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Kinetic equation for noninteracting electrons in the presence of strongly disordered magnetic impurities

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We derive a kinetic equation for noninteracting electrons acted upon by an external (longitudinal) field slowly varying in space and time, in the presence of strongly disordered magnetic impurities. We show that this equation is of the Boltzmann type with an effective scattering kernel which is *nonlocal* in time *and* space. Implications for the physical mechanism leading to localization are discussed in conjunction with general symmetry arguments.

Electronic localization effects have traditionally been studied by determination of the hydrodynamic limit of the response functions,[1] which evidences the localization through a critical slowing down of the diffusion coefficient. Recently, however, there has been increasing interest in the inclusion of localization effects in the more conventional Boltzmann description of transport processes,[2-4] an approach which is relevant insofar as it can give a deeper physical understanding of the microscopic processes which are involved in the electronic localization. The first successful attempt in this direction has been made for the nonmagnetic impurity case by Hershfield and Ambegaokar.[2] They derived a Boltzmann-type equation whose (effective) scattering kernel is sharply enhanced in the backscattering direction, in agreement with the standard interpretation of localization in terms of quantum interference.[5]

In this Rapid Communication we extend the Boltzmann-type description to the localization in the magnetic impurity case which had so far no simple interpretation in terms of quantum interference. Specifically, we will show that the interplay of two or more diffusion processes yields a reflection of the incident wave over a broad region of phase space. As a consequence, the effective scattering kernel of the Boltzmann equation becomes *nonlocal* in space within a distance of the order of the mean free path. The nonlocality of the scattering kernel is indeed *a peculiar feature* of the localization in the magnetic impurity case, even though in the standard classical regime the short range of the potential would ensure locality.[6] In the nonmagnetic impurity case,[2] the nonlocality in space is instead suppressed by symmetry considerations involving the interchange of the initial and final directions in the scattering processes.

The tendency toward localization in the nonmagnetic impurity case is signaled (near two dimensions) by the occurrence of an infrared divergency of the crossed-ladder contribution in the backscattering channel. This feature is shared by the ordinary diagrammatic perturbation theory[1] as well as by the Kadanoff and Baym approach[7] that has been adopted by Hershfield and Ambegaokar in their treatment of the kinetic equation.[2] In the presence of (quenched) magnetic impurities, however, this singularity is cutoff by the appearance of masses in both singlet and triplet particle-particle channels,[8] and one is thus forced to consider more complex diagrammatic structures such as the crossing of two or more particle-hole ladder propagators.[1,9] In particular, one has to calculate all relevant (two-loop) contributions of second order in the expansion parameter t, which in two dimensions is given by $2(k_F l)^{-1}$ where l is the mean free path. For this reason, we found it more convenient to derive the kinetic equation in the presence of magnetic impurities by an approach that relies on the ordinary diagrammatic perturbation theory which is usually adopted to treat localization problems,[1] rather than attempting to generalize the treatment by Hershfield and Ambegaokar to two-loop order. Our results will specifically hold within linear response in the limit of slowly varying perturbations.

The strategy we adopt is the following. (i) A distribution function is suitably introduced to overcome the difficulties one would face with the more conventional Wigner distribution function due to the lack of momentum conservation. (ii) Diagrammatic perturbation theory is then used within linear response theory to derive an integral (Bethe-Salpeter) equation for the distribution function near two dimensions to second order in t. (iii) The integral equation is finally cast in the form of a Boltzmann-type equation with an effective scattering kernel which includes quantum-interference effects.

The distribution function we consider hinges on an idea by Prange and Kadanoff[10] and is adopted to overcome the lack of momentum conservation in the presence of strong disorder:[2]

$$n(\mathbf{k};\mathbf{R},T)=g[\hat{\mathbf{k}},\varepsilon_{\mathbf{k}}+\phi_{\mathrm{ext}}(\mathbf{R},T);\mathbf{R},T]\,, \tag{1}$$

where

$$g(\hat{\mathbf{k}},\omega;\mathbf{R},T)=\int\frac{d\varepsilon_{\mathbf{k}'}}{2\pi}\int d\rho\, e^{-i\hat{\mathbf{k}}|\mathbf{k}'|\cdot\rho}\int dt\, e^{i\omega t}\tfrac{1}{2}\langle[\psi^{\dagger}(\mathbf{R}-\rho/2,T-t/2)\psi(\mathbf{R}+\rho/2,T+t/2)$$
$$-\psi(\mathbf{R}+\rho/2,T+t/2)\psi^{\dagger}(\mathbf{R}-\rho/2,T-t/2)]\rangle\,, \tag{2}$$

with $\varepsilon_{\mathbf{k}}=\mathbf{k}^2/2m$ and $\phi_{\rm ext}$ being an external (scalar) potential.[11] In Eq. (2) the energy is fixed in a coarse-grained way [corresponding to the "slow" position ($\mathbf{R}$) and time (T) variables] by the frequency ω; in Eq. (1) this energy is then portioned into a kinetic and a potential term. In the absence of impurities, whereby the wave vector $\mathbf{k}$ is a good quantum number, g itself would implicitly define a dispersion relation $\omega=\varepsilon_{\mathbf{k}}+\phi_{\rm ext}(\mathbf{R},T)$. In the presence of impurities, on the other hand, the average over the impurity configurations is understood to be taken in Eq. (2) after the quantum-mechanical average $\langle\cdots\rangle$ over the perturbed ground state. Equation (1) is then required to define locally an effective dispersion relation along a fixed direction $\hat{\mathbf{k}}$, which will thus be the only variable affected by the scattering processes.[12] One may further verify that the total number density and current can be obtained from the distribution function (1) in the usual way.[13]

The variation of the function (2) can be evaluated to first order in the external potential by linear response techniques, and then related to a time-ordered function which admits a representation in terms of standard Feynman diagrams. After Fourier transformation of the "slow" variables $\mathbf{R}$ and T to the external momentum $\mathbf{Q}$ and frequency Ω, this procedure results in the same diagrammatic structure used for the response functions but of a final integration over the direction $\hat{\mathbf{k}}$. Specifically, in the presence of magnetic impurities the relevant irreducible scattering terms consist, up to second order in the expansion parameter t, of the (isotropic) Born collision contribution [Fig. 1(a)] and of the diagrams obtained by intersecting two and three direct ladders [Figs. 1(b) and 1(c), respectively] plus the decorations needed to keep the approximation conserving. In each term the total scattering time τ combines the contributions of the nonmagnetic (τ_0) and magnetic (τ_m) impurities, where we assume $\tau_0\ll\tau_m$. Taking the electronic spin into proper account further requires us to multiply each direct ladder [as defined in Fig. 1(d)] by a factor $\frac{1}{2}$, as well as to multiply the three-ladder diagrams of Fig. 1(c) by an overall factor of 2.

To disentangle the above irreducible scattering terms from the distribution function, thereby mapping the diagrammatic structure onto the collision integral of the Boltzmann equation, it is sufficient to evaluate this structure up to the required order in t. With this procedure one safely keeps all relevant contributions in $\mathbf{Q}$ and Ω, which will eventually be required to recover the diffusive form of the density-density response function as well as to render the theory renormalizable in the usual way. The final equation for the distribution function (1) can then be cast into the general form (after back Fourier transformation from $\mathbf{Q}$ to $\mathbf{R}$)[14]

$$[-i\Omega+v_F\hat{\mathbf{k}}\cdot\nabla_{\mathbf{R}}-\nabla_{\mathbf{R}}\phi_{\rm ext}(\mathbf{R},\Omega)\cdot\nabla_{\mathbf{k}}]n(\mathbf{k};\mathbf{R},\Omega)=-\int\frac{d\hat{\mathbf{k}}'}{S_d}\int d\mathbf{R}'W(\hat{\mathbf{k}},\hat{\mathbf{k}}';\mathbf{R}-\mathbf{R}',\Omega)[n(\mathbf{k};\mathbf{R}',\Omega)-n(\mathbf{k}';\mathbf{R}',\Omega)]\,, \tag{3}$$

where v_F is the Fermi velocity, S_d stands for the solid angle in d dimensions, and $|\mathbf{k}|=|\mathbf{k}'|$. In Eq. (3) the mixed space ($\mathbf{R}$) and frequency (Ω) representation is kept in order to use Ω as the infrared cutoff of the theory, according to a standard procedure in localization theory.

In the hydrodynamic regime the spatial dependence of the effective scattering kernel W is characterized by its first two moments[15]

$$W_0(\hat{\mathbf{k}},\hat{\mathbf{k}}';\Omega)=\int d\mathbf{R}'W(\hat{\mathbf{k}},\hat{\mathbf{k}}';\mathbf{R}-\mathbf{R}')\,, \tag{4a}$$

$$\mathbf{W}_1(\hat{\mathbf{k}},\hat{\mathbf{k}}';\Omega)=\int d\mathbf{R}'W(\hat{\mathbf{k}},\hat{\mathbf{k}}';\mathbf{R}-\mathbf{R}')(\mathbf{R}'-\mathbf{R})\,, \tag{4b}$$

which naturally appear once the function $n(\mathbf{k};\mathbf{R}',\Omega)-n(\mathbf{k}';\mathbf{R}',\Omega)$ at the right-hand side of Eq. (3) is expanded in powers of $\mathbf{R}-\mathbf{R}'$.

In the case of magnetic impurities we find

$$W_0(\hat{\mathbf{k}},\hat{\mathbf{k}}';\Omega)=\frac{1}{\tau}\{1-\tfrac{1}{2}t^2I_d^2(\Omega)[1+2(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')]\}\,, \tag{5a}$$

$$\mathbf{W}_1(\hat{\mathbf{k}},\hat{\mathbf{k}}';\Omega)=-\frac{1}{\tau}\frac{1}{2}t^2I_d^2(\Omega)[1+\epsilon/8+2(1+\tfrac{3}{8}\epsilon)(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')]\mathbf{l}(\hat{\mathbf{k}}+\hat{\mathbf{k}}')\,, \tag{5b}$$

to order $\epsilon=d-2$ in ϵ expansion, where

$$I_d(\Omega)=\int\frac{d\mathbf{q}}{(2\pi)^d}\frac{1}{\mathbf{q}^2-i\Omega} \tag{6}$$

is logarithmically singular in two dimensions. The result (5) has to be contrasted with its counterpart in the presence of

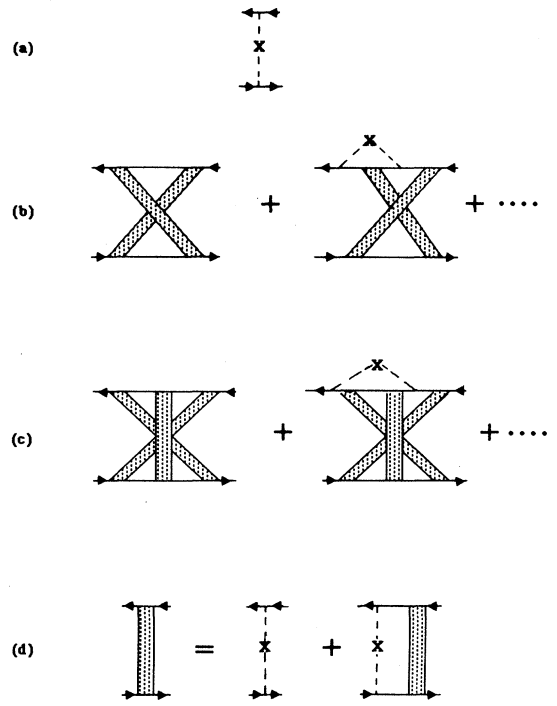

FIG. 1. (a) Irreducible scattering process within the Born approximation; (b) two and (c) three intersecting ladders' contributions of order t^2; (d) integral equation for the direct ladder.

nonmagnetic impurities only[2]

$$W_0(\hat{\mathbf{k}},\hat{\mathbf{k}}';\Omega)=\frac{1}{\tau}\{1+2tI_d(\Omega)[S_d\delta(\hat{\mathbf{k}}+\hat{\mathbf{k}}')-1]\}\,, \tag{7a}$$

$$\mathbf{W}_1(\hat{\mathbf{k}},\hat{\mathbf{k}}';\Omega)=0\,, \tag{7b}$$

which exhibits a marked backscattering effect in accordance with the standard interpretation of localization in terms of quantum interference.[5] Equation (5b), in particular, shows that the breaking of time-reversal symmetry, because of the presence of magnetic impurities, induces a *nonlocality* of the scattering probability W which couples scattering processes occurring in the neighborhood of a given $\mathbf{R}$ within a range of the order of the mean free path $l=\tau v_F$. In fact, as the averaging over the impurity configurations restores the symmetry of the effective scattering kernel under the interchange $\hat{\mathbf{k}}\leftrightarrow\hat{\mathbf{k}}'$ (which would otherwise hold only for single impurity events[6]), the first moment $\mathbf{W}_1$ can be directed only along the direction $\hat{\mathbf{k}}+\hat{\mathbf{k}}'$. For this reason $\mathbf{W}_1$ cannot survive [as in Eq. (7b)] when time-reversal symmetry requires, in addition, the scattering kernel to be symmetric under the interchange $\hat{\mathbf{k}}\leftrightarrow-\hat{\mathbf{k}}'$. The vanishing of $\mathbf{W}_1$ is also implicit in the (isotropic) Born approximation

$$W(\hat{\mathbf{k}},\hat{\mathbf{k}}';\mathbf{R}-\mathbf{R}',\Omega)=\frac{1}{\tau}\delta(\mathbf{R}-\mathbf{R}') \tag{8}$$

that disregards quantum-interference effects altogether. In this case, the presence of the spatial δ function arises from the classical approximation of our considering each scattering process as an independent event.

Equations (5) also show that, in the presence of magnetic impurities, W_0 is only weakly enhanced in the back direction $\hat{\mathbf{k}}'=-\hat{\mathbf{k}}$ and that $\mathbf{W}_1$ vanishes in that direction. An effective reflection of the incident wave can thus occur in this case only over a *broad region* of phase space, whereby to alternative microscopic scattering channels are associated different relaxation times. In order to obtain a limiting macroscopic relaxation process (on the hydrodynamic scale), one then has to average over the allowed region of phase space. In the present context this corresponds to averaging with equal weight over all possible directions $\hat{\mathbf{k}}$ on the Fermi surface. In this way, one also circumvents the problem of the two moments leading to nonrenormalizable processes when taken separately because their first significant term would be proportional to the square of a logarithmic singularity. Once the averaging is carried out one recovers from Eq. (3) the diffusion equation, where the diffusion coefficient has the standard form[1]

$$D=D_0\left[1+\frac{1}{16\pi^2}t^2\ln(\Omega\tau)\right]\,, \tag{9}$$

with the characteristic logarithmic term adding to the Born collision contribution D_0.[16]

In conclusion, we have derived a Boltzmann equation for noninteracting electrons in the presence of magnetic impurities, and shown that localization does not appear in this case as a simple backscattering enhancement but rather as a building up of the reflected wave that occurs over an extended region of phase space. Our analysis thus provides an understanding at a microscopic level of the processes leading to electronic localization when time-reversal invariance is lacking.

[1]See, e.g., *Anderson Localization,* edited by Y. Nagaoka and H. Fukuyama (Springer-Verlag, New York, 1982).

[2]S. Hershfield and V. Ambegaokar, Phys. Rev. B **34**, 2147 (1986).

[3]J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986).

[4]V. K. Dugaev and D. E. Khmelnitskii, Zh. Eksp. Teor. Fiz. **90**, 1871 (1986) [Sov. Phys. JETP **63**, 1097 (1986)].

[5]G. Bergmann, Phys. Rep. **107**, 1 (1984); B. L. Altshuler, A. G. Aronov, D. E. Khmelnitskii, and A. I. Larkin, in *Quantum Theory of Solids,* edited by I. M. Lifshitz (Mir Publishers, Moscow, 1982), p. 130.

[6]See, e.g., N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia, PA, 1976), Chap. 16; see also E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics* (Pergamon, Oxford, 1981), Sec. 16.

[7]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, Menlo Park, CA, 1962); D. C. Langreth, in *Linear and Nonlinear Electron Transport in Solids,* edited by J. T. Devreese and E. van Doren (Plenum, New York, 1976), p. 3.

[8]See, e.g., the second part of Ref. 5. We adopt in this paper the usual assumptions of the theory of localization, whereby mag-

netic impurities are considered to be quenched. They thus effectively act as a random magnetic field that violates time-reversal invariance.

[9]S. Hikami, Phys. Rev. B **24**, 2671 (1981).

[10]R. E. Prange and L. P. Kadanoff, Phys. Rev. **134**, A566 (1964).

[11]We set $\hbar = 1$ throughout.

[12]The procedure we have adopted to define the dispersion relation in the presence of strong disorder bears some analogy with the approach by O. Betbeder-Matibet and P. Nozières [Ann. Phys. **37**, 17 (1966)]: Our function δg corresponds to their $\delta\bar{n}$ (the deviation of the distribution function from local equilibrium) and Eq. (1) recovers the total δn from the knowledge of $\delta\bar{n}$.

[13]The dependence of the Fermi field ψ (and hence of the distribution function) on the spin projection has not been indicated explicitly in Eqs. (1) and (2). Since the coupling to the external agent is represented by a scalar potential, we need only consider in the following the singlet scattering channels of the electron-hole pair excitations.

[14]G. Strinati, C. Castellani, and C. Di Castro (unpublished).

[15]We note that the second moment of W is not needed, at leading order in the small external wave vector $\mathbf{Q}$ and frequency Ω, since W multiplies the difference $n(\mathbf{k}) - n(\mathbf{k}')$ which is already of first order in $\mathbf{Q}$ and Ω.

[16]It is a matter of straightforward algebra to derive from Eq. (3) the diffusion equation for the angular average of $n(\mathbf{k};\mathbf{R},\Omega)$. Making use of Eq. (5) at d dimensions, one obtains $D - D_0 \sim (\frac{1}{2} - 1/d) I_d^2$, and Eq. (9) is thus recovered in the context of dimensional regularization.