = \hat{H}_o + \hat{V} \qquad V.2$$

and is defined by

$$\hat{G}(z) = (z - \hat{H})^{-1} . \qquad V.3$$

In the coordinate representation, the Green's function

$$G(\vec{r}, \vec{r}', z) = \langle \vec{r} | \hat{G}(z) | \vec{r}' \rangle \qquad V.4$$

satisfies the equation

$$(z-\hat{H})G(\vec{r}, \vec{r}', z) = \delta(\vec{r} - \vec{r}') . \qquad V.5$$

Also G(z) satisfies the following identities:

$$\begin{aligned} G(z) &= G_o(z) + G_o(z)VG(z) \\ &= G_o(z) + G(z)VG_o(z) \end{aligned} \qquad V.6$$

where $G_o(z)$ is the Green's function corresponding to the unperturbed Hamiltonian, H_o.

Also we can write

$$G(z) = G_o(z) + G_o(z)T(z)G_o(z) \qquad V.7$$

since

$$G(z)V = G_o(z)T(z),$$

and from which we get the Lippman-Schwinger equation for the t-matrix:

$$T(z) = V + VG_o(z)T(z). \qquad V.8$$

With the assumption that the scattering potential

$$V(\vec{r}) = \sum_{j=1} v(\vec{r} - \vec{R}_j) \qquad V.9$$

is a sum of isolated single site potentials, we can express the scattering matrix T(z) in terms of the single site scattering matrix t_i i.e.

$$T(z) = \sum_{j=1} t_i(z) + \sum_{i\neq j} t_i(z)G_o(z)t_j(z) + \ldots \quad , \qquad V.10$$

where $t_i(z)$ satisfies the Lippmann-Schwinger equation

$$\begin{aligned} t_i(z) &= v(\vec{r} - \vec{R}_i) + v(\vec{r} - \vec{R}_i)\, G_o(z)\, t_i(z) \\ &= v(\vec{r} - \vec{R}_i) + t_i(z)\, G_o(z)\, v(\vec{r} - \vec{R}_i) \quad . \end{aligned} \qquad V.11$$

Furthermore, we are interested in the dilute impurity concentration limit, so that, following Luttinger and Kohn (Luttinger 1957), we can approximate T(z) by

$$T(z) \tilde{=} \sum_{i=1} t_i(z) \quad . \qquad V.12$$

In this expression, we have neglected contributions from successive scatterings between two or more impurity centers. This is consistent with the dilute impurity approximation.

Substituting Eqs. V.7 and V.12 into the expression for $\sigma_{\mu\nu}(0)$, one can distinguish between three types of terms:

a) a term independent of the t-matrix

b) two terms linear in the t-matrix

c) and finally a term quadratic in the t-matrix.

The term quadratic in the t-matrix arises from scattering between two different atoms and also from repeated scattering on the same impurity. Consistent with Eq. V.12 only the latter contribution is significant. But this term also identically vanishes in the s-wave approximation (m=0). This is due to the velocity operator selection rule and is fully discussed in Appendix A. Hence, the effect of the impurity system is simply the sum of the effect of each individual impurity center.

Thus Eq. V.13 can be rewritten as

$$T(z) = N_I t(z) \qquad \text{V.13}$$

where t(z) is the t-matrix due to an impurity center located as the origin and N_I is the number of impurity centers in the volume V. Therefore, we have

$$\sigma_{\mu\nu}(o) = \sigma^{(0)}_{\mu\nu}(0)+\Delta\sigma_{\mu\nu}(0) \ , \qquad \text{V.14}$$

where

$$\sigma^{(0)}_{\mu\nu} = \frac{-ie^2\hbar}{V\pi} \int_{-\infty}^{\infty} dE \ f(E)Tr[v_\mu ImG^{(0)}(E)v_\nu \frac{d}{dE} G_R^{(0)}(E)$$

$$- v_\mu \frac{d}{dE} G_A^{(0)}(E)v_\nu ImG^{(0)}(E)]. \qquad \text{V.15}$$

The term $\Delta\sigma_{\mu\nu}(0)$ is linear in the t-matrix and could further be decomposed into:

$$\Delta\sigma_{\mu\nu}(0) = \sigma^{(1)}_{\mu\nu}(0) + \sigma^{(2)}_{\mu\nu}(0), \qquad \text{V.16}$$

where

$$\sigma_{\mu\nu}^{(1)} = - n_I \frac{ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E) \frac{d}{dE}\ S_{\mu\nu}(E), \qquad V.17$$

$$S_{\mu\nu}(E) = Tr\{v_\mu ImG^{(0)}(E)v_\nu[G_R^{(0)} t_R G_R^{(0)}]-v_\mu[G_A^{(0)} t_A G_A^{(0)}]$$

$$x\ v_\nu ImG^{(0)}(E)\}\ , \qquad V.18$$

and

$$\sigma_{\mu\nu}^{(2)}(0) = \frac{n_I ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E)\ Im[Z_{\mu\nu}(E) - Z_{\nu\mu}(E)], \qquad V.19$$

with

$$Z_{\mu\nu}(E) = Tr\{v_\mu \frac{dG^{(0)}(E)}{dE}\ v_\nu[G^{(0)}(E)T(E)G^{(0)}(E)]\}. \qquad V.20$$

Evidently, $\sigma_{\mu\mu}^{(2)}(0) = 0$ and in fact

$$\sigma_{\mu\mu}(0) = \sigma_{\mu\mu}^{(1)}(0)$$

for the transverse components, since $\sigma_{xx}^{(0)}(0) = \sigma_{yy}^{(0)}(0) = 0$.

In the dilute limit of short ranged impurity potential, the Hall conductivity can be written as

$$\sigma_{xy}(0) = \sigma_{xy}^{(0)}(0) + \Delta\sigma_{xy} \qquad V.21$$

where

$$\Delta\sigma_{xy}(0) = \sigma_{xy}^{(1)}(0) + \sigma_{xy}^{(2)}(0) \qquad V.22$$

and the diagonal elements of the transverse magnetoconductivity are given by

$$\sigma_{xx}(0) = \sigma_{yy}(0) = \sigma_{xx}^{(1)}(0)$$

$$= \frac{-n_I i e^2 \hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E)\ \frac{d}{dE}\ S_{xx}(E)\ . \qquad \text{V.23}$$

In all these results, we have ignored the electron spin.

It is illustrative to point out that the first term in Eq. V.21 is nothing more than the semiclassical result for the Hall conductivity, i.e.

$$\sigma_{xy}^{(0)}(0) = \frac{-nec}{B} \qquad \text{V.24}$$

where n is the electronic density and B is the magnetic field strength. This result will be explicitly obtained in the next chapter. However, it is important to note here that scattering is necessary for the existence of conduction in the high magnetic field limit, whereas scattering reduces conduction in the low magnetic field limit.

CHAPTER VI

THE TRANSVERSE COMPONENTS OF THE MAGNETOCONDUCTIVITY TENSOR

Returning to the expressions obtained for the transverse components of the magnetoconductivity tensor in Chapter V and bearing in mind the Lifshitz ansatz made in Chapter IV to simplify the matrix elements for the various potential models, the t-matrix for the system can now be written in a closed form. This is a consequence of the separability of the impurity potential matrix elements. Thus the Born series involved in the expression for the single site t-matrix can now be summed for each potential model. The calculation is done in Appendix A.

As was pointed out in Chapter IV, the Lifshitz ansatz is exact in the case of the cut-off delta function potential model. In this case the t-matrix is given by:

VI.1

$$t_{n,n'}(\eta) = \begin{cases} \dfrac{(\alpha/2\pi)V_o}{1 + \sum_{n_1=0}^{N_T} \dfrac{P}{\sqrt{n_1+\frac{1}{2}-\eta}}} & ; \quad n,n' \leq N_T \\ 0 & ; \quad \text{otherwise} \end{cases}$$

where V_o is the potential strength in Eq. IV.1 which can be expressed in terms of the scattering amplitude f of a zero energy electron in the absence of the magnetic field as

$$V_o = \frac{\hbar^2 f}{M} \quad .$$

One can introduce a dimensionless potential strength parameter, P, defined as

$$P = \frac{f}{\ell\sqrt{2}} = \frac{MV_o}{\hbar^2\ell\sqrt{2}} \quad . \qquad \text{VI.2}$$

Here again ℓ is the classical radius of the Landau ground state orbit, and

$$\eta = \frac{E}{\hbar\omega_c} \qquad \text{VI.3}$$

is the dimensionless energy parameter.

The expression for the t-matrix in the case of the dispersive potential models is given by:

$$t_{nn'}(\eta) = \frac{\hbar^2}{\pi M}\sqrt{\alpha/2}\;\frac{Pg_n g_{n'}}{1+P\sum_{n_1=0}^{\infty}\frac{g_{n_1}^2}{\sqrt{n_1+\frac{1}{2}}-\eta}} \qquad \text{VI.4}$$

where the g_n's are the Lifshitz factors defined in Eq. IV.50 for the various potential models of interest.

It is noteworthy to point out here that in the case of the cut-off delta function potential model, the Lifshitz factors impose a cut-off both in the numerator and in the denominator of Eq. VI.4 which is logically consistent with their derivation, and thus gives back Eq. VI.1. This result is in sharp contrast to that used by Nozieres and co-authors (Bastin 1971) where a cut-off was imposed "artificially" in the denominator to avoid its divergence and was completely ignored in the numerator. This is similar to the cut-off parameter suggested by Skobov (Skobov 1960) where $N_T=n_c+1$ and n_c is the largest quantum number

for which the expression $(\eta-n-\frac{1}{2})$ is positive. Such a choice of the cut-off parameter is not usually accurate.

Although the imposition of the Lifshitz ansatz simplifies the expression for the t-matrix, it, however, has other consequences. The approximation resulting from this ansatz would be justifiably correct if the potential is non-local, short-ranged and square integrable. The nonlocality of the potential in turn implies noncommutativity of the position operator with the scattering potential operator. Therefore, it is pertinent and illustrative to consider each case separately, since the velocity operator is different in each case.

A. Local Potential Model.

For a local potential, the velocity operator has its usual form (as the position operator commutes with the potential energy operator) and is expressed as:

$$\hat{\vec{v}} = \frac{i}{\hbar} [\hat{H},\hat{\vec{r}}] = \frac{i}{\hbar} [\hat{H}_o,\hat{\vec{r}}] , \qquad \text{VI.5}$$

where $\hat{H}_o$ is again the Hamiltonian of an electron in a magnetic field and

$$\hat{H} = \hat{H}_o + \hat{V}(\vec{r})$$

is the total Hamiltonian of the system. Using the matrix elements of the velocity operator, which are given by

$$\langle n'm'k'|v_x|nmk\rangle = \frac{1}{i} \frac{\hbar}{M} \sqrt{\alpha/2} \left[\sqrt{n}\, \delta_{n',n-1}\delta_{m',m-1} - \sqrt{n+1}\, \delta_{n',n+1} \right.$$

$$\left. \times \delta_{m'm+1} \right] \delta_{k'k}, \qquad \text{VI.6}$$

$$\langle n'm'k'|v_y|nmk\rangle = \frac{\hbar}{M}\sqrt{\alpha/2}\ \left[\sqrt{n}\ \delta_{n',n-1}\delta_{m',m-1} + \sqrt{n+1}\ \delta_{n',n+1}\right.$$

$$\left. \times\ \delta_{m',m+1}\right]\delta_{k'k}\ , \qquad \text{VI.7}$$

we evaluate the various terms contributing to the Hall conductivity in Appendix B,

$$\sigma_{xy}^{(0)}(0) = -\frac{ec}{H}\frac{(2\alpha)^{3/2}}{(2\pi)^2}\sum_{n=0}^{n_c}\sqrt{\eta_F - n - \tfrac{1}{2}} \qquad \text{VI.8}$$

where η_F is the dimensionless energy parameter at the Fermi level

$$\eta_F = \frac{\varepsilon_F}{\hbar\omega_c}\ ,$$

ε_F is the Fermi energy,

$\omega_c = \frac{eB}{Mc}$ is the cyclotron frequency, and

n_c is the largest Landau number for which the radicand in Eq. VI.8 is positive.

The $\sigma_{xy}^{(0)}(0)$ obtained above agrees with the usual semiclassical result for the Hall conductivity,

$$\sigma_{xy}^{sc}(0) = -\frac{ec}{B}n_e$$

where n_e is the carrier density, as

$$n_e = \frac{(2\alpha)^{3/2}}{(2\pi)^2}\sum_{n=0}^{n_c}\sqrt{\eta_F - n - \tfrac{1}{2}}\ . \qquad \text{VI.9}$$

Similarly, we have (from Appendix B) VI.10

$$\sigma_{xy}^{(1)}(0) = \frac{-n_I e^2}{\hbar\alpha}\int_{-\infty}^{\infty} dE\ \frac{df}{dE}\sum_{n,k}\delta[E-\varepsilon_n(k)]\,\mathrm{Re}\{(n+1)t_{n+1,k}(E) - n t_{n-1,k}(E)\}$$

and

$$\sigma_{xx}^{(1)}(0) = \frac{n_I e^2}{\hbar\alpha}\int_{-\infty}^{\infty} dE \frac{df}{dE} \sum_{n,k} \delta[E-\epsilon_n(k)]\mathrm{Im}\{(n+1)t_{n+1,k}(E) + n\, t_{n-1,k}(E)\}\,, \qquad \text{VI.11}$$

where $t_{n,k}(E)$ are the diagonal elements of the t-matrix taken between the unperturbed states.

It is interesting to note that due to the delta functions in Eqs. VI.10 and VI.11, $\sigma_{xy}^{(1)}(0)$ and $\sigma_{xx}^{(1)}(0)$ have a dissipative character. In particular, only states in the neighborhood of the Fermi energy contribute to these terms. On the contrary, $\sigma_{xy}^{(2)}(0)$ involves integration over all energies and thus has a dispersive nature. Thus the Hall conductivity consists of a dissipative term and a dispersive term, represented by $\sigma_{xy}^{(1)}(0)$ and $\sigma_{xy}^{(2)}(0)$, respectively.

These results Eqs. VI.10 and VI.11 constitute a generalization of the results obtained by Nozieres and co-workers (Bastin 1971). In the present approximation of short-ranged potential, there is no contribution from terms quadratic in the t-matrix. There however, exists a contribution to the Hall conductivity which is linear in the t-matrix but arises solely from the finite range and it is given by:

$$\sigma_{xy}^{(2)}(0) = \frac{n_I e^2}{\pi\hbar\alpha}\left(\frac{\alpha\hbar^2}{M}\right)^2\int_{-\infty}^{\infty} dE\, f(E)\,\mathrm{Im} \sum_{n,k} \left\{\frac{(n+1)t_{n+1,k}(E)}{[E-\epsilon_n(k)]^2[E-\epsilon_{n+1}(k)]^2} - \frac{n t_{n-1,k}(E)}{[E-\epsilon_n(k)]^2[E-\epsilon_{n-1}(k)]^2}\right\}\,. \qquad \text{VI.12}$$

Substituting the general expression for the t-matrix into formulas (VI.10) and VI.11) and assuming that T=0, the integration over energy in the expressions for σ_{xx}, and $\sigma_{xy}^{(1)}$ can easily be carried out. On integrating over the z-component of the linear momentum, k , the transverse components of the magnetoconductivity tensor can finally be written as:

$$\sigma_{xx}(0) = \frac{n_I e^2}{\pi\hbar\alpha} \frac{F_I}{(1+F_R)^2+(F_I)^2} \sum_{n=0}^{n_c} \frac{P\{(n+1)g_{n+1}^2 + ng_{n-1}^2\}}{\sqrt{\eta_F - n - \frac{1}{2}}} , \quad \text{VI.13}$$

and

$$\sigma_{xy}^{(1)}(0) = \frac{n_I e^2}{\pi\hbar\alpha} \frac{(1+F_R)}{(1+F_R)^2+(F_I)^2} \sum_{n=0}^{n_c} \frac{P\{(n+1)g_{n+1}^2 - ng_{n-1}^2\}}{\sqrt{\eta_F - n - \frac{1}{2}}} , \quad \text{VI.14}$$

where F_R and F_I are the real and imaginary parts of F, which in turn is defined as

$$F = \sum_{n=0}^{\infty} \frac{Pg_n^2}{\sqrt{n+\frac{1}{2}-\eta_F}} \equiv F_R + iF_I , \quad \text{VI.15}$$

so that

$$F_R = P \sum_{n=n_c+1}^{\infty} \frac{g_n^2}{\sqrt{n+\frac{1}{2}-\eta_F}} , \quad \text{VI.16}$$

and

$$F_I = P \sum_{n=0}^{n_c} \frac{g_n^2}{\sqrt{\eta_F - n - \frac{1}{2}}} . \quad \text{VI.17}$$

Here again, n_c is the largest Landau number for which the radicand in Eq. VI.17 is positive. At this juncture, it is illuminating to consider the cut-off delta function potential model separately from the other three dispersive potential models, so as to complete the comparison between the delta function model used in the present work and that used by previous authors, and also to contrast the delta function model with all the

other dispersive models. The conductivities for the cut-off delta function potential model can be written as:

$$\sigma_{xx}(0) = \frac{n_I e^2}{\pi\hbar\alpha} \frac{F_I}{(1+F_R)^2+(F_I)^2} \sum_{n=0}^{n_c} \frac{P(2n+1)}{\sqrt{n_F-n-\frac{1}{2}}} , \qquad \text{VI.18}$$

and

$$\sigma_{xy}^{(1)}(0) = \frac{n_I e^2}{\pi\hbar\alpha} \frac{F_I(1+F_R)}{(1+F_R)^2+(F_I)^2} . \qquad \text{VI.19}$$

The expression for $\sigma_{xy}^{(2)}(0)$ given by Eq. VI.12 vanishes in the case of a delta function potential, since the t-matrix is just a constant independent of the indices. The other contribution to the change in the Hall conductivity, $\sigma_{xy}^{(1)}$ would also vanish in this model, because the sum in Eq. VI.16, F_R, diverges and consequently $\sigma_{xx}(0)$ and $\sigma_{xy}^{(1)}(0)$ will both vanish. Thus the effect of impurity scattering on the conductivity is strongly related to the finite range of the scattering potential.

On the other hand, expression VI.4 for the t-matrix, implies the presence of a pole in the case of an attractive potential which means that there are bound states in the problem. But according to Eq. VI.12, $\sigma_{xy}^{(2)}$ involves an integration of the t-matrix over all energy, it therefore follows that, there is a contribution to the Hall conductivity arising from the poles of the t-matrix. This is contradictory to the initial assumption that the impurity concentration is low and as such, there should be no current contribution from the bound states.

Such a contribution would vanish only in the case of a true delta function potential. Thus, for any finite ranged potential model (the COD model included), there is a nonvanishing contribution from the

bound states. This is due to the fact that we used non-local potentials (implied by the separable form) but defined the velocity operator, in a way which is true for only local potentials. Hence, there is a need to do this in a consistent fashion and that is the topic of the next section.

B. Non-Local Potential Model.

In this case the velocity operator is determined not only by the unperturbed Hamiltonian but also by the perturbing potential. Hence, the velocity operator in the non-local potential approximation is given as

$$\hat{\vec{v}}_{N-L} = \frac{i}{\hbar}[\hat{H}_o, \hat{\vec{r}}] + \frac{i}{\hbar}[\hat{V}, \hat{\vec{r}}], \qquad \text{VI.20}$$

or simply

$$\hat{\vec{v}}_{N-L} = \hat{\vec{v}}_L + \hat{\vec{v}}_V \ . \qquad \text{VI.21}$$

In terms of the eigenstates of the unperturbed Hamiltonian, the matrix elements of this velocity operator can be written as:

$$\langle n'm'k' | \hat{\vec{v}}_{N-L} | nmk \rangle = \langle n'm'k' | \hat{\vec{v}}_L | nmk \rangle + \langle n'm'k' | \hat{\vec{v}}_V | nmk \rangle \ . \qquad \text{VI.22}$$

Evaluation of these matrix elements require the knowledge of the matrix elements of the position operator and these are given by:

$$\langle n'm'k' | x | nmk \rangle = \frac{1}{\sqrt{2\alpha}} \{ [\sqrt{n+1}\ \delta_{n',n+1} - \sqrt{n-m}\ \delta_{nn'}] \delta_{m',m+1}$$

$$- [\sqrt{n}\ \delta_{n',n-1} - \sqrt{n-m+1}\ \delta_{n'n}] \delta_{m',m-1} \} \delta_{k',k} \ , \qquad \text{VI.23}$$

VI.24

$$\langle n'm'k' \,|y|\, nmk \rangle = -\frac{i}{\sqrt{2\alpha}} \{[\sqrt{n+1}\ \delta_{n',n+1} - \sqrt{n-m}\ \delta_{nn'}]\delta_{m',m+1}$$

$$-[\sqrt{n}\ \delta_{n',n-1} - \sqrt{n-m+1}\ \delta_{n'n}]\delta_{m',m-1}\delta_{k'\,k} \ .$$

Thus the matrix elements of the potential-dependent part of the velocity operator can then be written as:

VI.25

$$\langle n'm'k' \,|v_V^x|\, nmk \rangle = \frac{i}{h}\frac{V_o}{\sqrt{2\alpha}}\delta_{k'\,k}\ \{g_{n'}\sqrt{n+1}\ (g_{n+1}-g_n)\delta_{m'o}\delta_{m',m+1}$$

$$+ g_{n'}\sqrt{n}\ (g_{n-1}-g_n)\delta_{m'o}\delta_{m',m-1} - g_n\sqrt{n'}\ (g_{n'-1}-g_{n'})$$

$$\times\ \delta_{mo}\delta_{m,m'-1} - g_n\sqrt{n'+1}\ (g_{n'+1}-g_{n'})\delta_{mo}\delta_{m,m'+1}\},$$

and

VI.26

$$\langle n'm'k' \,|v_V^y|\, nmk \rangle = \frac{V_o}{h\sqrt{2\alpha}}\ \delta_{k'\,k}\ \{g_{n'}\sqrt{n+1}\ (g_{n+1}-g_n)\delta_{m',o}\delta_{m',m+1}$$

$$- g_{n'}\sqrt{n'}\ (g_{n-1}-g_n)\delta_{m'o}\delta_{m',m-1} - g_n\sqrt{n'}\ (g_{n'-1}-g_{n'})$$

$$\times\ \delta_{m,o}\delta_{m,m'-1} + g_n\sqrt{n'+1}\ (g_{n'+1}-g_{n'})\delta_{m,o}\delta_{m,m'+1}\} \ .$$

These matrix elements vanish in the case of a delta function potential model for which all the Lifshitz factors, g_n, are equal. Substituting the matrix elements of $\vec{v}_{N-L}$ into the formula for the magnetoconductivity tensor, and using the explicit expression for the t-matrix, the diagonal element of the transverse magnetoconductivity tensor, $\sigma_{xx}(0)$, can then be written as:

$$\sigma_{xx}(0) = n_I \frac{e^2}{\pi\hbar\alpha} \frac{F_I}{(1+F_R)^2+F_I^2} \sum_{n=0}^{n_c} \frac{Pg_n^2(2n+1)}{\sqrt{n_F-n-\frac{1}{2}}} \qquad \text{VI.27}$$

where F_R and F_I are the real and imaginary parts of the sum defined earlier. Details of the calculation are in Appendix C.

This result is very similar to expression VI.13 obtained in the "local" potential approximation and it is identical with it if the potential is a delta function. In fact the non-local potential approximation result Eq. VI.15 can be obtained from Eq. VI.13 simply by making the substitution:

$$(n+1)g_{n+1}^2 + ng_{n-1}^2 \rightarrow (2n+1)g_n^2 .$$

Actually, for N_T=n=5 (for the Thomas-Fermi potential model) these two results differ only by about 0.8%. This fact is aptly demonstrated by the similarity of the curves in the Figs. 4 and 5. Eq. VI.15 further confirms the fact that the transverse component of the magneto-conductivity tensor starts from the second order term in the Born series, and this is well displayed in Fig. 6. Finally, it is observed that if the Fermi energy level is just between the ground state and the first excited state, the Thomas-Fermi model gives a $\sigma_{xx}(0)$ similar to that obtained from the cut-off delta function potential model.

In the case of the Hall conductivity the difference in the results between the local and non-local potential approximation is very striking. The change in the Hall conductivity is evaluated in the same way as was done for $\sigma_{xx}(0)$, and the details are given in Appendix C. The

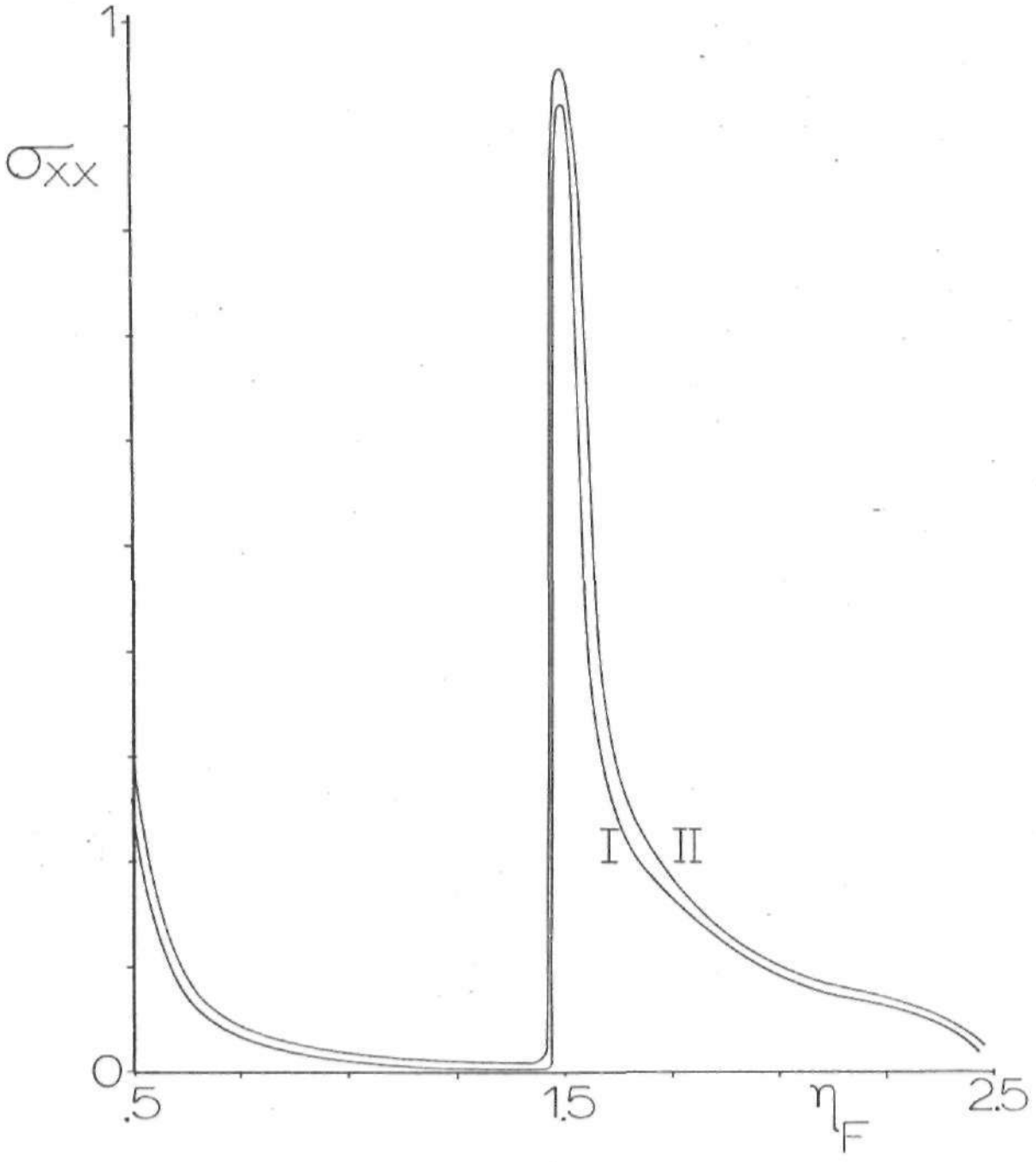


Fig. 4. The diagonal element of the transverse magnetoconductivity tensor, σ_{xx} as a function of η_F using the Thomas-Fermi model with $N_T = 10$ and $P = 1$.

I - Local potential approximation.

II - Non-local potential approximation.

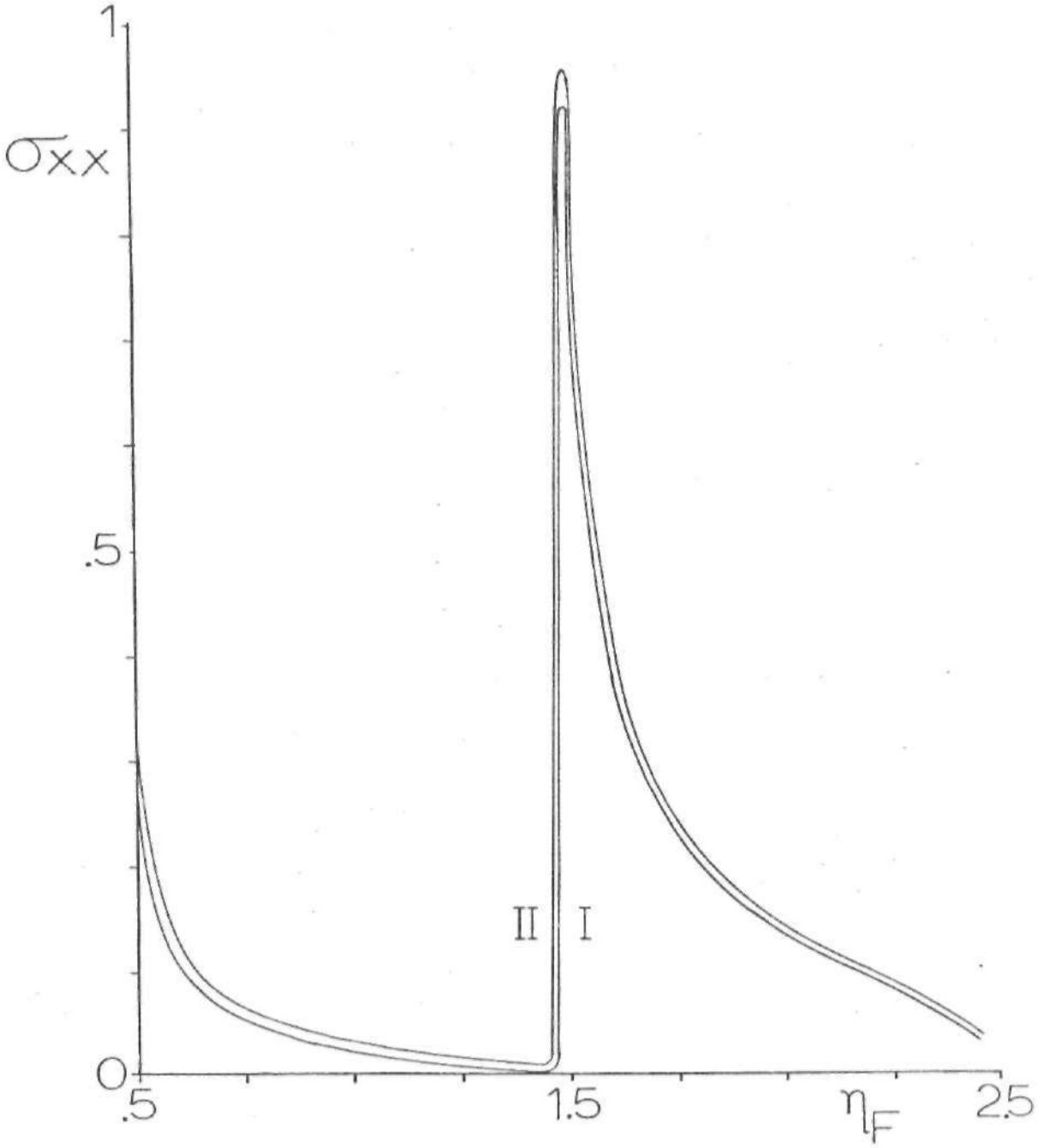


Fig. 5. The diagonal elements of the transverse magnetoconductivity, σ_{xx} as a function of η_F using the Thomas-Fermi model with N_T = 10 and P = 10:

I - Local potential approximation.

II - Non-local potential approximation.

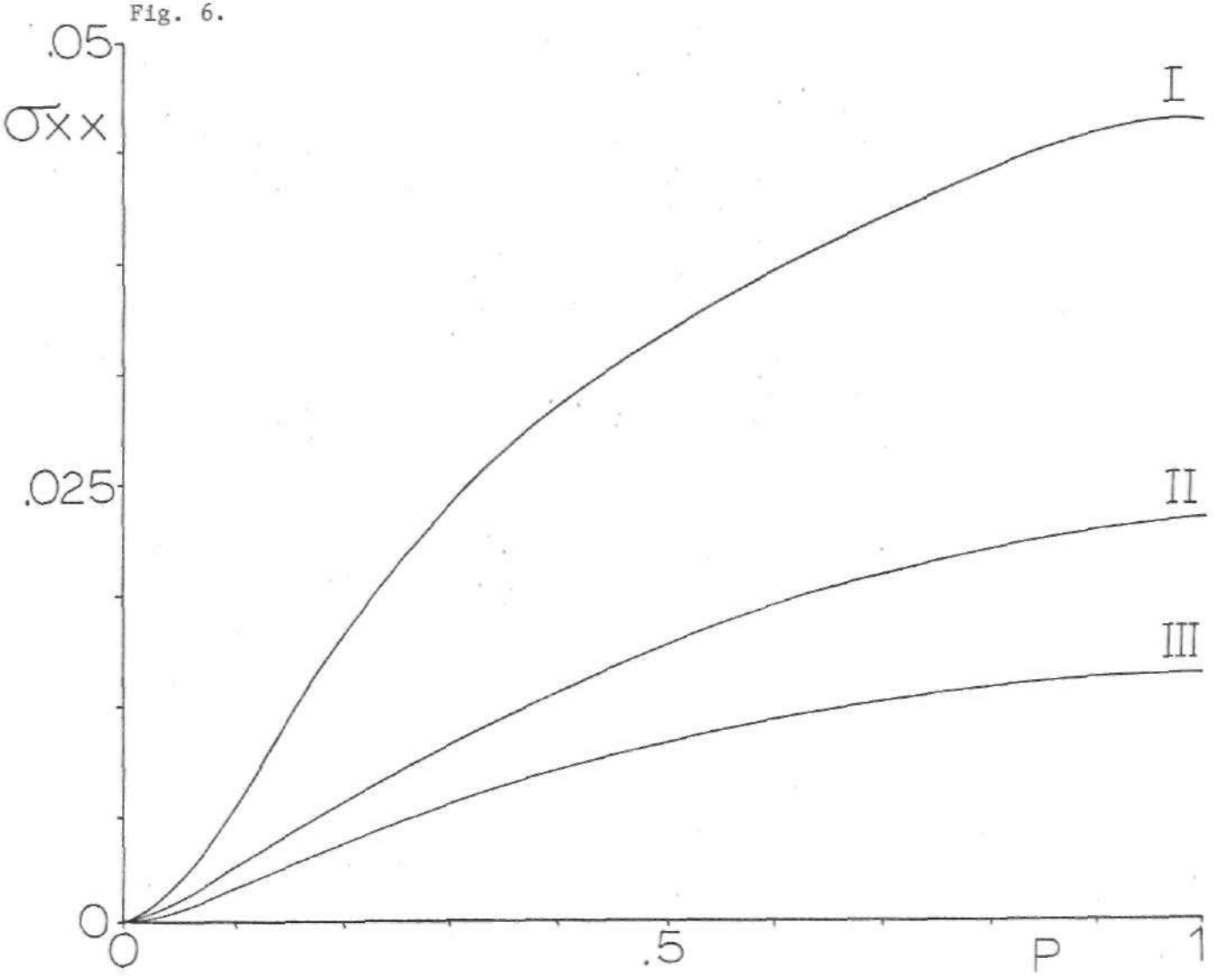
Fig. 6. The diagonal element of the transverse magnetoconductivity tensor, σ_{xx} as a function of P using the Thomas-Fermi model with $N_T = 10$ for various values of η_F:

I - $\eta_F = .7$

II - $\eta_F = .9$

III - $\eta_F = 1.1$.

Fig. 6.



result is expressed as:

VI.28

$$\Delta\sigma_{xy}(0) = \sigma_{xy}(0)-\sigma_{xy}^{(0)}(0) = \frac{n_I e^2}{\pi\hbar\alpha}\frac{(1+F_R)F_I}{(1+F_R)^2+F_I^2} + \frac{n_I e^2}{\pi\hbar\alpha} F_R \sum_{n=0}^{n_c}$$

$$\times \frac{P\{(n+1)(g_{n+1}-g_n)^2-n(g_{n-1}-g_n)^2\}}{\sqrt{\eta_F-n-\frac{1}{2}}} - \frac{2n_I e^2}{\pi\hbar\alpha} P^2 \sum_{n=0}^{n_c}\sum_{n'=n_c+1}^{\infty}$$

$$g_n^2, \{(n+1)(g_n-g_{n+1})^2-n(g_{n-1}-g_n)^2\} \frac{\sqrt{\eta_F-n-\frac{1}{2}}}{(n'-n)\sqrt{n'+\frac{1}{2}-\eta_F}} .$$

This expression is much simpler than its corresponding counterpart in the local potential approximation for the simple reason that all the integrations involved can be and have been carried out analytically. Moreover, this expression reduces to that obtained in the local potential approximation if, again, the potential model is a Dirac delta function, thereby reinforcing the need to consider a finite ranged potential model.

To facilitate the comparison between the results obtained from these two approximations and that obtained semiclassically, it is convenient to introduce the change in the carrier density, ΔN, in the system due to the impurities. Neglecting the electron spin, this quantity is derived in Appendix D and is given by:

$$\Delta N = -\frac{n_I}{\pi} \tan^{-1}\left(\frac{F_I}{1+F_R}\right) . \qquad \text{VI.29}$$

So that the semiclassical result for the change in the Hall conductivity can be written in the form:

$$\Delta\sigma_{xy}^{sc}(0) = -\frac{ec}{B}\Delta N . \qquad \text{VI.30}$$

Similarly, the change in the Hall conductivity obtained in the local and non-local potential approximations can be reduced to a form in which the semiclassical result is expressed, i.e.

$$\Delta\sigma_{xy}^{LOC}(0) = -\frac{ec}{B}\ \Delta N_H^{(LOC)}, \qquad \text{VI.31}$$

and

$$\Delta\sigma_{xy}^{N-L}(0) = -\frac{ec}{B}\ \Delta N_H^{(N-L)} \quad . \qquad \text{VI.32}$$

These relations define ΔN_H, of course. It is convenient to introduce a parameter R, which is the ratio of the change in the carrier density, ΔN_H, extracted from the Hall conductivity to the actual change in carrier density, ΔN:

$$R = \frac{\Delta N_H}{\Delta N} \quad . \qquad \text{VI.33}$$

This quantity is independent of the impurity concentration and from here on, we shall consider all the quantities per impurity, i.e.

$$\Delta N_H = n_I \cdot \Delta n_H$$

and $\Delta N = n_I \cdot \Delta n$

with $R = \frac{\Delta n_H}{\Delta n}$.

In the "local" potential approximation, the COD model gives a ratio R very close to unity for most values of P and η_F except in the neighborhood of the Landau levels. This is well illustrated in Figs. 7, 8 and 9. For this potential model, the major contribution to the Hall conductivity comes from the dissipative term $\sigma_{xy}^{(1)}(0)$. This is also

Fig. 7. A comparative plot of the ratio $R = \Delta N_H/\Delta N$ obtained in the local potential approximation as a function of $\eta_F = \varepsilon_F/\hbar\omega_c$ at $N_T = 10$ and $P = 1$:

I - Cut-off delta function model.

II - Thomas-Fermi potential model.

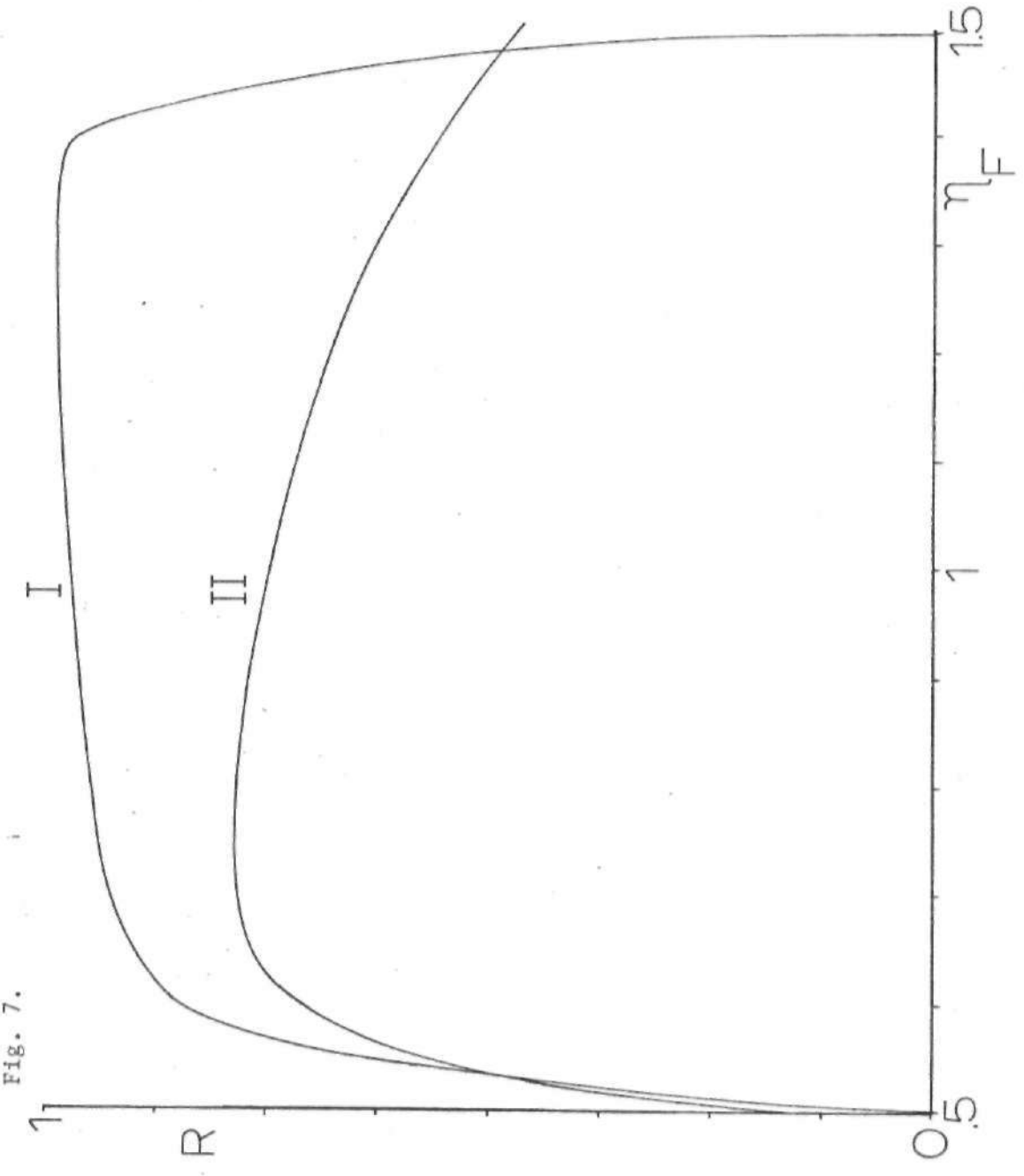


Fig. 7.

true for all values of P, and in fact the ratio of the dispersive term, $\sigma_{xy}^{(2)}$ to the dissipative term $\sigma_{xy}^{(1)}(0)$ is less than .01%.

This is in sharp contrast to the case of the TF model or any dispersive model for that matter, in which case both terms have the same order of magnitude. Hence, one concludes that the dispersive contribution to the Hall conductivity is negligible only in the COD model. Similarly, the ratio R is very different from unity and it is very sensitive to the values of P and N_T used. Its dependence on these parameters are demonstrated by the curves in Figs. 8 and 9.

Just as one would expect, the dissipative term in the Hall conductivity obtained in the local potential approximation (Eq. VI.14) is very similar to that obtained in the non-local potential approximation. In fact, the latter result could be obtained by substituting

$$(n+1)g_{n+1}^2 - ng_{n-1}^2 \rightarrow g_n^2$$

into Eq. VI.14 and the sum becomes just the definition of F_I. The two results (obtained in the local and non-local approximation) are identical in the COD model if $N_T > n_c$, and in the TF model, they differ only by about 1% for N_T=10.

However, that is the end of the similarity between the two results for the Hall conductivity obtained from the two approximations. The difference between $\Delta\sigma_{xy}^{(LOC)}$ and $\Delta\sigma_{xy}^{(N-L)}$ lies mainly in the behavior of the dispersive terms. In the case of the non-local potential, there are two dispersive terms, both of which are quadratic in the dimensionless potential strength, P. These terms have opposite signs and as a

Fig. 8. A plot of the ratio $R = \Delta N_H / \Delta N$ obtained in the local Thomas-Fermi potential model as a function of $\eta_F = \varepsilon_F / \hbar\omega_c$ at $N_T = 10$:

I - P = 0.1

II - P = 1.0

III - P = 10.0 .

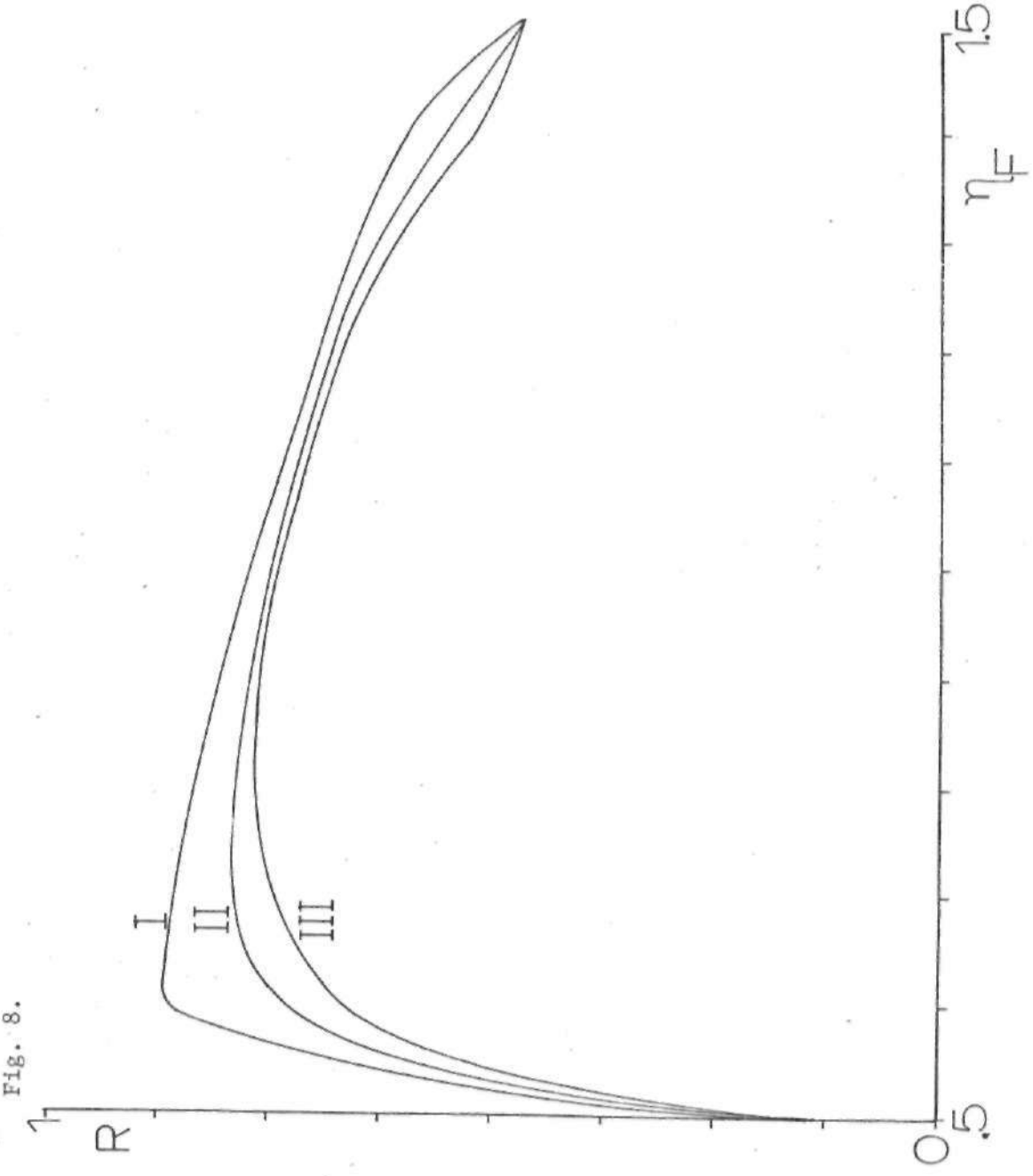


Fig. 8.

Fig. 9. A plot of the ratio $R = \Delta N_H/\Delta N$ obtained in the local Thomas-Fermi potential model as a function of $\eta_F = \varepsilon_F/\hbar\omega_c$ for P = 1 and the following values of N_T:

I - $N_T = 30$

II - $N_T = 10$

III - $N_T = 5$.

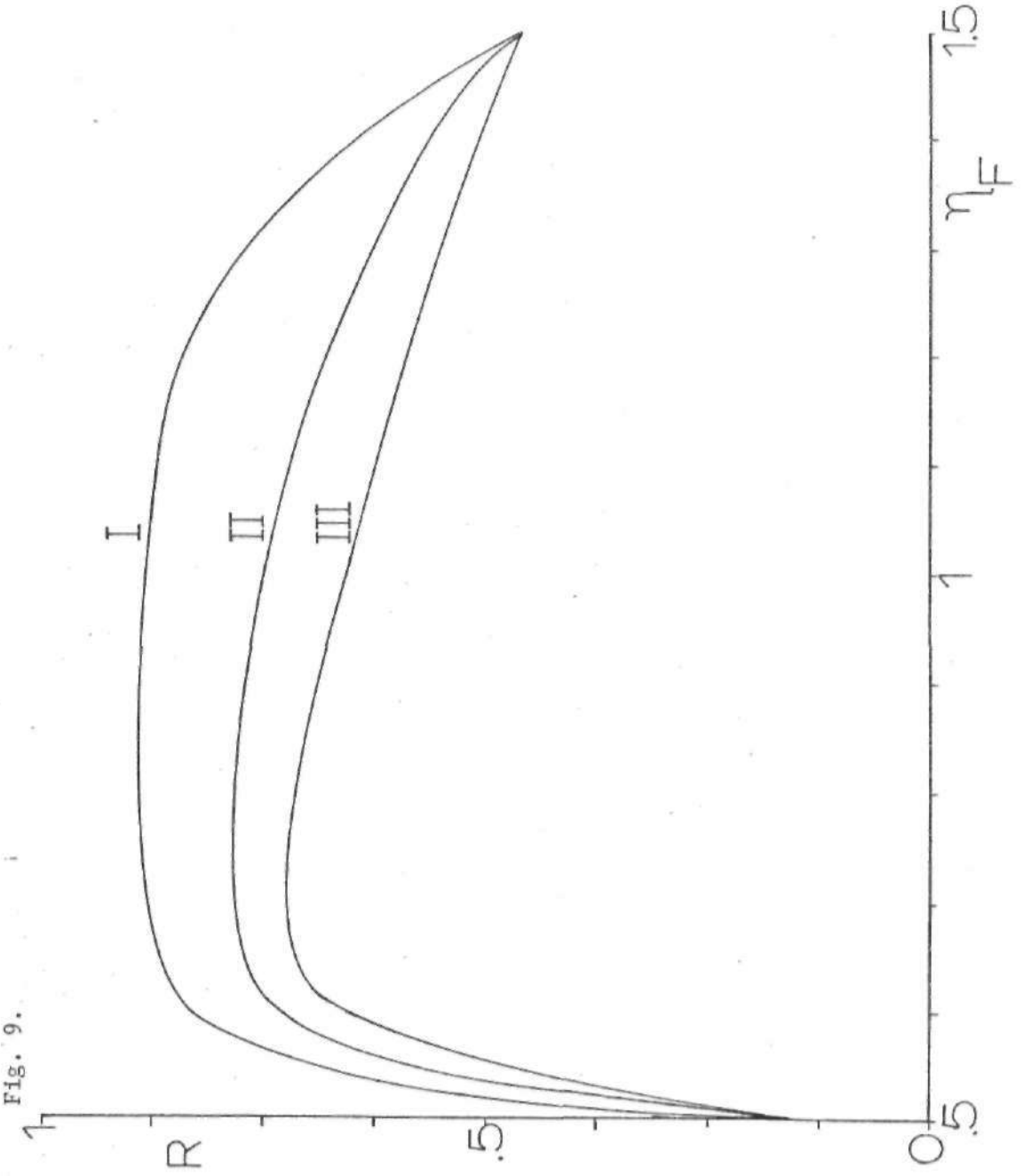


Fig. 9.

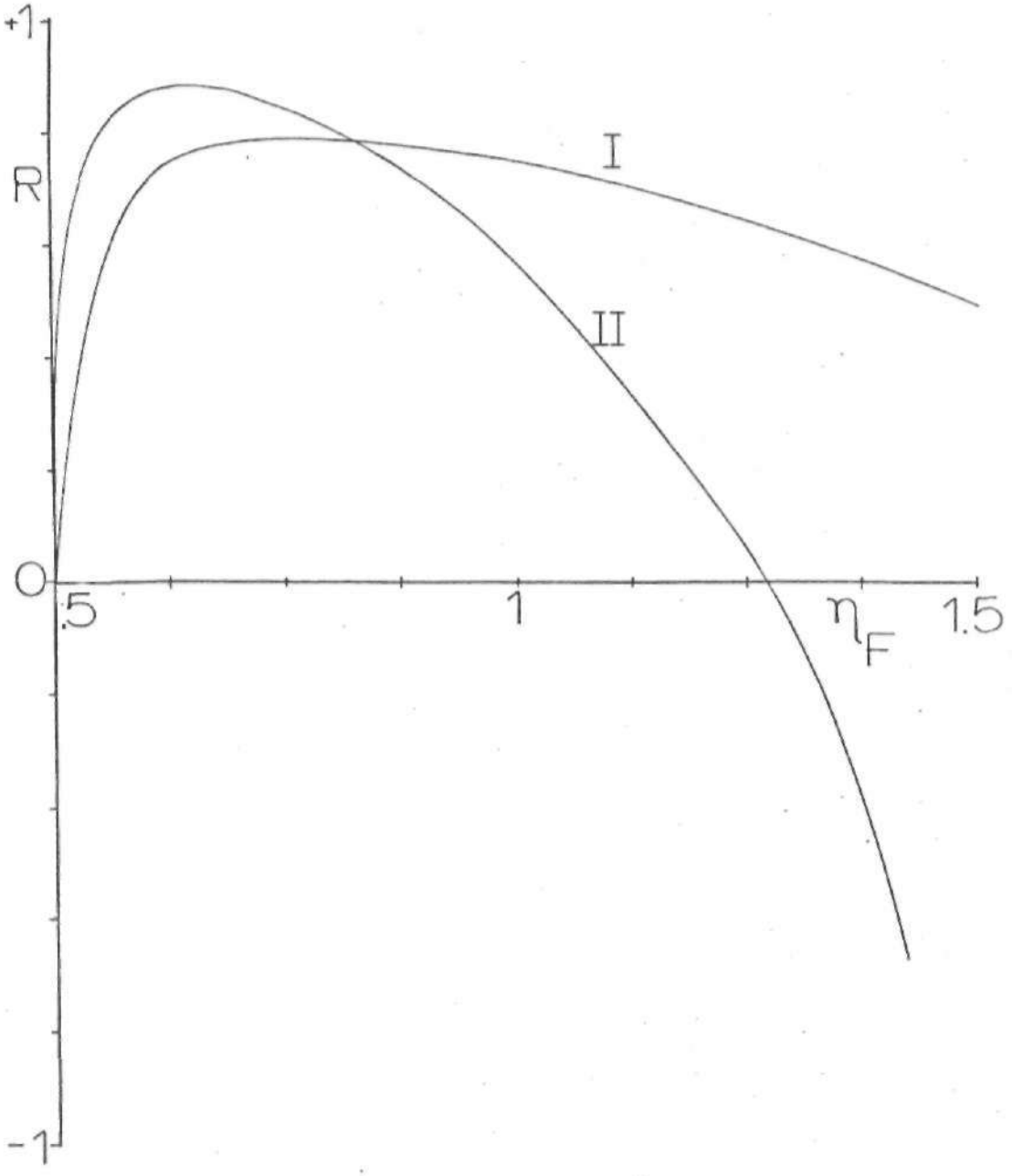


Fig. 10. A comparative plot of the ratio $R = \Delta N_H/\Delta N$ obtained in the Thomas-Fermi potential model as a function of $\eta_F = \varepsilon_F/h\omega_c$ for $N_T = 10$ and $P = 1$:

I - Local potential approximation.

II - Non-local potential approximation.

result, their contribution is only about 18% of the dissipative term, in the region $n_F \leq 1$ and for $P < 1$. This is illustrated in Fig. 10 by comparing the ratio R obtained in this approximation using the TF model. The curves in Figs. 11 and 12 demonstrate the sensitivity of R to the values of the two parameters in the theory, P and N_T, and also the fact that R changes sign regardless of the sign of P. It is interesting to note that the ratio R has the Born approximation value (R=1) for small P, however it changes drastically for larger values of P.

This result can further be illuminated by introducing an angle ϕ defined as

$$\phi = \tan^{-1} \frac{F_I}{1+F_R} \quad . \qquad \text{VI.34}$$

The change in the number of carriers due to the impurities is then given by

$$\Delta N = -\frac{n_I}{\pi} \phi \quad . \qquad \text{VI.35}$$

In this definition of the angle ϕ, it is necessary to stay just on the first Riemann sheet of arctangent, so that in the case of attractive potential, we count only the contributions from states in the continuum. This is important because the bound states cannot contribute to conduction in the dilute impurity limit. This is reminiscent of the phase shift δ, due to the impurity scattering, and in fact it is the phase shift defined by Kubo (Kubo 1965) and numerically evaluated by Doar (1972) for the case when the Fermi level lies between the ground state and the first excited state of the Landau levels. On the other

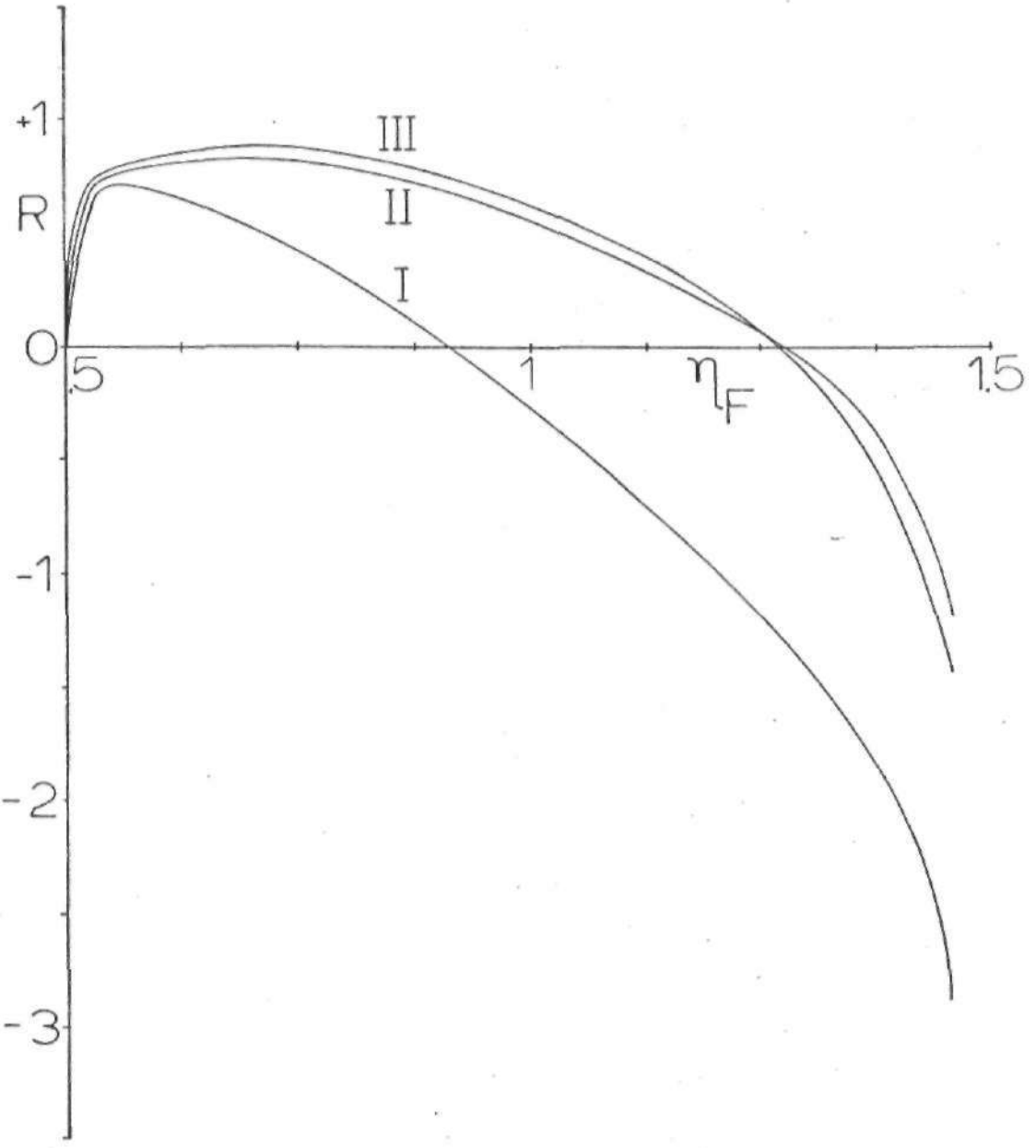


Fig. 11. A plot of the ratio $R = \Delta N_H/\Delta N$ obtained in the non-local Thomas-Fermi potential model as a function of $\eta_F = \varepsilon_F/\hbar\omega_c$ for $P = 1$ and the following values of N_T:

I - $N_T = 30$

II - $N_T = 10$

III - $N_T = 5$.

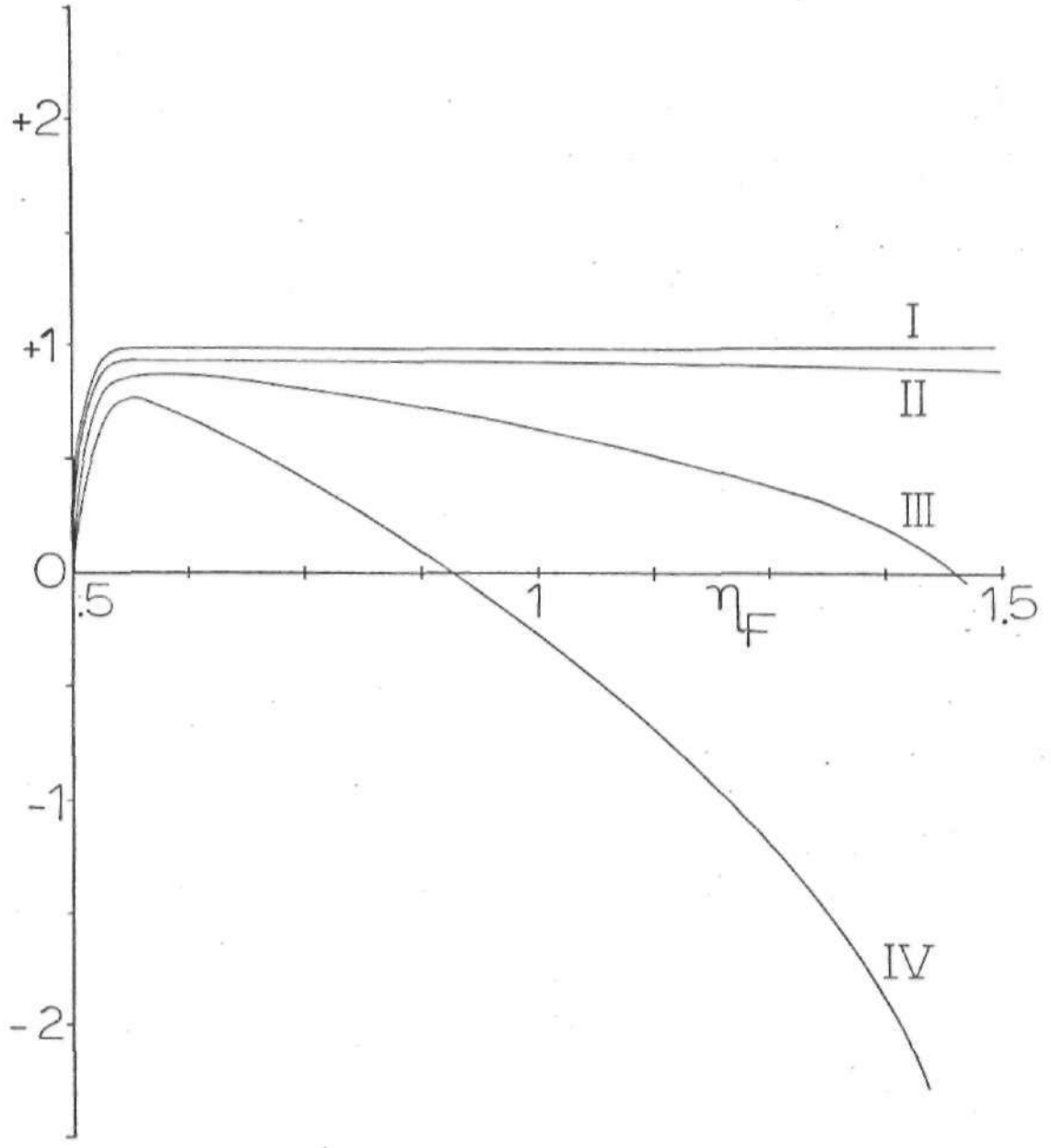


Fig. 12. A plot of the ratio $R = \Delta N_H/\Delta N$ obtained in the non-local Thomas-Fermi potential model as a function of $\eta_F = \varepsilon_F/\hbar\omega_c$ at $N_T = 30$ with the following values of P:

I - P = 10^{-4}

II - P = .1

III - P = .5

IV - P = 1.

hand, the expressions for $\sigma_{xx}(0)$ and $\Delta\sigma_{xy}^{N-L}$ can also be written in terms of this angle, thus facilitating the comparison between these results and those obtained by earlier workers. Eq. VI.27 becomes

$$\sigma_{xx} = n_I \frac{ec}{B} \frac{\sin^2\phi}{\pi} \quad . \qquad \text{VI.36}$$

This is in full agreement with the result of Kubo et al (1965), except that we considered only the m=0 partial waves, we ignored the spin degeneracy in all our calculations, and the Kubo result holds only for $\frac{1}{2} < \eta < 3/2$.

Similarly, the expression for $\Delta\sigma_{xy}^{N-L}$ in Eq. IV.28 can also be written in terms of the angle ϕ as

$$\Delta\sigma_{xy}^{N-L} = n_I \frac{ec}{B} \frac{\sin(2\phi)}{\pi} + \Delta^* \equiv \Delta\sigma_{xy}^{(1)} + \Delta^*, \qquad \text{VI.37}$$

where Δ^* is the second and third terms on the right hand side of Eq. VI.28 and is given by (for n_c=0):

$$\Delta^* = \frac{n_I}{\pi} \frac{ec}{B} (1-g_1)^2 F_R F_I - \frac{2n_I}{\pi} \frac{ec}{B} P^2 (1-g_1)^2 \sqrt{\eta_F - \tfrac{1}{2}} \sum_{n=1}^{\infty} \frac{g_n^2}{n\sqrt{n+\frac{1}{2}-\eta_F}} \quad . \qquad \text{VI.38}$$

This term does not have a simple expression in terms of ϕ, however it is pertinent to point out that it distinguishes our result from that obtained by Nozieres and co-workers (Bastin 1971). This term is due to the dispersive character of the scattering potential and dominates in the case of large P, since it grows with P^2. The dissipative term, $\Delta\sigma_{xy}^{(1)}$, on the contrary saturates at large P; and for small

P, this is the dominant contribution. In such a case, ϕ is small and so

$$\frac{\sin(2\phi)}{2\pi} \rightarrow \frac{\phi}{\pi}$$

$$\Delta\sigma_{xy} \rightarrow n_I \frac{ec}{B} \frac{\phi}{\pi} = -\frac{ec}{B} \Delta N \qquad \text{VI.39}$$

which agrees with the result of semiclassical approximation.

In the case of an attractive potential, one observes a gradual deviation from the semiclassical result as the potential scattering gets stronger. Thus for each value of N_T there is a value of P beyond which the ratio, R, can change sign. This is well displayed in Fig. 13.

It is also worthwhile to consider the materials for which the EQL (Extreme Quantum Limit) can be realized in the laboratory. These materials are all semimetals and their relevant parameters are tabulated in Table 2 along with the values for other materials that are usually of interest in this type of calculation. In Table 2, one observes that bismuth and graphite are the leading candidates for which the condition $\eta_F \tilde{<} 1$ can be most easily realized. The condition that N_T be much greater than one is, however better satisfied in graphite. Fig. 14 compares the ratio $R = \Delta N_H/\Delta N$ for graphite by varying the effective charge ΔZ.

Fig. 13. A plot of the ratio $R = \Delta N_H/\Delta N$ obtained in the case of attractive non-local Thomas-Fermi potential model as a function of $\eta_F = \varepsilon_F/\hbar\omega_c$ at $N_T = 10$ with the following values of P:

I - P = -0.0001

II - P = -0.1

III - P = -0.15

IV - P = -0.2

V - P = -0.5

VI - P = -1.0 .

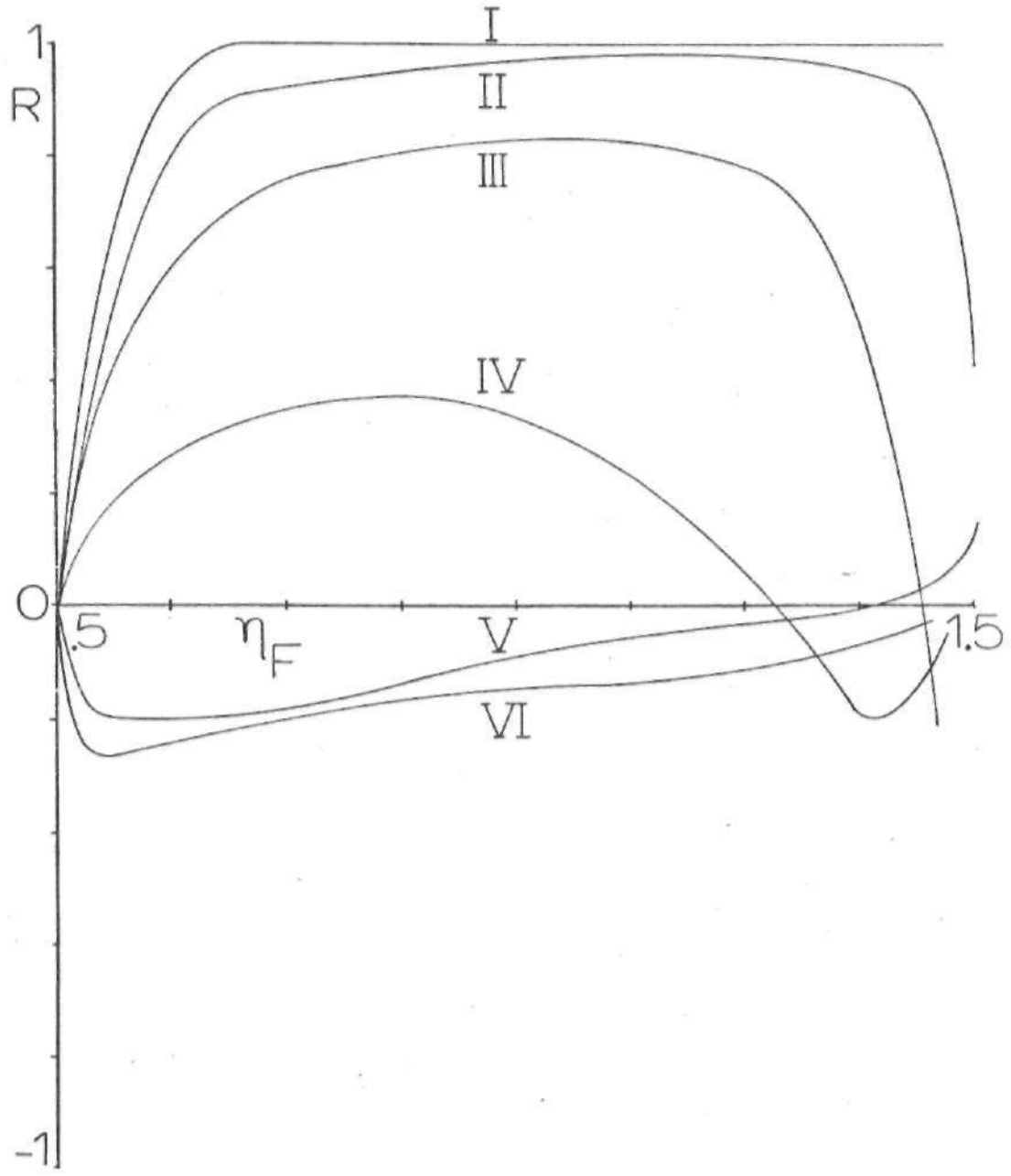


Fig. 13.

Fig. 14. A plot of the ratio $R = \Delta N_H/\Delta N$ obtained for graphite by using the parameters given in Table 2 with the following values of P and ΔZ:

I - P = .063 ; $\Delta Z = 1$

II - P = .32 ; $\Delta Z = 5$

III - P = -.32 ; $\Delta Z = -5$.

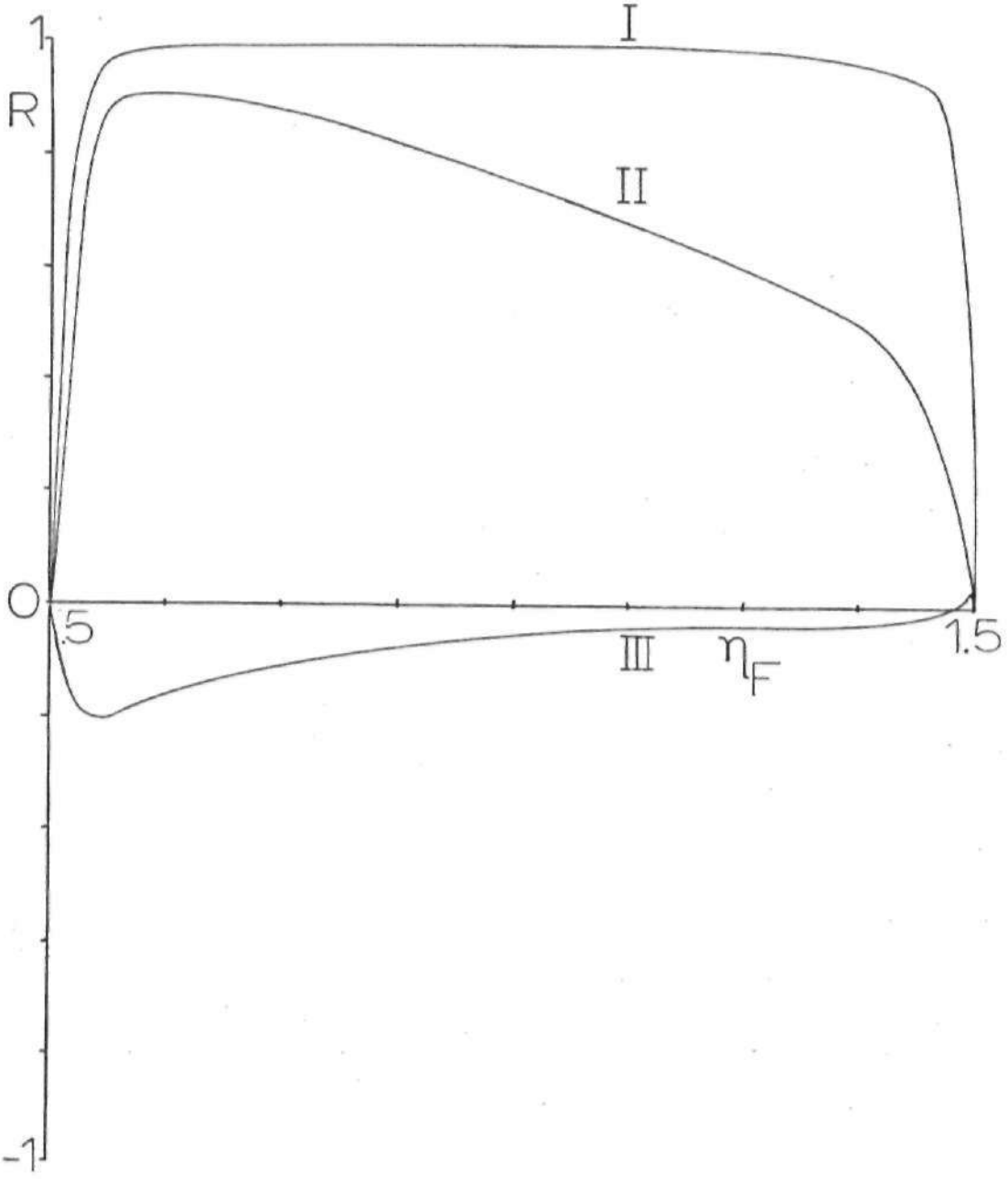


Fig. 14.

TABLE 2. Data used in the calculation.

Material	Carrier	Mz/Me	M^*/Me	ϵ_b	a(Å) (b)	ϵ_F(eV)	η_F	P (i)	N_T (a)
Antimony	Electrons	.080[c]	.320[c]	80[d]	16	.090[c]	194.72	.047	13
Bismuth	Holes	.064[e]	.210[e]	100[f]	93	.012[e]	0.66	.044	3
Graphite	Holes	.050[g]	.670[g]	9[g]	97	.020[g]	0.87	.063	34
PbTe[(h)]	Holes	.015	.012	10	45	.200	2.08	.090	2

The calculated values of η_F, P and N_T correspond to a field value of B = 100 kG. (The field is perpendicular to the crystalline c axis for all.)

(a) Calculated from Eq. IV. 4.

(b) Calculated from Eq. IV. 33.

(c) M. S. Dresselhaus, Proc. Conf. Phys. Semimetals and Narrow-Gap Semiconductors, Dallas, 1970 (Pergamon Press, New York, 1971) 3-39.

(d) C. Nanney, Phys. Rev. 139, 109 (1963).

(e) G. E. Smith, G. A. Baraff, and J. M. Rowell, Phys. Rev. 135A, 1118 (1964).

(f) W. S. Boyle and A. D. Brailsford, Phys. Rev. 120, 1943 (1960).

(g) D. E. Soule, J. W. McClure, and L. B. Smith, Phys. Rev. 134A, 453 (1964).

(h) R. L. Aggarwal, U. Smith, and B. Lax, Proc. IX Intern. Conf. Phys. Semicond., Moscow, 1968 (Nauka, Leningrad, USSR, 1968), Pt. I, 337.

(i) Calculated from Eq. IV. 48.

CHAPTER VII

DISCUSSION

The effect of impurity scattering on the Hall conductivity has been investigated using fairly realistic short-ranged potential models. This is an improvement on the treatment of this problem by previous authors (Bastin 1971, Skobov 1960), who used the Dirac delta function potential model. It is shown in the present work that, starting with a model such as the Thomas-Fermi potential, one can, after a series of systematic approximations, develop a representation in which the t-matrix has an exact form. Most crucial of these approximations is the assumption that the potential is short-ranged, which implies that the amplitude of the wave functions near the impurity will be very small except for the m=0 partial waves. Thus only the m=0 matrix elements of the potential are significant. It turns out, however, that such a simple short-ranged potential can only be non-local. The non-locality of the potential alters the velocity operator which in turn changes the transport properties of the system. The single-site t-matrix obtained in this formulation can also be used in the case of high impurity concentration.

In the dilute impurity regime, we obtained a significant contribution to the Hall conductivity due to impurity scattering. The dispersive term in $\Delta\sigma_{xy}$ given by Eq. VI.28 shows a very strong dependence on the potential strength and it is the dominant contribution in the case of strong scattering. It is this term that distinguishes our

results from those obtained by previous authors (Bastin 1971). Our results for σ_{xx} and $\Delta\sigma_{xy}^{(1)}$ are, however, similar to that of Nozieres and collaborators (Bastin 1971) but are numerically very different. This is partly due to the logical inconsistency in their calculation and also due to the arbitrary cut-off introduced in the summation for F_R. This point can be further elucidated by comparing numerical values that would be obtained in the present scheme for a COD model with the result obtained for a Dirac delta function model using the Skobov (1960) cut-off parameter, in the setting used by Nozieres (1971). Thus at η=.75 and P=1, we have F_R=3.75 using the physically derived N_T=5 in contrast to F_R=1.15 obtained by using the Skobov's arbitrary cut-off parameter, $N_T=n_c+1$. For weak scattering, our result for σ_{xx} is also similar to that obtained by Adams and Holstein (Adams 1959) in their Born approximation treatment of the problem.

In view of all the approximations made to arrive at the major results of this work, it is helpful to test for the self consistency of this model calculation by invoking the Friedel Sum Rule (Friedel 1954). This is a consequence of the fact that the total screening charge must equal the charge screened (Ziman 1960), and the fact that the number of new stationary states created by the introduction of a scattering potential depends on the phase shift. Barnes (1967) derived the Friedel Sum Rule in the quantum limit case for a system having cylindrical symmetry, and it is given by:

$$\Delta Z = \frac{2}{\pi} \sum_{m=0}^{\infty} [\delta_m^s(k_F) + \delta_m^a(k_F)] \quad , \qquad \text{VII.1}$$

where $\delta_m^s(k_F)$ and $\delta_m^a(k_F)$ are respectively the symmetric and antisymmetric phase shift corresponding to the m^{th} partial wave. The 2 on the right hand side accounts for the spin degeneracy. The sum represents the total amount of charge in the screening clouds of electrons, while the ΔZ on the left hand side represents the magnitude of the point charge which is being screened. In our case we consider a short-ranged potential, so that only the δ_o^s is significant. Thus, depending on whether we take into consideration the spin degeneracy or not, we get, for $\Delta Z=1$,

$$\delta_o = \begin{cases} (\pi/2) & \text{, considering spin degeneracy} \\ (\ \pi\ ) & \text{, no spin degeneracy} \end{cases} \qquad \text{VII.2}$$

and correspondingly, for σ_{xx} we have

$$\sigma_{xx} = \begin{cases} n_I(2/\pi) \quad (ec/B), & \text{spin degeneracy} \\ 0 \qquad\qquad\ \ , & \text{no spin degeneracy} \end{cases} \qquad \text{VII.3}$$

and for $\Delta\sigma_{xy}^{(1)}$, we have

$$\Delta\sigma_{xy}^{(1)} = 0, \text{ for either statistics.}$$

The result expressed in Eq. VII.3 is not physically reasonable and are suggestive of the necessity to include other partial waves in order to have a consistent short-ranged potential.

Finally, we have shown that there is a substantial reduction in the semiclassical value for the Hall conductivity, especially in the case of strong attractive potential. Although this is not a conclusive explanation of the magnetic freeze out, it is however, suggestive of some improvements on the results obtained by Fukuyama and collaborators (Shiba 1971) in the case of high impurity concentra-

tion, starting with the improved single-site t-matrix, developed here.

In the future, we shall like to consider the $m \neq 0$ matrix elements of the potential, so that the effect of interference between scattered waves could well be considered. It is also of importance to relax the condition that the potential be short-ranged in the direction of the magnetic field. We also propose to calculate the magnetoconductivity tensor using our new improved Lifshitz separable potential form which mimicks the true potential very closely both along the edges, as well as along the diagonal of the potential matrix. Besides, our development of the single-site t-matrix can also be used in the case of two dimensional electron gas, for which our approximation of the short-range in the direction of the field would even be more valid.

APPENDIX A

DERIVATION OF THE ONE-IMPURITY T-MATRIX IN THE NON-LOCAL POTENTIAL APPROXIMATION

An electron in a magnetic field is being scattered by an impurity located at the same origin as the vector potential. The system can be described by the Hamiltonian H_1 given by

$$H_1 = H_o + V(\vec{r}) \qquad A.1$$

where H_o is again the Hamiltonian of an electron in a magnetic field and without any impurities, and $V(\vec{r}) = V(\rho, |z|)$ is the impurity potential which is assumed to be short-ranged.

The wave function ψ describing the scattering is a solution of the Schroedinger equation

$$H\psi = E\psi \qquad A.2$$

for positive energy ($E > 0$) which at large distances must be a superposition of an incident and scattered waves. This equation does not have a simple solution for any type of scattering potential. Formally, the solution of Eq. A.2 which obeys the aforementioned boundary conditions is given by the - Lippmann-Schwinger equation:

$$\psi^{\pm}_{nmk}(\vec{r}) = \phi_{nmk}(\vec{r}) + \int d\vec{r}\,' G^{o}(\vec{r},\vec{r}\,', E^{\pm}) V(\vec{r}) \psi^{\pm}_{nmk_z}(\vec{r}\,') \qquad A.3$$

where '+' corresponds to incident wave plus outgoing scattered wave and '-' corresponds to incident wave plus incoming scattered wave $\phi_{nmk_z}(\vec{r})$ is the general solution of the unperturbed Schroedinger equation

$$H_o \phi_{nmk}(\vec{r}) = \varepsilon_n(k)\phi_{nmk}(\vec{r}) \qquad A.4$$

and $G^{o}(\vec{r},\vec{r}',E)$ is the unperturbed Green function satisfying the inhomogeneous equation

$$(E-H_o)G^{o}(\vec{r},\vec{r}',E) = \delta(\vec{r}-\vec{r}'). \qquad A.5$$

Explicit expressions for $\varepsilon_n(k)$ and $\phi_{nmk}(\vec{r})$ are given by Eqs. III.6 and III.7. The scattering operator t satisfies the integral equation

$$t = V + VG_o t \qquad A.6$$

and can be represented in the form of an infinite series

$$t = V + VG_oV + VG_oVG_oV + \ldots \qquad A.7$$

Due to the rotational symmetry of the scattering potential, the matrix elements of the potential and consequently those of the scattering operator are diagonal in the azimuthal quantum number m. Hence the matrix elements of the scattering operator t(E) is

$$\langle n,m,k\,|t(E^{+})|n'mk'\rangle = \int \phi^{*}_{nmk}(\vec{r}')V(\vec{r})\psi^{+}_{n'mk'}(\vec{r}')d\vec{r}' \,. \qquad A.8$$

Using an abbreviated notation for the quantum numbers

$\nu \equiv (n,m,k)$

we can rewrite Eq. A.8 as

$$t^{(E^{+})}_{\nu\nu'} = \int \phi^{*}_{\nu}(\vec{r}')V(\vec{r})\psi^{+}_{\nu'}(\vec{r}')d\vec{r}' \qquad A.9$$

which on using the Lippmann-Schwinger equation can be written as

$$t^{(E^{+})}_{\nu\nu_1} = V_{\nu\nu'} + \sum_{\nu_1} \frac{V_{\nu\nu_1}V_{\nu_1\nu'}}{E-\varepsilon_{\nu_1}} + \sum_{\nu_1,\nu_2} \frac{V_{\nu\nu_1}V_{\nu_1\nu_2}V_{\nu_2\nu'}}{(E^{+}-\varepsilon_{\nu_1})(E^{+}-\varepsilon_{\nu_2})} + \ldots \qquad A.10$$

The summation $\sum_{\nu} \equiv \sum_{n,m,k}$ means three summations over the three quantum numbers. $V_{\nu\nu'} \equiv \langle nmk|V|n'mk'\rangle$ is the matrix element of the scattering

potential. Eq. A.9 is an infinite series which in general cannot be summed or written in closed form for any arbitrary potential model. Hence we propose an improved version of the Lifshitz ansatz for which

$$V_{\nu\nu'} = V^{o}_{nn'} = V_o(g_n g_{n'} + f_n f_{n'}) \qquad \text{A.11}$$

defined in Eqs. IV.50-IV.52. In this case, we can solve the integral Eq. A.6 for t. Thus, we have

$$V_{\nu\nu'} + \sum_{\nu''} V_{\nu\nu''} G^{o}_{\nu''} t_{\nu''\nu'} = t_{\nu\nu'} \quad . \qquad \text{A.12}$$

We purpose a solution for $t_{\nu\nu'}$, as

$$t_{\nu\nu'} = a g_\nu g_{\nu'} + b(g_\nu f_{\nu'} + f_\nu g_{\nu'}) + c f_\nu f_{\nu'} \qquad \text{A.13}$$

where a,b,c are arbitrary constants that will be determined from the conditions that this solution obey Eq. A.6. Furthermore, we define

$$V_o \sum_{\nu''} g^2_{\nu''} G^{o}_{\nu''} = F_{11} \qquad \text{A.14}$$

$$V_o \Sigma_{\nu''} g_{\nu''} f_{\nu''} G^{o}_{\nu''} = F_{12} = F_{21} \qquad \text{A.15}$$

and

$$V_o \Sigma_{\nu''} f^2_{\nu''} G^{o}_{\nu''} = F_{22} \quad . \qquad \text{A.16}$$

Substituting Eq. A.12 into A.11 and comparing coefficients of the g's and f's we obtain

$$a = \frac{V_o(1-F_{22})}{D} \qquad \text{A.17}$$

$$b = \frac{V_o F_{12}}{D} \qquad \text{A.18}$$

$$c = \frac{V_o(1-F_{11})}{D} \qquad \text{A.19}$$

where

$$D \equiv (1-F_{11})(1-F_{22})-F_{12}^2 \quad . \tag{A.20}$$

Thus, we finally have for the improved separable potential model

$$t_{\nu\nu'} = \frac{V_o}{[(1-F_{11})(1-F_{22})-F_{12}^2]}[(1-F_{22})g_\nu g_{\nu'} + F_{12}(g_\nu f_{\nu'} + g_{\nu'} f_\nu) +$$

$$+ (1-F_{11})f_\nu f_{\nu'}] \quad . \tag{A.21}$$

In the limit of the f's $\to$ 0, so that F_{12} and F_{22} all go to zero, we obtain the t-matrix for the original formulation of the separable potential model:

$$t_{\nu\nu'} \to \frac{V_o}{1-F_{11}} \; g_n g_{n'} \quad .$$

Thus, in the case of an electron in a magnetic field in the dilute impurity regime, we have

$$t_{\nu\nu'} = g_\nu g_{\nu'} t_o(E) \tag{A.22}$$

where

$$t_o(E^+) = \frac{(\alpha/2\pi)V_o}{1-(\alpha/2\pi)V_o \sum_{n_1} \int dk_1 \frac{g_{n_1}^2}{E^+-\varepsilon_{n_1}(k_1)}} \quad . \tag{A.23}$$

Integrating over k_1 and introducing dimensionless parameters η and P, defined in Chapter VI, Eq. A.12 can be written as

$$t_o(\eta) = \frac{\frac{h^2\sqrt{2\alpha}}{M} P}{1 + P \sum_{n=0}^{\infty} \frac{g_{n_1}^2}{\sqrt{n_1 + \frac{1}{2} - \eta}}} \quad . \qquad \text{A.24}$$

This result, arrived at by using the Lifshitz ansatz, is exact for a Dirac delta function potential model. The problem in such a model arises from the fact that the summation in the denominator diverges and therefore has to be cut-off in a consistent fashion as was carried out in Chapter IV so that for any monotonously decreasing Lifshitz factor, this sum converges and the t-matrix gives a reasonable result free from any unphysical divergency.

APPENDIX B

DERIVATION OF $\Delta\sigma_{xy}(0)$ AND $\sigma_{xx}(0)$ IN THE LOCAL POTENTIAL APPROXIMATION

In Chapter III, we obtained a general expression for the static magnetoconductivity tensor:

$$\sigma_{\alpha\beta}(0) = \frac{ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E)\mathrm{Tr}\left[{}_{\alpha}\mathrm{Im}G(E)v_{\beta} \frac{dG_R}{dE}(E)-v_{\alpha} \frac{dG_A}{dE} v_{\beta}\mathrm{Im}G(E)\right]. \tag{B.1}$$

Substituting for G in terms of the scattering operator, and considering the case of the Hall conductivity, we obtain

$$\sigma_{xy}^{(0)} = \frac{ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E)\mathrm{Tr}\left[v_x \mathrm{Im}G^{o}(E)v_y \frac{dG_R^{o}}{dE}(E)-v_x \frac{dG_A^{o}}{dE} v_y \mathrm{Im}G^{o}(E)\right] \tag{B.2}$$

which is independent of the t-matrix, and

$$\sigma_{xy}^{(1)} = \frac{ie^2\hbar}{\pi} n_I \int_{-\infty}^{\infty} dE\ f(E) \frac{d}{dE} S_{xy}(E) \tag{B.3}$$

which after integrating by parts reduces to

$$\sigma_{xy}^{(1)} = -\frac{ie^2\hbar}{\pi} n_I \int_{-\infty}^{\infty} dE \frac{df}{dE} S_{xy}(E) \tag{B.3a}$$

where

$$S_{xy}(E) = Tr\{v_x \, ImG^o(E) v_y [G^o_R t_R G^o_R] - v_x \, [G^o_A t_A G^o_A] \, v_y \, ImG^o\} \, . \tag{B.4}$$

Here, we note that the integral in Eq. B.3a is simple to evaluate at T = 0, when

$$(-\frac{df}{dE}) = \delta(E - \varepsilon_F).$$

Hence $\sigma^{(1)}_{xy}$ is determined by the value of $S_{xy}(E)$ at the Fermi level, and it is linear in the t-matrix.

Besides $\sigma^{(1)}_{xy}$ there is another term linear in the t-matrix, and it is given by

$$\sigma^{(2)}_{xy} = -\frac{2ie^2\hbar N_I}{\pi} \int_{-\infty}^{\infty} dE \; f(E) ImZ_{xy}(E) \tag{B.5}$$

where

$$Z_{xy}(E) = \mathrm{Tr}\{v_x \frac{dG^o}{dE} \quad v_y[G^o t G^o]\} \quad . \qquad \text{B.6}$$

For the evaluation of these quantities, we make use of the velocity matrix elements given in Eqs. VI.6 and VI.7. Thus, for the unperturbed Hall conductivity, we obtain

$$\sigma_{xy}^{(0)} = -\frac{e^2}{\hbar\alpha} \int_{-\infty}^{\infty} dE\ f(E) \sum_{nmk} \delta(E-\varepsilon_n(k)) \quad . \qquad \text{B.7}$$

Integrating over k and summing over m, we obtain

$$\sigma_{xy}^{(0)} = -\frac{ec}{B} \frac{1}{(2\pi)^2} \sqrt{2M/\hbar^2} \sum_{n=0} \int_{-\infty}^{\infty} dE \ \frac{f(E)}{\sqrt{E-\varepsilon_n}} \qquad \text{B.7a}$$

where $\varepsilon_n = \hbar\omega_c(n+\frac{1}{2})$.

Integrating over E by parts and making use of the fact that at T=0,

$$-\frac{df}{dE} = \delta(E-\varepsilon_F)$$

we finally obtain

$$\sigma_{xy}^{(0)} = -\frac{ec}{B} \frac{(2\alpha)^{3/2}}{(2\pi)^2} \sum_{n=0}^{n_c} \sqrt{\eta_F - n - \tfrac{1}{2}} \qquad \text{B.8}$$

where we have introduced the dimensionless energy parameter at the Fermi level,

$$\eta_F = \frac{\varepsilon_F}{\hbar\omega_c}$$

and n_c is the largest integer for which the radicand in Eq. B.8 is positive.

Thus, we see that Eq. B.8 is nothing but the usual expression for the Hall conductivity:

$$\sigma_{xy}^{(s-c)} = -\frac{ecn_e}{B} \qquad \text{B.9}$$

where n_e is the number of electrons per unit volume.

To evaluate $S_{xy}(E)$ and $Z_{xy}(E)$, it is useful to introduce a creation and destruction operator in terms of v_x and v_y i.e.

$$v^{\pm} = (v_x \pm v_y)\frac{1}{C} \qquad \text{B.10}$$

such that $v^{+}|nmk\rangle = \sqrt{n+1}\ |n+1,m+1,k\rangle$ and B.11

$$v^{-}|nmk\rangle = \sqrt{n}\ |n-1,m-1,k\rangle \qquad \text{B.12}$$

and C is a normalizing constant.

Thus, we have for v_x and v_y:

$$v_x = (v^{+} + v^{-})\frac{c}{2} \qquad \text{B.13}$$

$$v_y = (v^{+} - v^{-})\frac{c}{2i} \ . \qquad \text{B.14}$$

Furthermore, we note that due to the rotational symmetry of the scattering potential and the consequent conservation of the azimuthal quantum number, m,

$$\langle n_1 m_1 k_1|t|n_2 m_2 k_2\rangle = \delta_{m_1 m_2}\langle n_1 m_1 k_1|t|n_2 m_1 k_2\rangle \ . \qquad \text{B.15}$$

Using the cyclic property of the trace, Eq. B.4 can be written as

$$S_{xy}(E) = \mathrm{Tr}\{\mathrm{Im}G^{o}(E)[v_y[G_R^{o}t_R G_R^{o}]v_x - v_x[G_A t_A G_A]v_y]\} \ .$$

In the above expression, we define $Q(E) = G^{o}tG^{o}$, so that on substituting for v_x and v_y in terms of v^{+} and v^{-} we obtain

$$S_{xy}(E) = \frac{c}{2} \mathrm{Tr}\{\mathrm{Im}G_o(E)\,\mathrm{Im}[v^+Qv^+ - v^-Bv^-] + \frac{1}{i}\,\mathrm{Re}[v^+Qv^- - v^-Qv^+]\} \,. \qquad \text{B.17}$$

But from Eq. B.15

$$\langle nmk|Q|n'm'k'\rangle = \delta_{mm'} \langle nmk|Q|n'mk'\rangle$$

and in view of Eqs. B.11 and B.12

$$\mathrm{Tr}\{\mathrm{Im}G_o(E)\,\mathrm{Im}(v^+Qv^+)\} = \mathrm{Tr}\{\mathrm{Im}G_o(E)\,\mathrm{Im}(v^-Qv^-)\} = 0 \qquad \text{B.18}$$

while

$$\mathrm{Tr}\{\mathrm{Im}G_o\mathrm{Re}[v^+Qv^-]\} = -i\pi \sum_{mmk} \delta\,E-\varepsilon_n(k)\;\mathrm{Re} \sum_{\substack{m_1 n_1 k_1 \\ m_2 n_2 k_2}} \delta_{n_1,n-1}\,\delta_{m_1,m-1} \times$$

$$\times\ \delta_{k_1 k}(v^+)^{n,m}_{n-1,m-1}\,Q_{n-1,m-1,k}\,(v^-)^{n-1,m-1}_{n,m}\,\delta_{n_2,n-1}\,\delta_{m_2,m-1}\,\delta_{k_2 k} \qquad \text{B.19}$$

and

$$\mathrm{Tr}\{\mathrm{Im}G_o(E)\mathrm{Re}[v^-Qv^+]\} = -i\pi \sum_{nmk} \delta[E-\varepsilon_n(k)]\mathrm{Re} \sum_{\substack{n_1 m_1 k_1 \\ n_2 m_2 k_2}} \delta_{n_1,n+1}\,\delta_{m_1,m+1} \times$$

$$\times\ \delta_{k_1 k}\,(v^+)^{n,m}_{n+1,m+1}Q_{n+1,m+1,k}(v^-)^{n+1,m+1}_{n,m} \,. \qquad \text{B.20}$$

Hence, we finally have

$$S_{xy}(E) = \frac{\pi}{i\alpha\hbar^2} \sum_{n_1 m_1 k_1} \delta[E-\varepsilon_n(k)]\mathrm{Re}\{(n+1)t_{n+1,m+1,k}(E) - n t_{n-1,m-1,k}(E)\} \qquad \text{B.21}$$

where $t_{n,m,k}(E)$ are the diagonal elements of the t-matrix corresponding to a single impurity located at the origin. Furthermore, we assume that, due to the short-ranged nature of the impurity potential, only $m = 0$

states do contribute and that the t-matrix is independent of k, i.e.

$$t_{n,m,k}(E) = t_n(E) \quad . \qquad \text{B.22}$$

Thus, in the limit of T = 0 and integrating over k, the expression for $\sigma_{xy}^{(1)}$ becomes

$$\sigma_{xy}^{(1)} = \frac{ec}{B} \frac{\alpha n_I}{(2\pi)^2} \sqrt{2M/\hbar^2} \; \mathrm{Re} \sum_{n=0}^{\infty} \left\{ \frac{(n+1)t_{n+1}(\varepsilon_F) - nt_{n-1}(\varepsilon_F)}{\sqrt{\varepsilon_F - \varepsilon_n}} \right\} . \qquad \text{B.23}$$

Similar to the case of $S_{xy}(E)$, we substitute for v_x and v_y in Eq. B.6 in terms of the raising and lowering operators v^+ and v^- and after a simple algebra, we obtain, in the same approximation as was carried out in Eq. B.22

$$\sigma_{xy}^{(2)} = -\frac{n_I e^2}{\pi\hbar\alpha} \left(\frac{\alpha\hbar^2}{M}\right)^2 \int_{-\infty}^{\varepsilon_F} dE \, \mathrm{Im} \sum_{n,k} \left\{ \frac{(n+1)t_{n+1}(E)}{[E-\varepsilon_{n+1}(k)]^2 [E-\varepsilon_n(k)]^2} - \right.$$

$$\left. - \frac{nt_{n-1}}{[E-\varepsilon_n(k)]^2 [E-\varepsilon_{n-1}(k)]^2} \right\} . \qquad \text{B.24}$$

Integrating over k in the above equation and defining

$$Z_n(\eta) \equiv 1/\sqrt{n+\tfrac{1}{2}-\eta} \qquad \text{and} \qquad K_n(\eta) \equiv 1/(n+\tfrac{1}{2}-\eta)^{3/2}$$

we finally obtain

$$\sigma_{xy}^{(2)} = \frac{-n_I}{2\pi} \frac{ec}{B} \int_{-\infty}^{\eta_F} d\eta \, \mathrm{Im} \sum_{n=0}^{\infty} (n+1)[t_{n+1}(\eta) - t_n(\eta)][K_n(\eta) + K_{n+1}(\eta)$$

$$- 4Z_n(\eta) + 4Z_{n+1}(\eta)] \quad . \qquad \text{B.25}$$

The general expression for the diagonal element of the transverse magnetoconductivity tensor, σ_{xx}, is given by

$$\sigma_{xx}(0) = \frac{e^2\hbar}{\pi} \int_{-\infty}^{\infty} dE \, \frac{df}{dE} \, Tr[v_x ImG(E) v_x ImG(E)]. \qquad B.26$$

Here again, we substitute for G in terms of the t-matrix and G_o. In this case, we note that $\sigma_{xx}^{(0)} = 0$; and in the limit of T = 0,

$$\sigma_{xx}(0) = \frac{e^2\hbar}{\pi} Tr[v_x ImG_o \; v_x Im(G_o t G_o)]_{E=\varepsilon_F} . \qquad B.27$$

Substituting for v_x in terms of the raising and lowering operators, given by Eqs. B.13 and B.14, and doing the trace, we obtain

$$\sigma_{xx}^{(1)}(0) = -\frac{ec}{B} \frac{\alpha n_I}{(2\pi)^2} \sqrt{2M/\hbar^2} \; Im \sum_{n=0}^{\infty} \frac{(n+1)t_{n+1}(\varepsilon_F) + n t_{n-1}(\varepsilon_F)}{\sqrt{\varepsilon_F - \varepsilon_n}} . \qquad B.28$$

APPENDIX C

DERIVATION OF $\Delta\sigma_{xy}(0)$ AND $\sigma_{xx}(0)$ IN THE NON-LOCAL POTENTIAL APPROXIMATION

In this case, the velocity operator depends on the scattering potential and consists of a kinematical part $\vec{v}_{H_o}$ and a dynamical part $\vec{v}_V$ i.e.

$$\vec{v} = \vec{v}_{H_o} + \vec{v}_V \equiv \vec{v}_1 + \vec{v}_2 \qquad \text{C.1}$$

where $\vec{v}_1 \equiv \vec{v}_{H_o}$ and $\vec{v}_2 \equiv \vec{v}_V$ and are defined by Eqs. VI.20 and VI.21. The change in the Hall conductivity $\Delta\sigma_{xy}$ can also be written as a sum as was done in Appendix B, except that in this case there are cross terms between the two velocity terms

$$\Delta\sigma_{xy} = \Sigma_{xy}^{(1)} + \Sigma_{xy}^{(2)} + (\Sigma_{xy}^{(0)} - \Sigma_{xy}^{(0)}) \qquad \text{C.2}$$

or

$$\sigma_{xy} - \sigma_{xy}^{(0)} = \frac{ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\, f(E) \{\frac{dS_{xy}}{dE} - 2\, \text{Im}\, Z_{xy}(E) + (\Sigma_{xy}^{(0)} - \sigma_{xy}^{(0)})\}$$

where $\Sigma_{xy}^{(0)}$ is interpreted as a term arising strictly from the unperturbed Green's function but depends on the scattering potential through $\vec{v}_2$, in contradistinction to $\sigma_{xy}^{(0)}$ which is independent of the scattering potential. Similarly, $S_{xy}(E)$ and $Z_{xy}(E)$ have cross-terms between $\vec{v}_1$ and $\vec{v}_2$ and as such more complex than the corresponding expressions in the local potential approximation. Thus we have

$$(\Sigma_{xy}^{(0)} - \sigma_{xy}^{(0)}) = \frac{ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E)\ Tr\{\ v_2^x ImG^o v_2^y\ \frac{dG_R^o}{dE} -$$

$$- v_2^x \frac{dG_A^o}{dE}\ v_2^y\ ImG^o\ \} + \frac{ie^2h}{\pi v} \int_{-\infty}^{\infty} dE\ f(E)\ Tr\ \ x$$

$$x\ \{v_1^x\ ImG^o v_2^y\ \frac{dG_R^o}{dE} - v_1^x\ \frac{dG_A^o}{dE}\ v_2^y\ ImG^o\} +$$

$$+ \frac{ie^2\hbar}{\pi} \int_{-\infty}^{\infty} dE\ f(E) Tr\ \{v_2^x ImG^o v_1^y\ \frac{dG_R^o}{dE} - v_2^x\ \frac{dG_A^o}{dE}\ \ x$$

$$x\ \ v_1^y\ ImG^o\}\ . \qquad C.3$$

We note that this term has both linear and quadratic dependence on the potential strength through the potential dependent velocity operator $\vec{v}_2$. Similarly, we have

$$S_{xy}(E) = Tr\{v_1^x\ ImG^o v_1^y [G_R^o t_R G_R^o] - v_1^x [G_A^o t_A G_A^o]\ v_1^y\ ImG^o\ \} +$$

$$+ Tr\{v_2^x\ ImG^o v_2^y [G_R^o t_R G_R^o] - v_2^x [G_A^o t_A G_A^o]\ v_2^y\ ImG^o\} +$$

$$+ Tr\{v_1^x\ ImG^o v_2^y [G_R^o t_R G_R^o] - v_1^x [G_A^o t_A G_A^o]\ v_2^y\ ImG^o\} +$$

$$+ Tr\{v_2^x\ ImG^o v_1^y [G_R^o t_R G_R^o] - v_2^x [G_A^o t_A G_A^o]\ v_1^y\ ImG^o\} \qquad C.4$$

and

$$Z_{xy}(E) = Tr\{v_1^x\ \frac{dG^o}{dE}\ v_1^y\ [G^o t G^o]\} + Tr\{v_2^x\ \frac{dG^o}{dE}\ v_2^y [G^o t G^o]\} +$$

$$+ Tr\{v_1^x\ \frac{dG^o}{dE}\ \ v_2^y\ [G^o t G^o]\} + Tr\{v_2^x\ \frac{dG^o}{dE}\ v_1^y [G^o t G^o]\}\ .$$

$$C.5$$

Again in this approximation of short-ranged potential, terms in $\Delta\sigma_{xy}$ quadratic in the scattering operator identically vanish.

Using the Lifshitz ansatz as it was developed in Appendix A and the velocity matrix elements for $\vec{v}_1$ and $\vec{v}_2$ given by Eqs. VI.25 and VI.26, each of the terms in Eqs. C.3 to C.5 can be evaluated. By so doing we have

$$(\Sigma_{xy}^{(0)} - \sigma_{xy}^{(0)}) = \frac{4e^2P}{\pi\hbar\alpha} \sum_{n=0}^{n_c} \sqrt{\eta_F - n - \tfrac{1}{2}} \; [(n+1)(g_n^2 - g_{n+1}^2) - n(g_{n-1}^2 - g_n^2)] -$$

$$- \frac{e^2P^2}{\pi\hbar\alpha} \sum_{n=n_c+1}^{\infty} \sum_{n_1=0}^{n_c} \frac{\sqrt{\eta_F - n_1 - \tfrac{1}{2}}}{(n-n_1)\sqrt{n+\tfrac{1}{2}-\eta_F}} \; x$$

$$x \; \{g_n^2 (n_1+1) g_{n_1+1} - g_{n_1})^2 - g_{n_1}^2 (n+1)(g_{n+1} - g_n)^2 +$$

$$+ g_{n_1}^2 n \; (g_{n-1} - g_n)^2 - g_n^2 n_1 (g_{n_1-1} - g_{n_1})^2\} \qquad \text{C.6}$$

$$\Sigma_{xy}^{(1)} = \frac{Pe^2}{\pi\hbar\alpha} (1 + F_R) \sum_{n=0}^{n_c} \frac{\{g_{n+1}^2 (n+1) - n g_{n-1}^2\}}{\sqrt{\eta_F - n - \tfrac{1}{2}}} - \frac{2e^2P}{\pi\hbar\alpha} F_R \; x$$

$$x \sum_{n=0}^{n_c} \frac{\{(n+1) g_n g_{n+1} - g_n g_{n-1}\}}{\sqrt{\eta_F - n - \tfrac{1}{2}}} + \frac{e^2}{\pi\hbar\alpha} - F_I \left[\frac{1+F_R}{(1+F_R)^2 + F_I^2} + \right.$$

$$\left. + (F_R - 1)\right] \qquad \text{C.7}$$

$$\Sigma_{xy}^{(2)} = \frac{e^2}{\pi\hbar\alpha} P \sum_{n=0}^{n_c} \frac{\{(n+1)(g_n^2-g_{n+1}^2)+n(g_{n-1}^2-g_n^2)\}}{\sqrt{\eta_F-n-\frac{1}{2}}} -$$

$$- \frac{4e^2P}{\pi\hbar\alpha} \sum_{n=0}^{n_c} \sqrt{\eta_F-n-\tfrac{1}{2}}\,\{(n+1)(g_n^2-g_{n+1}^2) - n(g_{n-1}^2-g_n^2)\} -$$

$$- \frac{e^2P^2}{\pi\hbar\alpha} \sum_{n=n_c+1}^{\infty} \frac{\{(n+1)(g_n-g_{n+1})^2-n(g_{n-1}-g_n)^2\}}{\sqrt{n+\frac{1}{2}-\eta_F}} \sum^{n_c} \frac{g_{n_1}^2\sqrt{\eta_F-n_1-\frac{1}{2}}}{(n-n_1)}$$

$$- \frac{e^2P^2}{\pi\hbar\alpha} \sum_{n=0}^{n_c} \{(n+1)(g_n-g_{n+1})^2-n(g_{n-1}-g_n)^2\} \sum_{n_1=n_c+1}^{\infty} \frac{g_{n_1}^2\sqrt{\eta_F-n-\frac{1}{2}}}{(n_1-n)\sqrt{n_1+\frac{1}{2}-\eta_F}} .$$

C.8

In these expressions, we have made use of the dimensionless potential strength parameter P defined by Eq. VI.2, the dimensionless Fermi energy given by Eq. VI.3 and also of the real and imaginary parts F_R and F_I of the sum

$$F = P \sum_{n=0}^{\infty} \frac{g_n^2}{\sqrt{n+\frac{1}{2}-\eta}} .$$

So that we finally have for the change in the Hall conductivity

$$\Delta\sigma_{xy} = \frac{e^2}{\pi\hbar\alpha} \frac{F_I(1+F_R)}{(1+F_R)^2+F_I^2} + \frac{e^2}{\pi\hbar\alpha} F_R P \sum_{n=0}^{n_c} \frac{\{(n+1)(g_{n+1}-g_n)^2-n(g_{n-1}-g_n)^2\}}{\sqrt{\eta_F-n-\frac{1}{2}}}$$

$$- \frac{2e^2}{\pi\hbar\alpha} P^2 \sum_{n=0}^{n_c} \sum_{n_1=n_c+1}^{\infty} \Sigma g_{n_1}^2 \{(n+1)(g_n-g_{n+1})^2-n(g_{n-1}-g_n)^2\} \times$$

$$\times \frac{\sqrt{\eta_F-n-\frac{1}{2}}}{(n_1-n)\sqrt{n_1+\frac{1}{2}-\eta}} .$$

C.9

The diagonal of the transverse magnetoconductivity tensor $\sigma_{xx}(0)$ has the same structure here as in the case of local potential approximation except for the cross terms between $\vec{v}_1$ and $\vec{v}_2$, and is given as

$$\sigma_{xx} = \frac{e^2\hbar}{\pi} \mathrm{Tr}\left[(v_1^x+v_2^x)\,\mathrm{Im}G(\varepsilon_F)(v_1^x+v_2^x)\,\mathrm{Im}G(\varepsilon_F)\right] \qquad \text{C.10}$$

$$\sigma_{xx} \quad \frac{e^2\hbar}{\pi} \mathrm{Tr}[v_1^x \mathrm{Im}G v_1^x \mathrm{Im}G] + \frac{e^2\hbar}{\pi} \mathrm{Tr}[v_2^x\ \mathrm{Im}G v_2^x\ \mathrm{Im}G]$$

$$+ \frac{2e^2\hbar}{\pi}\ \mathrm{Tr}\ [v_1^x \mathrm{Im}G v_2^x \mathrm{Im}\ G\ ]\ . \qquad \text{C.11}$$

Expressing the full Green's function in terms of the t-matrix

$$G = G_o + G_o t G_o$$

we can rewrite Eq. C.11 as

$$\sigma_{xx} = \frac{e^2\hbar}{\pi} \mathrm{Tr}[v_1^x \mathrm{Im}G_o v_1^x \mathrm{Im}\ G_o] + \frac{2e^2\hbar}{\pi}\ \mathrm{Tr}[v_1^x \mathrm{Im}G_o v_2^x \mathrm{Im}G_o]\ +$$

$$+ \frac{e^2\hbar}{\pi} \mathrm{Tr}[v_2^x \mathrm{Im}G_o v_2^x \mathrm{Im}G_o] + \frac{2e^2\hbar}{\pi}\ \mathrm{Tr}[v_1^x \mathrm{Im}G_o v_1^x \mathrm{Im}(G_o t G_o)]$$

$$+ \frac{2e^2\hbar}{\pi} \mathrm{Tr}[v_2^x \mathrm{Im}G_o v_2^x \mathrm{Im}(G_o t G_o)]\ + \frac{2e^2\hbar}{\pi} \mathrm{Tr}[v_1^x \mathrm{Im}G_o v_2^x \mathrm{Im}(G_o t G_o)] +$$

$$+ \frac{2e^2\hbar}{\pi}\ \mathrm{Tr}[v_1^x \mathrm{Im}(G_o t G_o) v_2^x \mathrm{Im}G_o]\ . \qquad \text{C.12}$$

Due to the selection rule on the $\vec{v}_1$ and $\vec{v}_2$ imposed by the azimuthal quantum number m the first two terms on the right hand side of Eq. C.12 vanish.

Carrying out the same procedure as was done for $\Delta\sigma_{xy}$, we finally have

$$\sigma_{xx} = \frac{F_I}{(1+F_R)^2+F_I^2} \sum_{n=0}^{n_c} \frac{Pg_n^2(2n+1)}{\sqrt{n_F-n-\frac{1}{2}}} \quad . \qquad \text{C.13}$$

APPENDIX D

NUMERICAL CALCULATION OF THE T-MATRIX AND OTHER RELATED QUANTITIES OF INTEREST

All the quantities of physical interest, i.e. $\Delta\sigma_{xy}$, σ_{xx}, and ΔN - the change in the number of carriers are all expressed in terms of the t-matrix. The t-matrix in turn involves an infinite summation, F defined by

$$F = P \sum_{n=0}^{\infty} \frac{g_n^2}{\sqrt{n+\frac{1}{2}-\eta_F}} = F_R + iF_I \quad . \qquad D.1$$

The real part of F,

$$F_R = P \sum_{n=n_c+1}^{\infty} \frac{g_n^2}{\sqrt{n+\frac{1}{2}-\eta_F}}$$

involves an infinite summation which can be carried out to some finite Landau number, N_B, and the remaining part of the sum is evaluated numerically by using the Euler-Maclaurin's formula. Since there are other infinite sums involved, in the results, it is therefore illustrative to consider a general sum

$$S = \sum_{n=n_c+1}^{\infty} h_n \quad . \qquad D.2$$

This sum is rewritten as

$$S = \sum_{n=n_c+1}^{N_B} h_n + \sum_{n=N_B+1}^{\infty} h_n = \sum_{n=n_c+1}^{N_B} h_n + \sum_{n=1}^{\infty} h_{n+N_B} \qquad D.3$$

where N_B is some large number beyond which the remainder is evaluated by using the Euler-Maclaurin summation formula as a correction.

So that

$$S = A + N \qquad D.4$$

where

$$A = \sum_{n_c+1}^{N_B} h_n \qquad D.5$$

and

$$N = \sum_{n=1}^{\infty} h_{n+N_B} \quad . \qquad D.6$$

Applying this summation formula to Eq. D.6, we have

D.7

$$N = \sum_{n=1}^{\infty} h_{n+N_B} = \int_0^{\infty} h(x+N_B)dx - \tfrac{1}{2}[h(N_B)+h(\infty)] + 1/12[h^1(\infty)-h^1(N_B)] -$$

$$- 1/720[h^{111}(\infty)-h^{111}(N_B)] + 1/30240\ [h^{(v)}(\infty)-h^{(v)}(N_B)] - \ldots$$

But since all the h_n's involved in the present theory are monotonically decreasing functions of n, hence

$$h(\infty) = h^1(\infty) = h^{111}(\infty) = h^{(v)}(\infty) = 0 \qquad D.8$$

and we finally have

$$N = \int_0^{\infty} h(x+N_B)dx - \tfrac{1}{2}h(N_B) - 1/12\ h^1(N_B) + \ldots \qquad D.9$$

Depending on the explicit form of the h_n's and of course on the Lifshitz factor used, the integral in Eq. D.9 can be carried out analytically and the result for N is written into a function subprogram. Actually there are four different types of the h's involved in the whole calculation for arbitrary Lifshitz factor, hence we have four function subprograms, viz. COR1, COR2, COR3, COR4.

Besides the various infinite cummations involved, there is also an integral over η in the expression for $\sigma_{xy}^{(2)}$ given by Eq. VI.12. This integral is carried out by using the subroutine package QSF*. The relationship between variables used in the computer program and those used in the text is:

Program	Text
NT	N_T
NB	N_B
ETA	η
ETAF	η_F
DETA	$d\eta$
ETAFϕ	η_o
ETAMAX	η_{max}
DEL	Δ
SIGMXX	$\sigma_{xx}/(e^2/\hbar\alpha)$
DNP	$\Delta\sigma_{xy}/(e^2/\hbar\alpha) = \Delta N_H$
DNE	ΔN
DREL	R

* IBM, System/360 Scientific Subroutine Package. (IBM, White Plains, New York, 1968) Manual No. H20-0205-3.

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