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The breakdown of weak-localisation theory in disordered conductors with magnetic or spin–orbit scattering

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Abstract. The wavelength dependence of quantum interference corrections to the diffusion constant is calculated in two dimensions, in the weak-localisation regime, using models belonging to the three universality classes for localisation. In each case, the corrections at second order in perturbation theory are much larger for finite wavevector than expected from previous results at zero wavevector. In two cases (systems without time-reversal invariance and systems with spin–orbit scattering), this wavevector dependence determines the way in which perturbation theory breaks down as the cut-off length for quantum interference increases. We speculate that these results may signal crossover from simple diffusive behaviour to a critical regime characterised by novel variation of the diffusion constant with wavevector and frequency.

1. Introduction

The central predictions of the scaling theory of localisation [1, 2], and the most fully tested experimentally, are for the length-scale dependence of the conductance. The same theoretical framework also leads to definite expectations for the frequency and wavevector dependence of the diffusion constant [3, 4, 5]. Although these are less accessible to direct observation (they *do* have immediate consequences for the temperature dependence of the inelastic scattering rate [6]), they form an integral part of current understanding of the mobility edge.

In this paper we calculate perturbatively the wavevector dependence of weak-localisation corrections to the diffusion constant in two-dimensional systems. We study models representing each of the three universality classes for localisation: systems with potential scattering only; those with a weak magnetic field or scattering by magnetic impurities; and those with spin–orbit scattering. Results can be reconciled with established expectations only in the first case. For systems with magnetic or spin–orbit scattering, we find that corrections at finite wavevector, which are much larger than anticipated from the length-scale dependence of the conductance, dominate behaviour as the inelastic scattering length (or other long-distance cut-off, L) increases.

Briefly, our results are the following. In principle, weak-localisation calculations of transport coefficients in two dimensions can generate terms at second order with the L-dependence $[\ln(L)]^2$. It is well known [7] that such terms are in fact absent from the conductivity. We find, however, that they *do* appear in the finite-wavevector diffusion constant.

Our calculations were motivated by related results obtained recently in a model for the integer quantum Hall effect [8]. Subsequent numerical simulations [9] in that context have revealed that the diffusion constant, D, at the mobility edge has a novel dependence on wavevector $\boldsymbol{q}$, and frequency, ω: D is constant for q^2/ω small, but $D \sim (q/\sqrt{\omega})^{-\eta}$ for q^2/ω large with $\eta \simeq 0.4$. We speculate that our present results may indicate crossover from conventional, diffusive behaviour to a similar critical regime in two-dimensional systems with spin-flip or spin–orbit scattering.

2. Calculation and results

We use for our calculations tight-binding models with n orbitals per lattice site as introduced by Wegner, Oppermann and Jüngling [10, 11, 12]. These models are solvable in the $n = \infty$ limit [10]. Quantum interference effects can be calculated perturbatively [11, 12] using an expansion in powers of $1/n$, which is equivalent to the $1/E_F\tau$ expansion for weak disorder [1, 7]. The $1/n$ expansion provides a particularly straightforward setting for our calculation but we expect that other approaches would lead to the same results. In the following we refer extensively to the earlier papers by Oppermann and Wegner ([11], denoted by OW) and by Jüngling and Oppermann ([12], denoted by JO), emphasising only the new features of the current work.

The models are defined, neglecting spin for the present, in terms of a set of basis states $\{|r\alpha\rangle\}$, where r is a site position on a simple square lattice and $\alpha = 1, 2, \ldots, n$ labels the orbitals at each site. The Hamiltonian is [10].

$$H = \sum_{r\alpha, r'\beta} n^{-1/2} f_{r\alpha, r'\beta} |r\alpha\rangle\langle r'\beta|. \tag{1}$$

The matrix elements $f_{r\alpha,r'\beta}$ are random variables with a probability distribution chosen to simplify calculations as much as possible. Their joint distribution is Gaussian with zero mean

$$[f_{r\alpha,r'\beta}]_{\text{av}} = 0 \tag{2}$$

and covariance

$$[f_{r\alpha,r'\beta} f_{r''\gamma,r'''\delta}]_{\text{av}} = \delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{rr'''}\delta_{r'r''}M(r-r') + \delta_{\alpha\gamma}\delta_{\beta\delta}\delta_{rr''}\delta_{r'r'''}M'(r-r'). \tag{3}$$

In the first model, intended to represent scattering by a random potential only, and known as the real matrix ensemble, the fs are real and $M'(r-r') = M(r-r')$. In the second model, representing systems without time-reversal invariance (because of magnetic impurities or a weak external magnetic field), and known as the complex matrix ensemble, the fs have random phases and $M'(r-r') = 0$. We refer the reader to OW for a discussion of the ideas of local gauge invariance that motivate these choices.

JO [12] have extended these models to include spin. Effort is economised by using the result [12, 13] that properties of a model with strong spin–orbit scattering, known as the spin-dependent complex matrix ensemble, can be expressed entirely in terms of those of the real matrix ensemble: see JO for further details.

We calculate the diffusion propagator, defined by (OW)

$$K(q, z, z') = \sum_{r\beta} [\langle 0\alpha|(z - H)^{-1}|r\beta\rangle\langle r\beta|(z' - H)^{-1}|0\alpha\rangle]_{\mathrm{av}}\, \mathrm{e}^{\mathrm{i}q\cdot r} \qquad (4)$$

where z and z' have imaginary parts of opposite sign. The diffusion constant, D is extracted from the behaviour of $K(q, z, z')$ in the hydrodynamic limit (q, $|z - z'|$ small). Writing $z = E + \omega/2$, $z' = E - \omega/2$, with $\mathrm{Im}(\omega) > 0$, in this limit

$$K(q, z, z') \simeq 2\pi\rho(-\mathrm{i}\omega + Dq^2)^{-1} \qquad (5)$$

where ρ is the density of states per orbital at energy E. The $1/n$ expansion for $K(q, z, z')$ centres on calculating an irreducible vertex, denoted as λ_c by OW. The diffusion constant is related to λ_c and the normalised Fourier transform of $M(r)$

$$m(q) = \tilde{M}(q)/\tilde{M}(0) \qquad (6)$$

with

$$\tilde{M}(q) = \sum_r \mathrm{e}^{\mathrm{i}q\cdot r} M(r)$$

essentially by

$$Dq^2 \simeq 2\pi\rho\tilde{M}(0)(1 - \lambda_c - m(q)) \qquad (7)$$

where we have neglected the n-dependence of ρ. Since λ_c vanishes for $n = \infty$, and at $q = 0$ for all n, one has, writing $\tilde{M}(q) = \tilde{M}(0) - Aq^2$ and omitting higher-order terms in q

$$D = D_0 - 2\pi\rho\tilde{M}(0)\lambda_c/q^2 \qquad (8)$$

with $D_0 = 2\pi\rho A$.

Although contributions to λ_c are small in $1/n$, for a two-dimensional system they diverge logarithmically with the long-distance cut-off, which is imposed physically by inelastic scattering or finite system size, and in our calculation by finite ω.

Earlier work has established the behaviour of D in the limit $q = 0$, in $2 + \varepsilon$ dimensions using n-orbital models [11, 12], and in two dimensions using the $1/E_F\tau$ expansion [1, 7, 14, 15]. The results are characteristic of the universality class to which a system belongs. The leading terms in each case are

$$D = D_0[1 - (1/\alpha n)\ln(D_0/\omega)] \qquad (9)$$

for potential scattering; and

$$D = D_0[1 - (1/\alpha n)^2 \ln(D_0/\omega)] \qquad (10)$$

without time-reversal symmetry; and

$$D = D_0[1 + (1/2\alpha n)\ln(D_0/\omega)] \qquad (11)$$

with spin–orbit scattering, where $\alpha = 4\pi^2\rho D_0$. Gor'kov and co-workers [7] have emphasised the significance for scaling of the fact that there is no term in $D(q = 0)$ proportional to (in our context) $n^{-2}[\ln(D_0/\omega)]^2$.

Our new results are for weak-localisation corrections to the diffusion constant in the opposite limit to that above: q, ω small, but $Dq^2/\omega \gg 1$, rather than $Dq^2/\omega \ll 1$. We find in each model that when $Dq^2/\omega \gg 1$ there are corrections to D proportional to $n^{-2}\ln^2(D_0q^2/\omega)$ and that the leading behaviour in this regime is

$$D = D_0[1 - (1/\alpha n)\ln(D_0/\omega) - (1/\alpha n)^2\ln^2(D_0q^2/\omega)] \tag{12}$$

for potential scattering; and

$$D = D_0[1 - \tfrac{1}{2}(1/\alpha n)^2\ln^2(D_0q^2/\omega)] \tag{13}$$

without time-reversal symmetry; and

$$D = D_0[1 + \tfrac{1}{2}(1/\alpha n)\ln(D_0\omega) - \tfrac{1}{4}(1/\alpha n)^2\ln^2(D_0q^2/\omega)] \tag{14}$$

with spin–orbit scattering.

The new terms arise in the calculation from the diagram denoted as ν_4 in OW's figure 20. Its evaluation involves the integral

$$I = \int d^2\boldsymbol{p}_1 \int d^2\boldsymbol{p}_2 \frac{|\boldsymbol{p}_1 - \boldsymbol{q}|^2(2\boldsymbol{q}\cdot\boldsymbol{p}_1 - q^2)}{(\omega + p_1^2)(\omega + p_2^2)(\omega + |\boldsymbol{p}_1 + \boldsymbol{p}_2 - \boldsymbol{q}|^2)} \tag{15}$$

with an O(1) upper cut-off to the momentum integrals (the lattice constant is unit length). The leading divergence as $\omega \to 0$ is

$$I = -2\pi \int d^2p \frac{p^2}{\omega + (p+q)^2} \ln\left(\frac{\omega + p^2}{\omega}\right) + \text{less singular terms.} \tag{16}$$

In the limit $q^2/\omega \ll 1$ we obtain

$$I \simeq -\pi^2q^2[\ln(1/\omega)]^2 + \text{less singular terms.} \tag{17}$$

In the opposite limit, $q^2/\omega \gg 1$, we find

$$I \simeq -\pi^2q^2\{[\ln(1/\omega)]^2 + [\ln(q^2/\omega)]^2\} + \text{less singular terms.} \tag{18}$$

Other diagrams have the same leading divergence in both limits. Combining the contributions we reach the expressions given in (12)–(14).

3. Discussion

The perturbation theory used to derive these results is presumably reliable when $(1/\alpha n)\ln(D_0/\omega)$ is small and corrections to $n = \infty$ behaviour are themselves small. In contrast, the important aspect of the interpretation is understanding implications for behaviour outside the perturbative regime.

Weak-localisation corrections to the zero-wavevector diffusion constant have previously been extrapolated into the strongly localised regime both using mode-coupling theory [16] and by integrating an approximate β-function [17], with similar results. The diffusion constant is renormalised, eventually to zero, in systems with potential scattering only and in systems without time-reversal invariance. The finite-wavevector quantum interference effects we have calculated will be unimportant if the diffusion constant is driven towards zero sufficiently rapidly with decreasing ω that (replacing D_0 by D) they are never much larger than the zero-wavevector corrections. As long as they are *not* important, eigenfunction correlations will be characterised completely by a scale-dependent diffusion constant. The wavevector and frequency dependence of the diffusion constant in these circumstances will be related to the system size dependence of the $q = \omega = 0$ value as elaborated by Abrahams and Lee [5].

In fact, it is only in the real matrix ensemble that renormalisation of the zero-wavevector diffusion constant is sufficiently rapid to control the divergence as $\omega \to 0$ of the finite-wavevector corrections we have obtained. In systems without time-reversal invariance or with strong spin–orbit scattering, perturbation theory breaks down because the diffusion constant naively evaluated at finite q approaches zero.

Related behaviour has been noted recently in a model for the integer quantum Hall effect [8]. Numerical simulation in that case [9] uncovered a power-law dependence of the diffusion constant on the scaling variable q^2/ω, for q^2/ω large. It seems likely that the present results are a signal of similar behaviour in two-dimensional systems with spin-flip or spin–orbit scattering. Although (13) and (14) alone do not point specifically to this conclusion, it is in fact difficult to suggest alternatives. Scaling ideas and particle number conservation [3, 5] allow generalisation of (5) in two dimensions only to the extent of replacing the diffusion constant by a function $D(q^2/\omega, q\xi)$, with ξ the localisation length. Our calculation is presumably relevant to $q\xi$ large. Since $D(x, y)$ should not diverge, one expects $D(x, y)$ to be approximately constant for $x \ll 1$, $y \gg 1$. The finite-wavevector corrections imply that $D(x, y)$ decreases with increasing x for large y, and $D \sim x^{-\eta/2}$ is the simplest possibility. If this is so, crossover to such a critical regime should be the first consequence of quantum interference effects, before the strong-localisation regime is reached.

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