QUANTUM TRANSPORT THEORY OF SEMICONDUCTORS IN MAGNETIC FIELDS

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1. INTRODUCTION

Several years have passed since the first formula for magnetoconductivity in the transverse configuration was proposed by Titeica [1] on intuitive grounds, but controversy regarding the quantum transport at high magnetic fields still remains. In subsequent years, a rigorous justification of Titeica's method has been given by the development of several quantum-theoretical formalisms [2] in the strict Born approximation (SBA). These works interpret the transverse magnetoresistance in terms of the migration of the centers of the cyclotron orbits and their subsequent scattering by imperfections in solids. A divergence difficulty encountered in these works was removed by the assumed existence of any of the cutoff mechanisms postulated, but no satisfactory explanation of the experimental results has been given in terms of the above theoretical picture. In particular, for acoustic-phonon scattering, the above theories predict a quadratic-in-magnetic-field dependence of the transverse magnetoresistance [2], whereas the experiments tend to indicate an approximate linear behavior at high magnetic fields.

On the other hand, by extending the scattering dynamics beyond the SBA, the results obtained [3,4] in the dressed Born approximation (DBA) are free from divergence difficulty and indicate a linear dependence on magnetic field for acoustic-phonon scattering, in agreement [5] with the experimental results on n-Ge [6]. Arora and co-workers [4] have indicated that the iterative solution of Liouville's equation for the density matrix in DBA has built into it a Breit–Wigner type of collision broadening, which is responsible for the removal of the divergence difficulty. A quantum-limit analysis [7] at high magnetic fields gives a linear-in-magnetic-field dependence of the magnetoresistance for acoustic-phonon scattering which is shown to dominate at sufficiently high fields.

More recently, Barker [8] and Hajdu [9] have attempted to resolve the controversies regarding quantum transport theories in crossed electric and magnetic fields. They indicate that the inclusion of the 'initial-state-correlation' effect produces significant modifications at intermediate and high-field strengths. This effect is equivalent to the interference effect described in detail by Hajdu and Keiter [10]. The conclusions arrived at by Barker [8] and Hajdu [9] are in favor of Titeica's formula [1]. But, unfortunately, as with previous works [2], these conclusions are not supported by the experimental observations on semiconducting materials. Furthermore, no quantum-limit analysis is made to study the magnetic field dependence at high magnetic fields.

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In the light of these conflicts, we review the assumptions and approximations in a magnetotransport theory, both in the SBA and the DBA, by using the more powerful superoperator technique originally used by Mori [11]. In Section 2, we present the solution of the density matrix in the SBA and emphasize the importance of the interference effect. In Section 3, we present the magnetoconductivity in the DBA by extending the scattering dynamics beyond the SBA. The results so arrived at are analyzed in the quantum limit. In the concluding section, we summarize the results and indicate the importance of a still better approximation—the generalized Born approximation (GBA), which is important for low-temperature quantum effects in degenerate semiconductors.

2. STRICT BORN APPROXIMATION

The Hamiltonian of an electron of effective mass m^* interacting with the lattice and externally applied electric field $\mathbf{E}$ in the presence of a magnetic field $\mathbf{B}$ in the z-direction with magnetic potential $\mathbf{A}=(0, Bx, 0)$ is given by:

$$\mathscr{H}=\mathscr{H}_0+\mathscr{H}'(t) \tag{2.1}$$

with

$$\mathscr{H}_0=(p_x^2+(p_y+m^*\omega_c x)^2+p_z^2)/2m^* \tag{2.2}$$

$$\mathscr{H}'(t)=V+F\mathrm{e}^{st}=V+e\mathbf{E}\cdot\mathbf{r}\mathrm{e}^{st},\ s\to 0^+ \tag{2.3}$$

$$\omega_c=eB/m^*c \tag{2.4}$$

where the time factor e^{st} describes the slow development of the system from time $t=-\infty$ when the electric field is applied to the steady state at $t=0$. V is the interaction potential of the electron interacting with various lattice imperfections. The eigenvalue solution of $\mathscr{H}_0$ is well known with eigenfunctions $\varphi_{nk}=|nk\rangle$ and eigenvalues ϵ_{nk} given by [7]

$$|nk\rangle=\exp[i(k_y y+k_z z)]\varphi_n((x-x_k)/\lambda),\quad n=0,\ 1,\ 2\ \ldots \tag{2.5}$$

$$\epsilon_{nk}=(n+\tfrac{1}{2})\hbar\omega_c+\hbar^2 k_z^2/2m^* \tag{2.6}$$

with

$$\lambda=(\hbar/m^*\omega_c)^{1/2} \tag{2.7}$$

$$x_k=-\lambda^2 k_y \tag{2.8}$$

where φ_n is the harmonic oscillator type wavefunction centered at x_k. k stands for (k_y, k_z). The matrix elements of the one-electron current operator $\mathbf{J}_{op}=-e\mathbf{v}_{op}$ are given by

$$\langle n'k'|J_x|nk\rangle=-(i\hbar e/2^{1/2}\lambda m^*)\times\{(n+1)^{1/2}\delta_{n',n+1}-n^{1/2}\delta_{n',n-1}\}\delta_{k'k} \tag{2.9}$$

$$\langle n'k'|J_y|nk\rangle=-(\hbar e/2^{1/2}\lambda m^*)\times\{(n+1)^{1/2}\delta_{n',n+1}+n^{1/2}\delta_{n',n-1}\}\delta_{k'k} \tag{2.10}$$

$$\langle n'k'|J_z|nk\rangle=-(e\hbar k_z/m^*)\delta_{n'n}\delta_{k'k} \tag{2.11}$$

The expectation value of the current J can be found from the statistical mechanics prescription:

$$\mathbf{J}=\mathrm{Tr}(\rho\mathbf{J}_{op})\equiv\sum_{\alpha\alpha'}\langle\alpha|\rho|\alpha'\rangle\langle\alpha'|J_{op}|\alpha\rangle \tag{2.12}$$

where the matrix elements $\langle\alpha|\rho|\alpha'\rangle$ of the density matrix ρ are obtained from the solution of Liouville's equation:

$$i\hbar\partial\rho/\partial t=[\mathscr{H},\rho] \tag{2.13}$$

in the representation of $\mathscr{H}_0(\alpha=nk)$. ρ is assumed to consist of an equilibrium part $\rho_0(\mathscr{H}_0+V)$ and non-equilibrium part ρ':

$$\rho=\rho_0(\mathscr{H}_0+V)+\rho'\mathrm{e}^{st} \tag{2.14}$$

Here the $\rho_0(\mathscr{H}_0+V)$ is chosen for the density matrix instead of $\rho_0(\mathscr{H}_0)$ in the previous work [7], in order to include the initial-state-correlation effect. By substituting Equations (2.1) and (2.14) in Equation (2.13) and defining superoperators denoted by carets as $\hat{A}B\equiv[A,B]$, we have for the formal solution of ρ' a superoperator equation:

$$\rho'=-R_F(s)\,\hat{F}\rho_0(\mathscr{H}_0+V) \tag{2.15}$$

with

$$R_F=(\hat{\mathscr{H}}_0+\hat{V}+\hat{F}-i\hbar s)^{-1} \tag{2.16}$$

$\rho_0(\mathscr{H}_0+V)$ can be expressed in terms of $\rho_0(\mathscr{H}_0)$ by assuming weak perturbation V and following the same procedure as used for F above:

$$\rho_0(\mathscr{H}_0+V)=\rho_0(\mathscr{H}_0)-R(s)\hat{V}\rho_0(\mathscr{H}_0)\quad s\to 0^+ \tag{2.17}$$

with

$$R=(\hat{\mathscr{H}}_0+\hat{V}-i\hbar s)^{-1} \tag{2.18}$$

Both R_F and R can be expanded into a perturbation series by using Dyson's Equation [12]:

$$R_F=R_0-R_0(\hat{V}+\hat{F})R_F \tag{2.19}$$

with

$$R_0=(\hat{\mathscr{H}}_0-i\hbar s)^{-1} \tag{2.20}$$

to give

$$R_F \approx R_0 - R_0(\hat{V}+\hat{F})\,R_0 + R_0(\hat{V}+\hat{F})R_0(\hat{V}+\hat{F})R_0 + \ldots \quad (2.21)$$

$$R \approx R_0 - R_0\hat{V}R_0 + R_0\hat{V}R_0\hat{V}R_0 - \ldots \quad (2.22)$$

In the Ohmic limit and the SBA, we keep terms linear in F and up to second order in V. The linear terms in V drop out in taking the ensemble average over the lattice quantum numbers. In this approximation, the density matrix ρ_{SBA} is given by

$$\rho_{SBA} = \rho_0(\mathscr{H}_0) - R_0\hat{F}\rho_0(\mathscr{H}_0) - R_0\hat{F}R_0\hat{V}R_0\hat{V}\rho_0(\mathscr{H}_0) - R_0\hat{V}R_0\hat{F}R_0\hat{V}\rho_0(\mathscr{H}_0) - R_0\hat{V}R_0\hat{V}R_0\hat{F}\rho_0(\mathscr{H}_0) \quad (2.23)$$

The matrix elements of the first equilibrium term $\rho_0(\mathscr{H}_0)$ are diagonal, diagonal elements being the Fermi–Dirac distribution function $f_\alpha = f(\epsilon_\alpha) = \{\exp[(\epsilon_\alpha - \zeta)/k_B T] + 1\}^{-1}$ where ζ is the Fermi energy:

$$\langle \alpha' | \rho_0(\mathscr{H}_0) | \alpha \rangle = f_{nk}\delta_{n'n}\delta_{k'k} \quad (2.24)$$

The matrix elements of the scattering-independent Hall term $R_0\hat{F}\rho_0$ by using the properties of superoperators [12], are given by

$$\langle \alpha' | R_0\hat{F}\rho_0 | \alpha \rangle = \frac{f_{\alpha'\alpha}}{\epsilon_{\alpha'\alpha}} F_{\alpha'\alpha} \quad (2.25)$$

with

$$f_{\alpha'\alpha} = f_{\alpha'} - f_\alpha, \quad \epsilon_{\alpha'\alpha} = \epsilon_{\alpha'} - \epsilon_\alpha \quad (2.26)$$

and $F_{\alpha'\alpha}$ are the matrix elements of $F = e\mathbf{E}\cdot\mathbf{r}$.

The term $R_0\hat{F}R_0\hat{V}R_0\hat{V}\rho_0(\mathscr{H}_0)$ is due to the change in the chemical potential [10] arising from the initial-state correlations and vanishes when the matrix elements are taken [10]. The matrix elements of the interference term $R_0\hat{V}R_0\hat{F}R_0\hat{V}\rho_0(\mathscr{H}_0)$, where $\hat{F}$ is sandwiched between two V's, for $\mathbf{E}\|\hat{x}$, are given by

$$\langle \alpha' | R_0\hat{V}R_0\hat{F}R_0\hat{V}\rho_0 | \alpha \rangle = \frac{i\pi e E_x}{\epsilon_{\alpha'\alpha}} \sum_\beta \left[(x_\alpha - x_\beta)\frac{df}{d\epsilon_\beta}\delta(\epsilon_{\alpha\beta}) + (x_{\alpha'} - x_\beta)\frac{df}{d\epsilon_\beta}\delta(\epsilon_{\alpha'\beta}) \right] V_{\alpha'\beta}V_{\beta\alpha} + \frac{f_{\alpha'\alpha}}{\epsilon_{\alpha'\alpha}} F_{\alpha'\alpha} i\pi \sum_\beta \left[|V_{\alpha'\beta}|^2\delta(\epsilon_{\beta\alpha}) + |V_{\alpha\beta}|^2\delta(\epsilon_{\beta\alpha'}) \right] \quad (2.27)$$

Here, we have used the properties of superoperators [12] and those of isotropic scattering interactions. The principal part in using the identity

$$\lim_{s\to 0+} (x - is)^{-1} = P(1/x) + i\pi\delta(x) \quad (2.28)$$

vanishes for isotropic scattering interactions in the elastic limit and is negligible for inelastic processes. The first term in Equation (2.27) involves the motion of the centers of the cyclotron orbits, whereas the second involves the motion about the center. The former gives the well-known Titeica formula [13, 14]. However, rigorous quantum transport theories justifying the method of Titeica neglect the latter. The latter term is, in fact, equivalent to the term obtained from expansion up to first order in $(\omega_c\tau)^{-1}$ of the previous results [4]. There is yet another way of writing Equation (2.27). With $\alpha' = (n+1, k)$ and $\alpha = nk$ and using the properties of isotropic scattering interactions [14], Equation (2.27) can be shown to be proportional to

$$\left(\frac{1}{2}\frac{df}{d\epsilon_{nk}}\tau_{nk}^{-1} + \frac{1}{2}\frac{df}{d\epsilon_{(n+1)k}}\tau_{(n+1)k}^{-1} - \frac{f_{(n+1),n}}{\hbar\omega_c}\tau_{nk,(n+1)k}^{-1} \right) \quad (2.29)$$

with

$$\tau_{nk,(n+1)k}^{-1} = \frac{1}{2}\tau_{nk}^{-1} + \frac{1}{2}\tau_{(n+1)k}^{-1} \quad (2.30)$$

$$\tau_{nk}^{-1} = \frac{2\pi}{\hbar}\sum_{n'k'} |\langle nk|V|n'k'\rangle|^2\delta(\epsilon_{nk,n'k'}) \quad (2.31)$$

It is clear from the above expressions that the interference effect vanishes for the classical case of large quantum numbers ($n+1 \approx n$). But for high magnetic fields when electrons populate the Landau levels with low n, this effect is appreciable. If the divergence arising from τ^{-1}, owing to the slowly moving electrons parallel to the magnetic field ($k_z \approx 0$), is removed by using a cutoff mechanism, the magnetoresistance arising from the former is proportional to B^2, whereas that obtained from the latter is proportional to B. In such cases, we can say that the motion about the center of the cyclotron orbit is negligible at high fields, justifying the validity of Titeica formulae which takes into account the motion of the center only.

We are still left with the last term in Equation (2.23) which we arbitrarily call the scattering-transport term. The matrix elements of this term are equal in magnitude but opposite in sign to that of the interference term given by Equation (2.27). The interference term thus has a destructive effect on the scattering-transport term and cancels it exactly, at least in the Ohmic limit and SBA. We thus conclude from the above results that no magnetoconductivity can be obtained in SBA; only the Hall conductivity is

obtained from the Hall term $R_0\hat{F}\rho_0$ in this approximation.

3. DRESSED BORN APPROXIMATION

In Section 2, we have shown that, by including the initial-state correlations, no magnetoconductivity can be obtained in SBA. In fact, considerable simplification could have been obtained if we chose from the beginning:

$$\rho(t) = \rho_0(\mathscr{H}_0) + \rho' e^{st},\ s \to 0^+ \tag{3.1}$$

a procedure which has been objected to by many workers as not being the correct one as it does not include the initial-state correlations. Actually, any choice of ρ_0 is a good choice provided consistent approximations are made. For example, if we choose $\rho_0(\mathscr{H}_0 + F)$, we should be aware of the nondiagonal matrix elements [15] it contains because of the presence of F; these were neglected in the work of Adams and Holstein [13]. It may also be noted that V is nondiagonal, whereas the electronic operators are all diagonal in lattice quantum numbers [4, 1975, p. 2287]. Therefore, $\hat{V}\rho_0(\mathscr{H}_0)$ vanishes identically when the trace over the lattice quantum numbers is taken. In this case the Ohmic-limit solution of the density matrix is

$$\rho = \rho_0(\mathscr{H}_0) - R\hat{F}\rho_0 \tag{3.2}$$

If R is analyzed using the Dyson Equation (2.19) up to second order in V, we have

$$R = R_0 - R_0\hat{V}R_0 + R_0\hat{V}R_0\hat{V}R \tag{3.3}$$

This equation is different from Equation (2.22) as this is exact, involving R at the end instead of R_0. If the trace over the lattice quantum numbers is taken in Equation (3.3), the linear term in V drops out. The resulting equation can be rewritten by using the Dyson Equation in reverse:

$$R = (\mathscr{H}_0 - \sum^{0}(s) - i\hbar s)^{-1} \tag{3.4}$$

with

$$\sum^{0}(s) = \hat{V}R_0\hat{V} \tag{3.5}$$

The same result could be obtained by the diagram method and can be made even more general [12]. We thus see R_0 in the Hall term $R_0\hat{F}\rho_0$ in SBA is now dressed by including $\Sigma^0(s)$ in the denominator, justifying the nomenclature DBA. The matrix elements of ρ obtained [4, 1980] by using the properties of superoperators are

$$\langle\alpha'|\rho|\alpha\rangle = f_\alpha\delta_{\alpha'\alpha} + \frac{\langle\alpha'|\hat{F}\rho_0|\alpha\rangle}{\epsilon_{\alpha'\alpha} - \Gamma^0_{\alpha'\alpha}} \tag{3.6}$$

$$\Gamma^0_{\alpha'\alpha} = i\hbar\,\tau^{-1}_{\alpha'\alpha} \tag{3.7}$$

$$\tau^{-1}_{\alpha'\alpha} = \frac{\pi}{\hbar}\sum_\beta\Big(|V_{\alpha'\beta}|^2\delta(\epsilon_{\beta\alpha}) + |V_{\alpha\beta}|^2\delta(\epsilon_{\beta\alpha'})\Big) - \frac{\pi}{\hbar}\sum_{\beta\beta'}\frac{\langle\beta'|\hat{F}\rho_0|\beta\rangle}{\langle\alpha'|\hat{F}\rho_0|\alpha\rangle}V_{\alpha'\beta}V_{\beta\alpha}\Big(\delta(\epsilon_{\beta\alpha'}) + \delta(\epsilon_{\beta\alpha})\Big) \tag{3.8}$$

The second term in Equation (3.7) vanishes for acoustic-phonon scattering, but makes an important contribution for ionized-impurity scattering. Equation (3.6) has built in it a collision broadening of the Breit–Wigner type in the denominator. This broadening is responsible for removal of the divergence difficulty. By using Equations (3.6) and (2.9)–(2.11) in Equation (2.12), the magnetoconductivity tensor σ defined by $\langle\mathbf{J}\rangle = \sigma\cdot\mathbf{E}$ is obtained as

$$\sigma = \begin{pmatrix} \sigma_1 & -\sigma_2 & 0 \\ \sigma_2 & \sigma_1 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix} \tag{3.9}$$

with

$$\sigma_1 = \frac{e^2}{m^*}\sum_{nks} f_{nk,(n+1)k}(n+1)\frac{\tau^{-1}_{nk,(n+1)k}}{\omega_c^2 + \tau^{-2}_{nk,(n+1)k}} \tag{3.10}$$

$$\sigma_2 = \frac{e^2}{m^*}\sum_{nks} f_{nk,(n+1)k}(n+1)\frac{\omega_c}{\omega_c^2 + \tau^{-2}_{nk,(n+1)k}} \tag{3.11}$$

$$\sigma_3 = -e^2\sum_{nks}(\hbar k_z/m^*)^2\tau_{nk}\frac{df}{d\epsilon_{nk}} \tag{3.12}$$

The expression for σ_3 could have been obtained from the Boltzmann transport equation because of the diagonal nature of the matrix elements for J_z. The above components reduce to those obtained from the Boltzmann transport equation in the low-field limit when $\tau_{nk} = \tau(\epsilon)$, where $\epsilon = \hbar^2k^2/2m^*$ is the classical energy of an electron. In the zero-field limit, σ becomes diagonal with all diagonal components equal to σ_0:

$$\sigma_0 = -\frac{e^2}{3}\sum_k(\hbar k/m^*)^2\frac{df}{d\epsilon}\tau(\epsilon), \tag{3.13}$$

where $k = (k_x, k_y, k_z)$ is the classical wavevector.

In the quantum limit ($\hbar\omega_c \gg k_BT$), only $n = 0$ level can be assumed to be appreciably populated. For acoustic-phonon scattering, the components in the

quantum limit are given by

$$\sigma_1 = \frac{2ne^2\hbar\tau_0^{-1}}{3\pi m^*\omega_c k_B T}\left[\ln\left(\frac{3\pi^{1/2}k_B T}{2\hbar/\tau_0}\right)^2 - \gamma\right] \quad (3.14)$$

$$\sigma_2 = n_e e^2/m^*\omega_c \quad (3.15)$$

$$\sigma_3 = 3n_e e^2\tau_0 k_B T/m^*\hbar\omega_c \quad (3.16)$$

with

$$\tau_0^{-1} = 3(2m^*k_B T)^{3/2}\mathscr{E}_1^2/8\pi^{1/2}\rho_d u^2\hbar^4$$

where $\gamma = 0.577$ is the Euler constant, τ_0 is the zero-field relaxation time, $\mathscr{E}_1$ is the deformation potential constant, ρ_d is the material density, and u the speed of sound. The magnetoresistivity ratios $\rho_{xx}/\rho_0 \approx \sigma_0\sigma_1/\sigma_2^2$ and $\rho_{zz}/\rho_0 = \sigma_0/\sigma_3$ are then given by

$$\rho_{xx}/\rho_0 = \frac{2\hbar\omega_c}{3\pi k_B T}\left[\ln\left(\frac{3\pi^{1/2}k_B T}{\hbar/\tau_0}\right)^2 - \gamma\right] \quad (3.17)$$

$$\rho_{zz}/\rho_0 = \hbar\omega_c/3k_B T \quad (3.18)$$

We thus see that the magnetoresistance, both transverse and longitudinal, is a linear function of the magnetic field, in agreement with actual observations. For ionized-impurity scattering, the magnetoresistance decreases with magnetic field [16]. Thus at high magnetic fields, the acoustic-phonon scattering always dominates.

4. CONCLUSIONS

We have shown that the SBA is not suitable for studying electronic transport at high magnetic fields. On the other hand, the DBA can be successfully used for describing electronic transport at high magnetic fields. In the above analysis, we have used the nondegenerate statistics. If electrons are degenerate, then an electron behaves like a quasi-particle in the field of many scatterers. In this case Γ^0 of Equation (3.7) needs to be dressed further involving the so-called generalized Born approximation (GBA). This GBA is necessary to include collision damping in the correct interpretation of low-temperature quantum effects of the oscillatory type [8, 12]. If the magnetic field is sufficiently high that the lowest Landau level is well above the Fermi level which may still be in the conduction band, a degenerate system will behave like a nondegenerate one. It is expected that in ultra-high magnetic fields, when $\hbar\omega_c \sim \zeta$ for metals, even these will behave like semiconductors. The DBA is thus expected to be a good approximation at high magnetic fields. With the availability of high magnetic fields, it is hoped that the above presentation will be useful for interpreting experimental results in terms of more realistic theoretical models.

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