Superoperator theory of magnetoresistance

Vijay K. Arora and Mohammad A. Al-Mass'ari
Department of Physics, University of Riyadh, P.O. Box 2455, Riyadh, Saudi Arabia
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A theory of Ohmic magnetoresistance is developed using the superoperator technique. This theory is found to be equivalent to that developed earlier when collision broadening is neglected.

The problem of Ohmic galvanomagnetic effects in semiconductors in quantizing magnetic field has been of interest for many years. Several theories (see Refs. 1 and 2 for useful references) have been developed to study the magnetoresistance as a function of magnetic field. A theory using the iterative solution of Liouville's equation for the density matrix was developed by Arora and Miller,[1] which was further elaborated by Arora and Peterson,[2] by extending the scattering dynamics beyond the strict Born approximation. In the "quantum limit" this theory predicted magnetoresistance linear in magnetic field in the regime where electron–acoustic-phonon scattering is considered to be the dominant mechanism of scattering,[3] in conformity with actual observations. Recently, Barker has critically discussed present controversies regarding quantum theories of crossed-field magnetoresistance.[4] He has presented the results of a new superoperator kinetic theory valid for arbitrary field strengths. No explicit functional dependence of the magnetoresistance on magnetic field is indicated in this work. Adams and Holstein's theory,[5] with suitable cutoff, gives a quadratic in magnetic field dependence of magnetoresistance for high magnetic fields, whereas high-field experiments indicate an approximate linear dependence.

Barker's theory includes the initial-state correlations by taking the unperturbed equilibrium density matrix as $\rho_0(H_0+V)$, in contrast to $\rho_0(H_0)$ taken in previous work.[1,2] This was done in previous work[1,2] on the understanding that in the absence of the perturbing electric field, the collisions will not change the distribution of electrons. Any change in ρ_0 due to inclusion of weak-scattering interaction is cancelled by a similar change in the Fermi energy leaving $\rho_0(H_0+V)\approx\rho_0(H_0)$. The electron-lattice interaction V and electron–electric-field interaction F were thus included in the perturbative part of the Hamiltonian and hence treated on the same footing. In steady state, our formalism[1,2] presented a familiar "gain-loss" picture, where the accelerating effect of the electric field was balanced by collision damping. The so-called "interference effect" was also found to be negligible in the development of the above formalism.

The use of superoperators in the theory of magnetoresistance does offer a distinct advantage in the fact that characteristic "gain-loss" relaxive structure associated with nonvanishing vertex corrections is built into formalism in a simple fashion. This gives "collision broadening," which is important in interpreting the low-temperature quantum transport effects of the Shubnikov–de Haas oscillations type and is normally included in a phenomenonlogical way. In the following, we rederive the nonequilibrium density matrix using the superoperator technique, but using essentially the same assumptions as used earlier.[2]

For a system of independent electrons interacting with the lattice in the simultaneous presence of an electric field and a magnetic field with magnetic potential $\vec{A}=(0,Bx,0)$, the electron current is obtained from[2]

$$\langle\vec{J}\rangle = \mathrm{Tr}(\rho\vec{J}_{op}), \tag{1}$$

where ρ is the steady-state solution of Liouville's equation

$$i\hbar\frac{\partial\rho}{\partial t}=[\hat{H}_0+\hat{H}'(t)]\rho\,, \tag{2}$$

where

$$H_0=[\vec{p}+(e/c)\vec{A}]^2/2m^*\,, \tag{3}$$

$$H'=F+V=e\vec{E}\cdot\vec{\gamma}+V\,. \tag{4}$$

Here carets denote the commutator-generating superoperators

$$\hat{A}B\equiv[A,B]\,. \tag{5}$$

All other symbols have the usual meaning.[2]

Assuming the time development of the system from an initial time $t=-\infty$ ($\rho=\rho_0$) to steady state at $t=0$ by switching on the perturbation as

$$H'(t)=H'\exp(\epsilon t/\hbar)\,, \tag{6}$$

we have for the steady-state density matrix ρ_s a solution

$$\rho_s = \rho_0 + \frac{i}{\hbar}\lim_{\epsilon\to 0^+}\int_{-\infty}^{0} dt\,[\hat{H}_0+\hat{H}'(t)]\rho(t)$$
$$= \rho_0 + \frac{i}{\hbar}\lim_{\epsilon\to 0^+}\int_{-\infty}^{0} dt\exp\frac{\epsilon t}{\hbar} \times \exp[-\frac{i}{\hbar}(\hat{H}_0+\hat{H}')t]\hat{H}'\rho_0\,, \quad (7)$$

which can be easily integrated to give

$$\rho_s = \rho_0 + \lim_{\epsilon\to 0^+}(\hat{H}_0+\hat{H}'-i\epsilon)^{-1}\hat{H}'\rho_0\,. \quad (8)$$

The field resolvent superoperator $(\hat{H}_0+\hat{H}'-i\epsilon)^{-1}$ can be expanded into a perturbation series, which can be partially summed by using the proper connected diagram technique[6] with the result

$$(\hat{H}_0+\hat{H}'-i\epsilon)^{-1} \simeq R_p(\epsilon)\,, \quad (9)$$

where

$$R_p(\epsilon) = [\hat{H}_0 - \Sigma(\epsilon) + \hat{F} - i\epsilon]^{-1}\,, \quad (10)$$
$$\Sigma(\epsilon) = [-V + VR_p(\epsilon)V - VR_p(\epsilon)VR_p(\epsilon)V + \cdots]\,. \quad (11)$$

Hence, the steady-state nonequilibrium part ρ' of the density matrix can be written as

$$\rho' \simeq [\hat{H}_0 - \Sigma(\epsilon) + \hat{F} - i\epsilon]^{-1}\hat{H}'\rho_0\,. \quad (12)$$

Equation (11) is a coupled equation in $\Sigma(\epsilon)$. To calculate the matrix elements of ρ', we need some approximations. Firstly, we make the linear approximation (Ohmic limit), and neglect $\hat{F}$ in the denominator of Eqs. (10) and (12). Secondly, we approximate $R_p(\epsilon)$ of Eq. (10) by neglecting $\Sigma(\epsilon)$, so that

$$R_p(\epsilon) \simeq (\hat{H}_0 - i\epsilon)^{-1} \equiv R_p^0(\epsilon)\,, \quad (13)$$
$$\Sigma(\epsilon) \simeq [-V + VR_p^0(\epsilon)V] \equiv \Sigma^0(\epsilon)\,, \quad (14)$$

where we have kept the terms up to second order in scattering interaction, assuming weak scattering. Now, we rewrite Eq. (12) as

$$[\hat{H}_0 - \Sigma^0(\epsilon) - i\epsilon]\rho' = \hat{H}'\rho_0\,, \quad (15)$$

and take the matrix elements. The required matrix elements of ρ' for averaging electronic current operator are diagonal in lattice quantum numbers and so is ρ_0, whereas V is nondiagonal in lattice quantum numbers. Hence, all the linear terms in V will drop out, giving for $\langle\alpha'|\rho'|\alpha\rangle$, where $|\alpha\rangle$ is the electronic state of the Hamiltonian H_0, the coupled equation

$$(\epsilon_{\alpha'\alpha} - i\epsilon)\langle\alpha'|\rho'|\alpha\rangle - \langle\alpha'|VR_p^0(\epsilon)V\rho'|\alpha\rangle = \langle\alpha'|\hat{F}\rho_0|\alpha\rangle\,, \quad (16)$$

with

$$\epsilon_{\alpha'\alpha} = \epsilon_{\alpha'} - \epsilon_\alpha\,, \quad (17)$$
$$\epsilon_\alpha = (n+\tfrac{1}{2})\hbar\omega_c + \hbar^2 k_z^2/2m^*\,. \quad (18)$$

All symbols have usual meaning as in Ref. 2. By using the properties of V, the second coupled term in Eq. (16) is approximated as[7]

$$\langle\alpha'|VR_p^0(\epsilon)V\rho'|\alpha\rangle \simeq \Gamma^{0*}_{\alpha'\alpha}\langle\alpha'|\rho'|\alpha\rangle\,, \quad (19)$$

where

$$\Gamma^{0*}_{\alpha'\alpha} = \lim_{\epsilon\to 0^+}\left[\sum_\beta \frac{|V_{\alpha'\beta}|^2}{\epsilon_\beta - \epsilon_\alpha - i\epsilon} - \sum_{\beta\beta'}\frac{\langle\beta'|\hat{F}\rho_0|\beta\rangle}{\langle\alpha'|\hat{F}\rho_0|\alpha\rangle}\frac{V_{\alpha'\beta'}V_{\beta\alpha}}{\epsilon_{\beta'} - \epsilon_\alpha - i\epsilon} + \sum_\beta \frac{|V_{\beta\alpha}|^2}{\epsilon_{\alpha'} - \epsilon_\beta - i\epsilon} - \sum_{\beta\beta'}\frac{\langle\beta'|\hat{F}\rho_0|\beta\rangle}{\langle\alpha'|\hat{F}\rho_0|\alpha\rangle}\frac{V_{\beta\alpha}V_{\alpha'\beta}}{\epsilon_{\alpha'} - \epsilon_\beta - i\epsilon}\right]. \quad (20)$$

The second and fourth terms in Eq. (20) are the anisotropic terms that vanish for isotropic scattering. $\Gamma^{0*}_{\alpha'\alpha}$ is the lowest-order complex broadening whose real part gives the shift in the unperturbed eigenvalues up to second order in scattering interaction, and the imaginary part gives the Breit-Wigner type of broadening. Equation (16) along with Eq. (19) can be quickly solved to give results identical to those obtained earlier[2,7]:

$$\langle\alpha'|\rho'|\alpha\rangle = \langle\alpha'|\hat{F}\rho_0|\alpha\rangle/(\epsilon_{\alpha'\alpha} - \Gamma^{0*}_{\alpha'\alpha})\,. \quad (21)$$

In conclusion, we have shown above that the more elegant superoperator technique gives essentially our earlier results if the collision broadening is neglected. In contrast, Adam and Holstein[5] take only the first few terms of the perturbative expansion of $R_p(\epsilon)$ given by Eq. (9) which leads to divergent results. This divergence is avoided by resuming the series as in Eq. (10). The detailed comparison with the divergent theories is not possible because the final results are sensitive to the cutoff used. The neglect of collision broadening in approximating $\Sigma(\epsilon) \approx \Sigma^0(\epsilon)$ may be justified at high and intermediate temperatures when $\hbar/\tau \ll k_B T$, but inclusion of this broadening may be necessary for quantum effects at low temperature. These studies will be reported in future communications.

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