Magnetoconductivity of a disordered electron system with N orbitals per site

S. G. Magalhães

Departamento de Matemática, Universidad Federal de Santa Maria, 97119-900 Santa Maria, Rio Grande do Sul, Brazil

Alba Theumann

Instituto de Física, Universidade Federal do Rio Grande do Sul, 91509-900 Porto Alegre, Rio Grande do Sul, Brazil (Received 2 April 1993; revised manuscript received 26 October 1993)

In the absence of a magnetic field, two formally equivalent expressions for the conductivity contribute different sets of Feynman diagrams, due to cancellations. We use this result to calculate the magneto-conductivity of the N-orbital model to O(1/N) and we show that it coincides with the result for a single-level system.

The purpose in this paper is to investigate the magnetoconductivity of Wegner's N-orbital model^{1,2} to order 1/N by means of the method proposed formerly by us;³ one that avoids the semiclassical approximation in favor of a formulation based on Landau levels. The first question we have to answer is, then, which are all the diagrams that contribute to the conductivity to order 1/N? To our surprise, we discovered that it depends on the choice between two equivalent expressions for the electrical conductivity: If the Einstein relations are used to relate the conductivity to the diffusion propagator,⁴ as was done in Ref. 2, then a certain series of diagrams are shown to contribute, but if instead the standard expression in Ref. 5 is used the family of contributing diagrams is highly reduced because many of them actually vanish, and the calculation is simplified. We show, in fact, that the magnetoconductivity of the model, to order 1/N, is given by the same expression obtained in Ref. 3 for a single-level system.

The N-orbital electron model proposed by Wegner¹ is generalized to include a constant magnetic field B in the z direction and it is described by the Hamiltonian:

$$H = -\frac{1}{2} \sum_{\alpha=1}^{N} \int d\mathbf{r} \, \psi_{\alpha}^{\dagger}(\mathbf{r}) \mathbf{D}_{r}^{2} \psi_{\alpha}(\mathbf{r})$$

$$+ \sum_{\alpha,\beta=1}^{N} \int d\mathbf{r} \, \psi_{\alpha}^{\dagger}(\mathbf{r}) \frac{1}{\sqrt{N}} V_{\alpha\beta}(\mathbf{r}) \psi_{\beta}(\mathbf{r}) , \qquad (1)$$

where we only considered the case of diagonal disorder and ψ_{α}^{\dagger} , ψ_{α} are the standard electron creation and destruction operators in the α orbital, $\alpha = 1...N$. We work in units in which $\hbar = c = 1$. The on-site random potential $V_{\alpha\beta}(\mathbf{r})$ scatters electrons among different orbitals, with mean and variance given by

$$\langle V_{\alpha\beta}(\mathbf{r})\rangle = 0$$
, (2)

$$\langle V_{\alpha\beta}(\mathbf{r})V_{\gamma\delta}(\mathbf{r}')\rangle = \delta(\mathbf{r} - \mathbf{r}')[M\delta_{\alpha\delta}\delta_{\beta\gamma} + M'\delta_{\alpha\gamma}\delta_{\beta\delta}],$$
 (3)

while

$$\mathbf{D}_r = \nabla_r - ie \; \mathbf{A}_0(\mathbf{r}) \; , \tag{4}$$

and $A_0(r)$ is the vector potential in the Landau gauge:

$$\mathbf{A}_0(\mathbf{r}) = (-By, 0, 0)$$
 (5)

Before proceeding to the calculation of the magnetoconductivity we are going to discuss the relevant contributions to the dc conductivity in the absence of a magnetic field, when A_0 vanishes in Eq. (4). In this way we may use translational invariance and Fourier transformation as powerful tools in the analysis of the contributing diagrams.

The diagrammatic expansion for the averaged one-particle Green function in powers of 1/N shows that $G_{\alpha\alpha} = O(1)$, with the leading contributions for the self-energy shown in Fig. 1(b), while $G_{\alpha\beta}$ for $\alpha \neq \beta$ is O(1/N). The contributions to the self-energy of the type shown in Fig. 1(b) have an independent summation over the orbital indices β and γ for each 1/N factor, while the crossed diagrams in Fig. 1(c) are O(1/N) due to the presence of δ functions that suppress some of the internal summations. To leading order, then, it is sufficient to consider the diagonal $G_{\alpha\alpha}$ with the self-energy given by the family of irreducible diagrams shown in Fig. 1(b).

A second important quantity in this theory is the configuration averaged product of two Green's functions:

$$\Pi_{\alpha\beta\beta\alpha}(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},\mathbf{r}_{4};\omega,\epsilon) = \langle G_{\alpha\beta}(\mathbf{r}_{1},\mathbf{r}_{2},\omega+\epsilon) \times G_{\beta\alpha}(\mathbf{r}_{3},\mathbf{r}_{4},\epsilon) \rangle_{C,A}, \qquad (6)$$

and some contributing diagrams are shown in Fig. 2. After summing over β , the contributions of diagrams in Figs. 2(a)-2(c) are O(1/N).

As it was shown in Ref. 5, linear-response theory may be used to derive the standard expression for the conductivity:

$$\sigma(\omega) = \lim_{\alpha \to 0} \frac{2e^2}{m} \frac{1}{\omega} \int_{-\omega}^{0} d\epsilon P(\mathbf{q}, \omega + \epsilon + i\delta, \epsilon - i\delta) , \qquad (7)$$

where in d dimensions and in momentum space

$$P(\mathbf{q},\omega+\epsilon+i\delta,\epsilon-i\delta)$$

$$= \frac{1}{d} \int \mathbf{p} \cdot \mathbf{p}' \sum_{\alpha,\beta} \Pi_{\alpha\beta\beta\alpha}(\mathbf{p},\mathbf{p}',\mathbf{q},\omega,\epsilon) d\mathbf{p} d\mathbf{p}' . \tag{8}$$

The function $P(\mathbf{q}, \omega + \epsilon + i\delta, \epsilon - i\delta)$ in Eq. (8) is related through analytical continuation to the retarded current-current correlation function:⁴

49

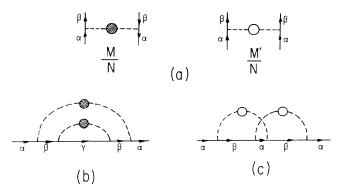


FIG. 1. (a) Diagrammatic representation of the average in Eq. (3). To the full and open dots correspond the factors M/N and M'/N, respectively. (b) and (c) contributions to the self-energy O(1) and O(1/N), respectively.

$$P^{R}(\mathbf{q},\omega) = \frac{1}{q^{2}} \sum_{\mu,\nu} q_{\mu} q_{\nu} \langle [j_{\mu}(\mathbf{q}), j_{\nu}(-\mathbf{q})] \rangle_{\omega}^{R} . \tag{9}$$

On the other hand, an equivalent formal expression for the conductivity may be derived by using Einstein relation with the diffusion propagator. Following closely the method in Ref. 4 we can prove the exact relation:

$$P(q=0,\epsilon+i\delta,\epsilon-i\delta)$$

$$= \lim_{\omega \to 0} \lim_{q \to 0} \frac{\omega^2}{2\pi} \frac{1}{q^2} \left\{ K(\mathbf{q}, \omega + \epsilon + i\delta, \epsilon - i\delta) - 2\pi i \frac{\rho(\epsilon)}{\omega} \right\}, \tag{10}$$

where the function K is given by

$$K(\mathbf{q},\omega+\epsilon+i\delta,\epsilon-i\delta) = \int d\mathbf{p} d\mathbf{p}' \sum_{\alpha,\beta} \Pi_{\alpha\beta\beta\alpha}(\mathbf{p},\mathbf{p}',q,\omega,\epsilon)$$
(11

and it is related through analytical continuation to the retarded density-density correlation function:

$$K^{R}(\mathbf{q},\omega) = \langle [\rho(\mathbf{q}), \rho(-\mathbf{q})] \rangle_{\omega}^{R}. \tag{12}$$

The function $\Pi_{\alpha\beta\beta\alpha}$ in Eq. (11) is the same that appears in Eq. (8) and was defined in Eq. (6). Conservation of particle number implies that⁴

$$K(0,\omega + \epsilon + i\delta, \epsilon - i\delta) = \frac{2\pi i \rho(\epsilon)}{\omega} . \tag{13}$$

By introducing Eqs. (13) and (10) into Eq. (7) we get the alternative expression for the conductivity:

$$\sigma(\omega) = \frac{e^2}{\pi m} \omega \int_{-\omega}^{0} d\epsilon \left[\frac{\partial}{\partial q^2} K(\mathbf{q}, \omega + \epsilon + i\delta, \epsilon - i\delta) \right]_{q=0}.$$
(14)

It is precisely Eq. (14) that has been used to calculate the conductivity of the N-orbital model to O(1/N) in Refs. 1, 2, and 6. The standard procedure to follow in order to obtain $\sigma(\omega)$ to O(1/N) is then to calculate all the contributions to $\Pi_{\alpha\beta\beta\alpha}$ in Fig. 2 to this order and to introduce the result either in Eq. (7) or in (14). However, the important point we want to stress here is that although both expressions are formally equivalent, due to the angular integration in Eq. (8), the contribution of many dia-

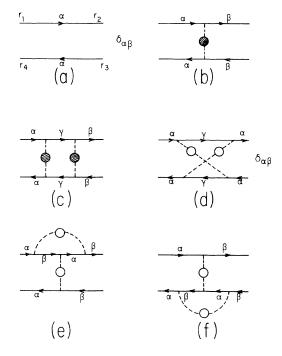


FIG. 2. Some diagrams contributing to $\Pi_{\alpha\beta\beta\alpha}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4,\omega,\epsilon)$. (a)-(c) are O(1) while (d)-(f) are O(1/N).

grams to $P(\mathbf{q},\omega+\epsilon,\epsilon)$ actually vanish for a contact potential, while the same diagrams will give a nonvanishing contribution to $K(\mathbf{q},\omega+\epsilon,\epsilon)$ in Eq. (11). It has been shown in Ref. 2 and Ref. 6 that all the contributions to $\Pi_{\alpha\beta\beta\alpha}(\mathbf{p},\mathbf{p}',\mathbf{q},\omega,\epsilon)$ of O(1) are those shown in Fig. 3, with the blocks representing the infinite partial sums of diagrams indicated in Fig. 4. However, many of these diagrams, although they are of O(1/N), will give a vanishing contribution due to the integration of two Green functions on the same side of the Fermi surface. For instance, the second diagram in Fig. 4(c) will have an internal integration:

$$\int d\mathbf{p}_1 G_{\gamma\gamma}(\mathbf{p}_1, \omega + \epsilon) G_{\gamma\gamma}(\mathbf{Q} - \mathbf{p}_1, \omega + \epsilon) \approx 0$$
 (15)

within the approximation of the constant density of states at the Fermi surface, and for the same reason all diagrams in Fig. 4(c) with more than one line crossing above the multiply crossed subdiagram will vanish. The same argument is of course valid for diagrams with lines that cross below, like in Figs. 3(g) and 3(h). By taking these considerations into account, we conclude that the relevant diagrams for the calculation of the conductivity are those in Fig. 5. The meaning of the crosses at the ends of the diagrams depend on whether we use Eq. (7) or (14) for the calculation of the conductivity. In the following we consider M = M'. For further use in our discussion, we need the momentum dependence of the ladder propagator in Fig. 4(a) and following standard procedures:

$$\Gamma_L(\mathbf{p}, \mathbf{p}', \mathbf{q}) \approx \frac{M}{\tau} \frac{1}{D_0 q^2 + i\omega}$$
, (16)

while the Cooperon or sum of maximally crossed diagrams in Fig. 4(b) gives

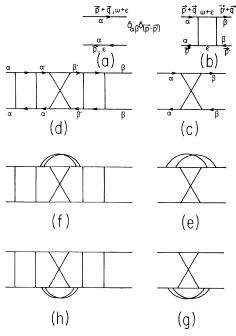


FIG. 3. Complete family of diagrams that contribute to the Fourier transformed $\Pi_{\alpha\beta\beta\alpha}(\mathbf{p},\mathbf{p}',\mathbf{q},\omega,\epsilon)$. The meaning of different blocks is indicated in Fig. 4.

$$\Gamma_C(\mathbf{p}, \mathbf{p}', \mathbf{q}) \approx \frac{M}{\tau} \frac{1}{D_0 |\mathbf{p} + \mathbf{p}' + \mathbf{q}|^2 + i\omega}$$
, (17)

where $D_0 = \kappa_F^2 \tau / d$ is the diffusion constant in d dimensions.

When we want to calculate $\sigma(\omega)$ by using Eq. (7), the "crosses" at the extreme of the diagrams in Fig. 5 indicate the internal product $\mathbf{p} \cdot \mathbf{p}'$ in Eq. (8). With the help of Eqs. (16) and (17) it is easy to check that the diagrams (b), and (d)-(h) in Fig. 5 give a vanishing contribution to $P(0,\omega+\epsilon+i\delta,\epsilon-i\delta)$ in Eq. (8) due to the angular integral over the angle between p and p'. The diagram in Fig. 5(a), however, gives the known Drude contribution due to the δ -function term, and Fig. 5(c) gives a finite contribution because, from Eq. (17), the singularity in the Cooperon for p and p' antiparallel may be approximated by a $\delta(p+p')$ factor that will also cancel the angular integration. We conclude that when the conductivity is calculated with the formula in Eq. (7), in the case of a contact potential, the only contributing diagrams are those in Figs. 5(a) and 5(c) of O(1) and O(1/N), respectively.

When the dc conductivity is given by Eq. (14) the diagrams in Fig. 5 represent the contributions of O(1) and O(1/N) to the function $K(0,\omega+\epsilon+i\delta,\epsilon-i\delta)$ in Eq. (11), provided the "crosses" are replaced by unity. We do not have an angular factor from $\mathbf{p}\cdot\mathbf{p}'$ and all diagrams contribute to the calculation, as has been shown in Refs. 2 and 6.

When the magnetic field is switched on, the calculation of diagrams becomes very difficult because of the lack of translational invariance and momentum conservation. However, under the assumption that the presence of a weak external magnetic field does not introduce new

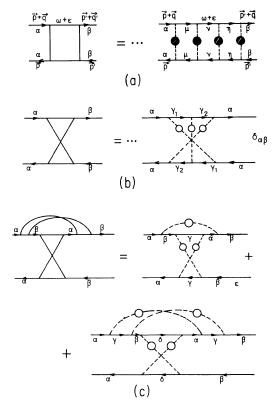


FIG. 4. Infinite partial sum of diagrams contributing to $\Pi_{\alpha\beta\beta\alpha}$ in Fig. 4. (a) is O(1) while the others are O(1/N).

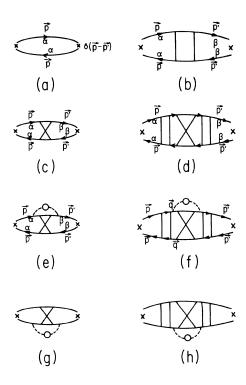


FIG. 5. Diagrams for the conductivity, with the notation of Figs. 3 and 4. (a) and (b) are O(1), all the others are O(1/N).

singularities, we argue that the arguments following Eq. (17) are still valid. This is plausible because the diagrams (c) to (h) in Fig. 3 exhibit a diffusion pole originating in the maximally crossed subdiagrams, and it is this singularity responsible for the nonanalytic behavior of the magnetoconductivity. The diagrams (d)–(h) can be obtained by "decorating" diagram (c) with ladders and they will not present new singularities. Given that they give a vanishing contribution at zero field, we argue that they give a small correction $O((\omega_c \tau)^2)$ to the leading diagram (c), where for weak fields $\omega_c \tau \ll 1$. Hence the magnetoconductivity tensor would be given to O(1/N) by the two diagrams in Figs. 5(a) and 5(c) if the calculation is performed with the analog of Eq. (7) in real space:⁵

$$(0)$$

$$(0)$$

$$(0)$$

$$(0)$$

$$(0)$$

$$(0)$$

$$(0)$$

$$(0)$$

$$(0)$$

FIG. 6. (a) and (b) are the only contributing diagrams to the magnetoconductivity to O(1) and O(1/N), respectively, when it is used Eq. (18). The differential operator is explicit in (c).

$$\sigma_{\mu\nu}(\omega) = \frac{2e^2}{m} \frac{1}{\omega} \int_{-\omega}^{0} d\epsilon \int d(\mathbf{r} - \mathbf{r}') P_{\mu\nu}(\mathbf{r} - \mathbf{r}', \omega + \epsilon + i\delta, \epsilon - i\delta) , \qquad (18)$$

where μ, ν indicate space directions and

$$P_{\mu\nu}(\mathbf{r}-\mathbf{r}',\omega+\epsilon+i\delta;\epsilon-i\delta) = \left\{ [D^{\mu}_{\rho}-D^{\mu*}_{r}][D^{\nu}_{\rho'}-D^{\nu*}_{r'}] \sum_{\alpha\beta} \Pi_{\alpha\beta\beta\alpha}(\mathbf{r},\mathbf{r}',\boldsymbol{\rho},\boldsymbol{\rho}';\epsilon,\omega) \right\}_{\substack{\rho=\mathbf{r}\\ \rho'=\mathbf{r}'}}.$$
 (19)

According to our conclusions above, the function $\Pi_{\alpha\beta\beta\alpha}(\mathbf{r},\mathbf{r}',\boldsymbol{\rho},\boldsymbol{\rho}';\epsilon,\omega)$ was defined in Eq. (6) and the only relevant contributions are those in Fig. 6, where (a) is O(1) and (b) is O(1/N). The explicit calculation of the contribution of these two terms to the magnetoconductivity was already performed by us in three dimensions (3D) and reported in Ref. 6. In this case the single-particle Green's function in Fig. 6 stands for

$$G_{\alpha\alpha}(\mathbf{r},\mathbf{r}',\epsilon) = \sum_{|\lambda|} \Psi_{\alpha}^{*}(\lambda,\mathbf{r})\Psi_{\alpha}(\lambda,\mathbf{r}') \left[\omega_{c} \left[n + \frac{1}{2} \right] + \frac{1}{2} \kappa_{z}^{2} - \epsilon_{F} - \epsilon - \frac{i}{2\tau} \operatorname{sgn}\epsilon \right]^{-1}, \tag{20}$$

where $\{\lambda\} = (n, \kappa_x, \kappa_z)$ indicates the set of Landau quantum numbers while $\Psi_\alpha(\lambda, \mathbf{r})$ is the wave function of an electron in level α , in a magnetic field. We indicate by $\omega_c = eB/m$ the cyclotron frequency and the inverse lifetime is given to O(1) by the imaginary part of the self-energy in Fig. 1(a).

We just quote the result for the 3D magnetoconductivity.

$$\sigma(\omega_c) - \sigma(0) \approx \frac{e^2 M}{\pi^4} \left[\pi 2^{-3/4} (\omega_c D_0 \tau)^{1/2} + O((\omega_c \tau)^2) \right] . \tag{21}$$

The main result of this paper is the observation that, in

the absence of a magnetic field, two formally equivalent expressions for the conductivity in Eqs. (7) and (14) contribute significantly different sets of Feynman diagrams due to cancellations. Hence all the relevant contribution to O(1) and O(1/N) are only those generally considered as responsible for the weak localization effect. Under the assumption that this property still holds in the presence of weak magnetic fields, we conclude that to the same order in 1/N the magnetoconductivity of the model in 3D is as calculated previously by us in Ref. 3.

This work was supported by Fianciadora de Estudos e Projetos (FINEP) and Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

¹F. J. Wegner, Phys. Rev. B 19, 783 (1979).

²R. Oppermann and F. Wegner, Z. Phys. B **34**, 327 (1979).

³A. Theumann and S. G. Magalhães, Phys. Rev. B **39**, 5798 (1989).

⁴S. V. Maleev and B. P. Toperverg, Zh. Eksp. Teor. Fiz. **69**, 1440 (1975) [Sov. Phys. JETP **42**, 734 (1976)].

⁵A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinsky, Methods of Quantum Field Theory in Statistical Physics (Prentice Hall, Englewood Cliffs, New Jersey, 1963).

⁶E. Fradkin, in Recent Advances in Field Theory and Statistical Mechanics, edited by J. B Zuber and R. Stora (Elsevier, New York, 1984).