On minimum metallic diffusivity in disordered conductors

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It is shown that the formal consistency of a locally diffusive motion on the metallic side of the mobility edge for a disordered system with the Schrödinger equation implies a minimum metallic diffusivity $D_{min} = \hbar/2m$. Its implification for the physics near the mobility edge is discussed.

METALLIC conductivity σ implies diffusivity D through the Einstein relation for the degenerate electron system, namely, $\sigma = e^2 D N_F$. For a quench-disordered conductor, this poses the question of formal consistency of the diffusive equation for the probability density with the Schrödinger equation for the probability amplitude. In what follows we address this question and find the surprising result that a necessary condition is $D_{min} = \hbar/2m$.

Consider a phase space wave packet initially localized around the origin and constituted from the extended energy eigenstates close to the Fermi energy (counted as zero of energy) which is taken to lie just on the metallic side of the mobility edge for the quench-disordered system.

Rewrite the Schrödinger equation for the wave packet

$$\psi(x, t) = R(x, t)\, e^{i\phi(x, t)} \equiv e^{\alpha(x, t) + i\beta(x, t)} \tag{1}$$

as

$$-\hbar\, \frac{\partial \phi}{\partial t} = \frac{\hbar^2}{2m} (\nabla \phi)^2 + V - \frac{\hbar^2}{2m}\, \frac{\nabla^2 R}{R} \tag{2}$$

along with the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\hbar}{m}\, \nabla \cdot (\rho \nabla \phi) = 0 \tag{3}$$

with $\rho = \psi^* \psi$.

Now, we would like the continuity equation for the probability density to converge asymptotically to the diffusive form

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho. \tag{4}$$

Comparing eqs. (3) and (4), we at once get a condition for this to be so in terms of α and β, which is

$$\frac{\hbar}{2m}\, \nabla \beta = D \nabla \alpha \tag{5}$$

assuming $\nabla \alpha$ to be irrotational.

We now substitute in eq. (2) from eq. (5) and rearrange

to get

$$-\hbar\, \frac{\partial \beta}{\partial t} = V - \frac{\hbar^3}{4m^2 D}\, \nabla^2 \beta + \frac{\hbar^2}{2m} \left(1 - \left(\frac{\hbar}{2mD} \right)^2 \right) (\nabla \beta)^2. \tag{6}$$

Now, averaging over the disorder V and noting that odd-symmetric quantities, i.e. $\langle \beta \rangle = \nabla^2 \langle \beta \rangle = \langle V \rangle = 0$, while $\langle (\nabla \beta)^2 \rangle \neq 0$, we necessarily have

$$D = \left(\frac{\hbar}{2m} \right). \tag{7}$$

Here, of course, we have regarded D as a self-averaging quantity. This is reasonable as we know that on the metallic side of the mobility edge in three dimensions the conductance fluctuations are universal ($\sim e^2/h$), but the conductivity fluctuation is $\sim (e^2/h) (1/L)$ and, therefore, vanishes in the infinite sample size (L) limit. We must note that our sample size L is always taken to be essentially infinite ($\gg$ any correlation length ξ that may exist as we approach the mobility edge). This ensures that we are always in the local diffusive regime in that the mean-squared displacement grows linearly in time as $2Dt$. For $L \leq \xi$, the diffusion constant itself can, of course, be L-dependent. This is, however, quite different from the anomalous diffusion, where the mean-squared displacement does *not* grow linearly with time. Further, we have insisted on the local diffusion equation (4) and this forces us physically to the limit when the mean free path equals the microscopic length – the Fermi wavelength $\sim$ the lattice discreteness. The latter implies that we should be closest to the mobility edge, but on the metallic side. Thus, $\hbar/2m$ is to be taken as the minimum possible value of D to ensure local diffusion.

As to the general conceptual question of how diffusion of an initially localized wave packet may come out of the Schrödinger equation with quenched (static) disorder, we consider the following. Of course, in the static random potential there is no dissipation and hence no irreversibility that one normally associates with the inelastic (incoherent) scatterings. Indeed, in the strictly fine-grained sense there is no irreversible diffusive spread of the electron wave packet, and eq. (3) is time-reversal-symmetric (i.e. under $t \to -t$ and $\phi \to -\phi$). This old problem[1] is the same as that discussed recently by Imry[2] in the context of the nonzero real part of the dc conductivity. The point is that for the extended states the level spacing scales to zero as the system size tends to infinity, i.e. the poles produce a cut. Then arbitrarily small level broadening will ensure the phase-mixed-upness of the otherwise pure state and thus ensure irreversibility in the long-time limit. This is really an analogue of the collisonless Landau damping! Indeed, Mott and Kaveh[3] have discussed the diffusion equation as arising from the Schrödinger equation for a disordered system.

The above derivation strongly suggests that there exists a minimum metallic diffusivity D_{min} having a universal value $\hbar/2m$ *whenever* a mobility edge is known to exist. The question now is whether or not this implies a minimum metallic conductivity[4] σ_{min} through the Einstein relation $\sigma = e^2 D N_F$. This brings us to an oft-stated but seldom proven theorem[5], namely, that the localized states cannot coexist with (be at the same energy) as the extended states. And this notwithstanding the well-known counterexamples of the Wigner–von Neumann construction of such states[6]. The latter seem to be dismissed as nongeneric. If the coexistence is denied, the N_F on the metallic side of the mobility edge counts the total density of states (there being no coexisting localized states) and then $D_{min} = \hbar/2m$ would imply a $\sigma_{min}^{3D} = e^2 D_{min} N_F$. In this connection it is worth noting that the ultrathin films of Bi on Ge substrate show[7] a limiting normal metallic conductivity of $4e^2/h$ (corresponding to a sheet resistance $\sim 6.5 \, k\Omega/\square$) for the separatrix dividing the insulating and the superconducting phases at $0\,K$. This may well be associated with the preexisting local electron pairs where the correlated motion of the pairing electron escapes the tyranny of two-dimensional (2D) localization. Now, it is interesting that our universal $D_{min} = \hbar/2m$, along with $N_F = (m/\pi\hbar^2)$ for $d = 2$ does indeed give $\sigma_{\square}^{2D} = 4e^2/h$. We would like to call it the σ_{min}^{2D} of Mott recovered through delocalization by pairing in two dimensions. This may be the case for all insulator–superconductor transitions with a normal-state separatrix for the ultrathin films.

There is, however, the question of the fine structure of the mobility edge for $d = 3$, where the conductivity is experimentally believed to vanish continuously[8] at the mobility edge in a narrow critical region with a critical exponent s. How is this consistent with $D_{min} \neq 0$? A possible solution consistent with $D_{min} \neq 0$ is to assume that $N_F = N_F(\text{localized}) + N_F(\text{extended})$. What then enters the Einstein relation is, of course, the $N_F(\text{extended})$, which can vanish at the mobility edge keeping the total N_F continuous and noncritical, as is known to be the case. It is not clear how this two-spectral fluid hypothesis[5], i.e. $N_F(E) = N_F(\text{localized}) + N_F(\text{extended})$, really differs from the asymptotic form of the resonance-like wave function in three dimensions adduced by Kaveh and Mott[9]. Such quasilocalized resonant states are strongly suggested by some recent works[10,11]. We think that a proper discussion on this point is yet to take place.

Finally, two technical remarks are in order. First, the validity of our eqn. (5) at any point x demands that x not be a node where $\psi(x)$ vanishes. But this condition is naturally obeyed by all diffusive states. Indeed, vanishing of $\psi(x)$ would imply vanishing of $\rho(x) = \psi^*(x)\,\psi(x)$, which is ruled out by the fact that $\rho(x)$ is requested to obey the diffusion equation (3).

The second point concerns the absolute value $4e^2/h$ for the sheet conductance of films referred to in the text, i.e. for Bi films on Ge. The point is that the effective band mass does not appear in the expression, and the correction to the density of states due to disorder or interaction is cancelled by the vertex correction, at least perturbatively – the well-known cancellation theorem valid in the absence of a pseudo gap[12].

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