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Transfer-matrix method for magneto-conductance of wires in longitudinal fields

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Abstract
We develop a transfer matrix method and calculate the magneto-conductance of a cylindrical wire in a longitudinal magnetic field for a wide range of magnetic fields and phase breaking times. The transfer matrix method is compared with the results of Al'tshuler *et al*, which were obtained by using the perturbation method. Good agreement is found in the limit where the magnetic field is weak and the phase breaking length is much greater than the wire dimensions. Generally, our study shows, in the case of a wire, that perturbation theory works well, and that it only overestimates magneto-conductance a little, or that, in terms of data analysis, the value of the phase breaking time fitted from the measured magneto-conductance using perturbation theory tends to be a slight underestimate. The method developed here is also applicable to the problem of the Aharonov–Bohm effect in a disordered metal ring.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Electrons move in solids as probability waves and, hence, display various interesting interference phenomena. An important phenomenon is backscattering interference between the quantum amplitudes of the clockwise and counterclockwise paths of particle diffusion, in association with the phenomenon of weak localization. This interference has attracted much attention, as it has a drastic effect on the electrical conductance, and can be varied or probed with an external magnetic field, as it changes the time allowed for interference from τ_ϕ (called the phase breaking time or dephasing time) to $(1/\tau_\phi + 1/\tau_B)^{-1}$, where τ_B is the magnetic dephasing time determined by the magnetic flux enclosed in the diffusion path. Extensive study of the magneto-conductance (MC) of disordered systems due to backscattering interference can be traced back to as early as the 1980s and is well documented in the literature [1–3]. For confined disordered systems, in particular, Al'tshuler *et al* [4] developed a perturbation method for weak magnetic fields. Beenakker *et al* [5] extended it to the ballistic regime. Lee *et al* [6] developed a numerical method for films and rectangular wires to cover a wide range of magnetic fields (with the field perpendicular in the case of a wire).

Interest in the magneto-conductance (MC) of films and wires seems to have revived recently, in connection with the issue of the experimental observation of dephasing time saturation, as the temperature drops [7, 8]. This has motivated us to extend the early perturbation-theoretical study of MC for confined systems. In particular, in this work we develop a transfer matrix method to calculate the MC of a cylindrical wire valid for a wide range of longitudinal magnetic fields and τ_ϕ which, to our knowledge, has never been attempted before, regardless of the shape of the wire's cross section. We believe that this extension is important for the analysis of experimental data recorded at relatively strong fields and high temperatures. In section 2, we describe the method. In section 3, we present the results and a discussion. In section 4, we conclude the study.

2. Calculational method

First, we briefly describe the quantum correction, due to backscattering, to the conductivity in a confined disordered

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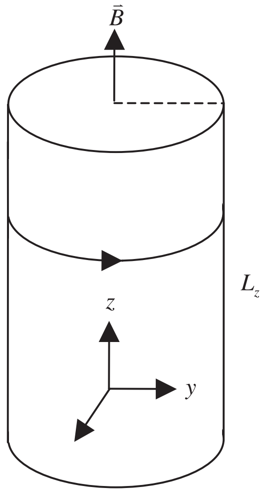

Figure 1. (a) A cylinder wire, with radius $= R$ and length $= L_z$, in an applied magnetic field parallel to the wire. The vector potential $\vec{A}(\vec{r}) = \frac{1}{2}\vec{B}\times\vec{r}$.

system with non-interacting electrons. The correction $\delta\sigma$ is the following [4]:

$$\delta\sigma(\vec{r}) = -\frac{2e^2}{\pi\hbar}D\tau C(\vec{r},\vec{r}), \tag{1}$$

where D is the diffusion coefficient, τ is the elastic scattering time, and the Cooperon $C(\vec{r},\vec{r}')$ obeys the equation

$$\left(L + \frac{1}{\tau_\phi}\right)C(\vec{r},\vec{r}') = \frac{1}{\tau}\delta(\vec{r}-\vec{r}') \tag{2a}$$

where $L \equiv D(\frac{1}{\mathrm{i}}\vec{\nabla} - \frac{2e}{\hbar c}\vec{A}(\vec{r}))^2$, with the boundary condition

$$\left(\frac{\partial}{\partial n} - \frac{\mathrm{i}2e}{\hbar c}\vec{A}(\vec{r})\cdot\hat{n}\right)C(\vec{r},\vec{r}')\Big|_S = 0 \tag{2b}$$

for a confined system. Here, τ_ϕ is the phase breaking time due to, for example, electron–electron or electron–phonon interaction, $\vec{A}(\vec{r})$ is the vector potential of the applied magnetic field, and $\hat{n}$ is the unit normal vector on boundary S of the system. The boundary condition, equation (2b), means that the normal component of diffusion current vanishes at the boundary. Note that $C(\vec{r},\vec{r}')$ is basically a Green's function, and hence can be expanded in terms of eigenfunctions of the auxiliary equation, as follows:

$$C(\vec{r},\vec{r}') = \frac{1}{\tau}\sum_\alpha \frac{\Psi_\alpha(\vec{r})\Psi^*_\alpha(\vec{r}')}{\lambda_\alpha + 1/\tau_\phi} \tag{3}$$

where λ_α and Ψ_α satisfy

$$L\Psi_\alpha(\vec{r}) = \lambda_\alpha\Psi_\alpha(\vec{r}) \tag{4a}$$

with the boundary condition

$$\left(\frac{\partial}{\partial n} - \frac{\mathrm{i}2e}{\hbar c}\vec{A}(\vec{r})\cdot\hat{n}\right)\Psi(\vec{r})\Big|_S = 0. \tag{4b}$$

We consider equations (4a) and (4b) for a cylindrical wire, with radius R, as shown in figure 1. We employ cylindrical coordinates (ρ,ϕ,z), and choose the gauge where the vector potential is

$$\vec{A}(\vec{r}) = \tfrac{1}{2}\vec{B}\times\vec{r} = \tfrac{1}{2}B\rho\hat{\phi}.$$

Then $L = L_0 + L_1 + L_2$, with

$$L_0 = -D\vec{\nabla}^2 = -D\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$L_1 = -D\frac{2eB}{\mathrm{i}\hbar c}\frac{\partial}{\partial\phi} = \mathrm{i}Dl_B^{-2}\frac{\partial}{\partial\phi}, \qquad l_B^{-2} = \frac{2eB}{\hbar c}$$

$$L_2 = D\left(\frac{2eB}{\hbar c}\right)^2\left(\frac{1}{2}B\rho\right)^2 = \frac{1}{4}Dl_B^{-4}\rho^2.$$

Next, we reduce the problem by using the method of separation of variables. Letting

$$\Psi_\alpha(\vec{r}) = \psi(\rho)\mathrm{e}^{\mathrm{i}m\phi}\mathrm{e}^{\mathrm{i}q_z z},$$

then

$$\left[\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\rho\frac{\mathrm{d}}{\mathrm{d}\rho} + k^2 - \frac{m^2}{\rho^2}\right) + l_B^{-2}\left(m - \frac{1}{4}l_B^{-2}\rho^2\right)\right]\psi(\rho) = 0,$$
$$k^2 = \lambda_\alpha/D - q_z^2 \tag{4a'}$$

with the boundary condition

$$\frac{\mathrm{d}}{\mathrm{d}\rho}\psi(\rho)\Big|_{\rho=R} = 0. \tag{4b'}$$

Equations (4a') and (4b') are the reduced equations, with ρ as the only variable now. In the absence of magnetic field, the solution is a Bessel function of the first kind, $\psi(\rho) = J_m(k_{mn}\rho)$, with $k = k_{mn}$ determined by the roots of the function's derivative, i.e.

$$k = k_{mn} = \beta_{mn}/R, \qquad \frac{\mathrm{d}}{\mathrm{d}x}J_m(x)\Big|_{x=\beta_{mn}} = 0.$$

Also, the eigenvalue is $\lambda_\alpha = D(k_{mn}^2 + q_z^2) = D(\beta_{mn}^2/R^2 + q_z^2)$. In the case of finite magnetic fields, however, there are no analytical solutions, and we solve them by using the transfer matrix method discussed below. We first rewrite the equation in terms of the dimensionless variable $\xi = \ln(\rho/R)$ (which maps $\rho\in[0,R] \Rightarrow \xi\in[-\infty,0]$):

$$\left[\left(\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \beta^2e^{2\xi} - m^2\right) + R_B^2e^{2\xi}\left(m - \frac{1}{4}R_B^2e^{2\xi}\right)\right]f(\xi) = 0, \tag{5a}$$

where $\beta \equiv kR$, $R_B \equiv R/l_B$, and $f(\xi) \equiv \psi(\rho(\xi))$. The boundary condition (4b') now becomes

$$\frac{\mathrm{d}f}{\mathrm{d}\xi}\Big|_{\xi=0} = 0. \tag{5b}$$

We also need a boundary condition at $\rho = 0$, i.e. $\xi\to-\infty$,

$$\begin{cases} m = 0, & \frac{\mathrm{d}f}{\mathrm{d}\xi}\Big|_{\xi\to-\infty} = 0 \\ m \neq 0, & f\Big|_{\xi\to-\infty} = 0. \end{cases} \tag{5c}$$

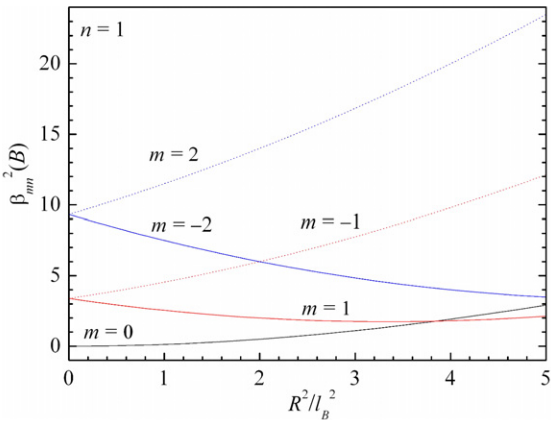

Figure 2. Variation of eigenvalues with magnetic field (since $R^2/l_B^2 \propto B$): $\beta_{mn}^2(B) = (\lambda_{mn}(B)/D - q_z^2)R^2$.

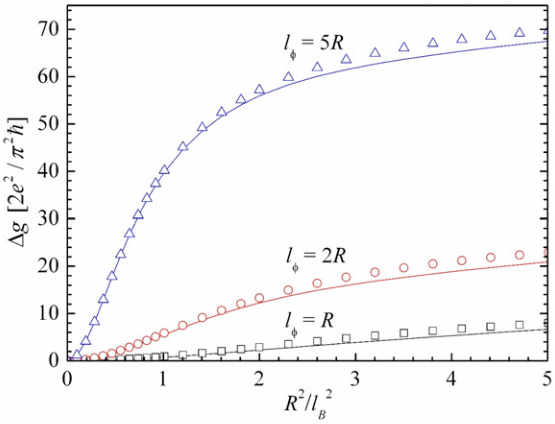

Figure 3. MC of the wire versus $R^2/l_B^2(\propto B)$ for various l_ϕ. Δg is in units of $2e^2/\pi^2\hbar$. Solid curves are obtained by using the transfer matrix method. Triangles, circles, and squares are obtained by using perturbation theory.

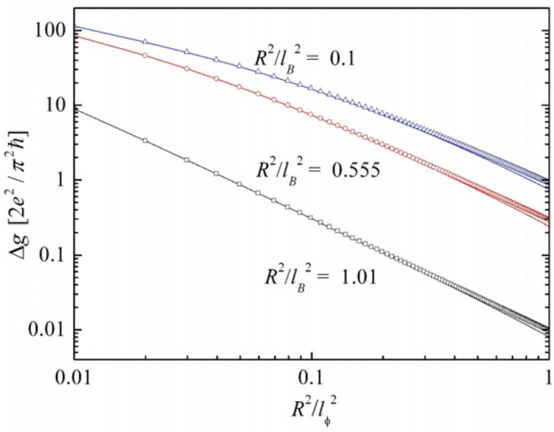

Figure 4. MC of the wire versus R^2/l_ϕ^2 for various l_B. Δg is in units of $2e^2/\pi^2\hbar$. Solid curves are obtained with the transfer matrix method. Triangles, circles, and squares are obtained by using the perturbation theory.

The derivation of equation (5*c*) is discussed in appendix A. Now, equation (5*a*) is analogous to the one-dimensional problem of a particle moving in a potential, and the standard numerical method of the transfer matrix can be employed to solve equations (5*a*)–(5*c*). A brief sketch is provided in appendix B. Note that the method developed here is also suited to the problem of the Aharonov–Bohm effect in a disordered metal ring where the domain $\rho \in [R_1, R_2]$ or $\xi \in [\ln(R_1/\rho), \ln(R_2/\rho)]$ is used, which was previously treated within the perturbation theory [1].

With the auxiliary eigenfunctions and eigenvalues solved, equations (1) and (3) are used to calculate δg, the quantum correction to conductance per unit length, as follows:

$$\delta g = \frac{1}{L_z}\int \delta\sigma(\vec{r})\,\mathrm{d}^3 r$$

$$= -\frac{2e^2}{\pi^2\hbar}\sum_{mn}\frac{R}{\sqrt{\beta_{mn}^2 + (R/l_\phi)^2}}\tan^{-1}\left(\frac{R/l}{\sqrt{\beta_{mn}^2 + (R/l_\phi)^2}}\right),$$

where L_z is the wire length, $l_\phi = \sqrt{D\tau_\phi}$ is the phase breaking length, and $\beta_{mn}^2 = (\lambda_{mn}/D - q_z^2)R^2$ is determined by the eigenvalue obtained. MC is then given by $\Delta g(B) \equiv \delta g(B) - \delta g(0)$. For comparison, the perturbation-theoretical result of Al'tshuler *et al* [4] gives, for weak magnetic fields and $l_\phi \gg R$,

$$\Delta g_{\text{pert}}(B) = \frac{e^2 l_\phi}{\pi\hbar}\left(1 - \frac{1}{\sqrt{1 + \tau_\phi/\tau_{\text{B}}}}\right), \qquad (6)$$

where $\frac{1}{D\tau_{\text{B}}} = \frac{1}{8}\frac{DR^2}{l_B^4}$.

3. Result and discussion

We present numerical results for the wire with $R = 10l$, where l = mean free path. In figure 2, we show the variation of eigenvalues with magnetic field, for various m with $n = 1$. Here, $\beta_{mn}^2(B) = (\lambda_{mn}(B)/D - q_z^2)R^2$ is basically the eigenvalue excluding the contribution from motion in the z-direction and is obtained by using the transfer matrix method.

In figure 3, we show the MC of the wire versus $R^2/l_B^2(\propto B)$ for various l_ϕ, calculated by using both the transfer matrix method and perturbation theory. As expected, the two theories converge at weak magnetic fields, and deviate somewhat from each other with increasing magnetic field. In fact, the perturbation theory slightly overestimates MC, as shown in the figure. For example, the relative differences between the two theories at $R^2/l_B^2 = 5$ are 19.5%, 9.4%, and 3.3% for $l_\phi = R$, $l_\phi = 2R$, and $l_\phi = 5R$, respectively. In terms of data analysis, this means that, with perturbation theory, the value of τ_ϕ fitted using equation (6) from the measured MC tends to be a slight underestimate.

In figure 4, we show the MC of the wire versus R^2/l_ϕ^2 for various l_B, calculated with both the transfer matrix method and perturbation theory. As shown in the figure, the two results converge when R/l_ϕ decreases, and deviate slightly from each other, with the relative difference increasing with R/l_ϕ.

4. Conclusion

We have developed a transfer matrix method to calculate the MC of disordered wires in longitudinal magnetic fields. The method extends the range of study with perturbation theory in this case, allowing a more extensive analysis of experimental data taken at high fields and high temperatures. A comparison of the perturbation-theoretical calculation versus the numerical method developed here shows that perturbation theory works well in general, and that the value of the phase breaking time fitted from the measured MC using perturbation theory tends to be a slight underestimate. The method developed here is also suited to the problem of the Aharonov–Bohm effect in a disordered metal ring.

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Appendix A

We derive equation (5*c*) here. We consider the auxiliary two-dimensional (2D) problem of a confined disc. First, we note, for a confined disc, that when τ_ϕ is short enough such that the phase breaking length is much less than the disc size, then $C(\vec{r} = \vec{r}' = 0)$ is physically expected to approach that of an infinite 2D system, that is, $\ln(\tau_\phi/\tau)$, a finite value. On the other hand, equation (3) expresses $C(\vec{r} = 0, \vec{r}' = 0)$ as a sum over discrete states, since the eigenvalue spectrum as determined in equations (4*a*) and (4*b*) is discrete for a confined disc. In order for the sum to be finite, each term must be finite. So, this requires $|\Psi_\alpha(\vec{r} = 0)|$ in the numerator of each term to be finite.

According to equation (5*a*), when $\xi \to -\infty$, we obtain asymptotically, for $m = 0$,

$$\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} f(\xi) \approx 0 \Rightarrow f(\xi) \approx C_1\xi + C_0.$$

Also, $C_1 = 0$, following the requirement of $|\Psi_\alpha(\vec{r} = 0)|$ to be finite. In other words,

$$\frac{\mathrm{d}}{\mathrm{d}\xi} f(\xi \to -\infty) = 0 \qquad \text{for } m = 0.$$

Similarly, for $m \neq 0$, equation (5*a*) gives asymptotically, when $\xi \to -\infty$,

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} - m^2\right) f(\xi) \approx 0 \Rightarrow f(\xi) \approx C_+\mathrm{e}^{m\xi} + C_-\mathrm{e}^{-m\xi}.$$

The requirement of finite $|\Psi_\alpha(\vec{r} = 0)|$ results in $C_- = 0$, or

$$f(\xi \to -\infty) = 0 \qquad \text{for } m \neq 0.$$

Appendix B

The domain $\xi \in [-\infty, 0]$ is approximated as $\xi \in [-\xi_0, 0]$, where ξ_0 is a large positive number (chosen in such a way that the numerical result stays about the same when ξ_0 is further increased). We divide the interval into N equal segments. In the limit $N \to \infty$, equation (5*a*) is approximated as

$$\left[\left(\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \beta^2\mathrm{e}^{2\xi_i} - m^2\right) + R_B^2\mathrm{e}^{2\xi_i}\left(m - \frac{1}{4}R_B^2\mathrm{e}^{2\xi_i}\right)\right] f^i(\xi) = 0 \tag{B.1}$$

in the ith segment, where $\beta^2 = \beta^2(\lambda_{mn}) = (\lambda_{mn}/D - q_z^2)R^2$ is λ_{mn}-dependent (with λ_{mn} being a given trial value), $f^i(\xi)$ is the solution in the segment, and ξ_i is a representative constant (say, the value at the left endpoint) of the segment. $f^i(\xi)$ consists of two parts, i.e. a right-moving part $\phi^i(\xi)$ and a left-moving part $\tilde{\phi}^i(\xi)$, with

$$f^i(\xi) = \phi^i(\xi) + \tilde{\phi}^i(\xi). \tag{B.2}$$

In the transfer matrix formalism [9, 10], the value $f(-\xi_0)[=\phi^1(-\xi_0) + \tilde{\phi}^1(-\xi_0)]$ at the left endpoint of the domain is linearly related to the value $f(0)[=\phi^N(0) + \tilde{\phi}^N(0)]$ at the right endpoint by the following formula:

$$\boldsymbol{\psi}_R = \mathbf{M}_N\boldsymbol{\psi}_L \tag{B.3}$$

where

$$\boldsymbol{\psi}_L = \begin{pmatrix}\phi^1(-\xi_0)\\ \tilde{\phi}^1(-\xi_0)\end{pmatrix} \equiv \begin{pmatrix}\phi_L\\ \tilde{\phi}_L\end{pmatrix}$$
$$\boldsymbol{\psi}_R = \begin{pmatrix}\phi^N(0)\\ \tilde{\phi}^N(0)\end{pmatrix} \equiv \begin{pmatrix}\phi_R\\ \tilde{\phi}_R\end{pmatrix}.$$

$\mathbf{M}_N$ is the overall transfer matrix, consisting of a sequence of matrices described in the following. We note that the solution vector at the left end of the ith segment, represented as $\boldsymbol{\psi}_i = (\phi^i(\xi_i), \tilde{\phi}^i(\xi_i))^{\mathrm{T}}$, is related to $\boldsymbol{\psi}_{i+1}$ by the following formula:

$$\boldsymbol{\psi}_{i+1} = \mathbf{B}_i\mathbf{C}_i\boldsymbol{\psi}_i.$$

Here, $\mathbf{C}_i$ is the matrix connecting $f^i(\xi)$ at the left endpoint to $f^i(\xi)$ at the right endpoint of the ith segment, and $\mathbf{B}_i$ is the matrix of the boundary condition—continuity of the solution and its derivative across the ith/$(i+1)$th boundary. Explicitly, $\mathbf{M}_N$ is expressed as

$$\mathbf{M}_N = \mathbf{C}_N\mathbf{B}_{N-1}\mathbf{C}_{N-1}\cdots\mathbf{B}_1\mathbf{C}_1.$$

Note that each factor matrix in the product depends on λ_{mn}, and so does M_N.

Last, we impose the boundary condition of equations (5*b*) and (5*c*) on both ends of the domain. At $\xi = -\xi_0$, the vector $\boldsymbol{\psi}_L$ is, for $m = 0$, chosen to be

$$\boldsymbol{\psi}_L = \begin{pmatrix}\phi_L\\ \tilde{\phi}_L\end{pmatrix} = \begin{pmatrix}1\\ 1\end{pmatrix}$$

such that

$$\left.\frac{\mathrm{d}}{\mathrm{d}\xi} f\right|_{\xi=-\xi_0} \propto \phi_L - \tilde{\phi}_L = 0$$

satisfying (5*c*). For $m \neq 0$,

$$\boldsymbol{\psi}_L = \begin{pmatrix}\phi_L\\ \tilde{\phi}_L\end{pmatrix} = \begin{pmatrix}1\\ -1\end{pmatrix}$$

such that

$$f|_{\xi=-\xi_0} \propto \phi_L + \tilde{\phi}_L = 0,$$

as required by (5*c*). ψ_R is then obtained by multiplying $\mathbf{M}_N$ on ψ_L according to equation (B.3). Now, if

$$\frac{d}{d\xi} f(\xi)\bigg|_{\xi=0} \propto \phi_R - \tilde{\phi}_R$$

happens to vanish, then the boundary condition (5*b*) at $\xi = 0$ is also satisfied and the trial value λ_{mn} is accepted as an eigenvalue.

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