Brief Reports

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Connection of localization with the problem of the bound state in a potential well

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It is shown that the problem of electron localization in a random potential is formally equivalent to the problem of finding a bound state in a shallow potential well.

Recently, significant advances have been made[1,2] in understanding Anderson's localization in disordered systems. Much of the work has been based on the idea[3] that the extended or localized nature of the eigenstates can be determined by a single scaling variable, the dimensionless conductance $g(L)$ of a system of length L. By assuming that the quantity $\beta(g) \equiv d\ln g/d\ln L$, which describes the length dependence of g, is a monotonic and nonsingular function of g only, one obtains that $g \to 0$ as $L \to \infty$ for any disordered system of dimensionality lower or equal to two.

A self-consistent perturbation theory[4] has been developed for the localization problem which gives results in agreement with scaling theory. The conductance g obeys a scaling equation as proposed by Abrahams *et al.*[1] for all dimensions d.

It has been shown,[4] within the weak-scattering limit, that the frequency-dependent diffusion coefficient $D(\omega)$ in the long-wavelength limit ($q \to 0$) is given by

$$D(\omega) = D_0 - \frac{1}{(2\pi)^d \pi\hbar\rho} \int_{q_{\min}}^{q_{\max}} \frac{d\vec{q}}{q^2 - i\omega/D_0} \quad , \tag{1}$$

where D_0 is the bare diffusion constant, which is related with the conductivity σ_0 by the Einstein relation $\sigma_0 = 2e^2 D_0\rho$. Here ρ is the density of states (DOS) per spin per unit volume (area, length), and d is the dimensionality. The DC conductivity σ_0 in the weak-scattering limit is

$$\sigma_0 = \frac{2}{(2\pi)^d d} \frac{e^2}{\hbar} l S_F \quad ,$$

where l is the mean free path and S_F is the Fermi surface. (For $d=2$, S_F is the length of the Fermi line, and for $d=1$, $S_F=2$.) The upper cutoff $q_{\max} = 1/L_{\min}$, where $L_{\min}$ is believed to be very close to the mean free path l; here we assume $L_{\min} = (D\tau)^{1/2} = l/\sqrt{d}$. The lower cutoff $q_{\min} = 1/L_{\max}$, where $L_{\max}$ is dominated by the shortest of several upper cutoff lengths which may be present in the system. Such lengths are the diffusion length during the inelastic relaxation time τ_i in $L_T = (D\tau_i)^{1/2}$, and the diffusion length during the time ω^{-1}, where ω is the frequency of an external ac field, $L_\omega = (D/\omega)^{1/2}$; the presence of an external magnetic field H introduces the cyclotron radius $L_H = (\hbar c/eH)^{1/2}$.

As we have already mentioned, Eq. (1) is correct for the weak-scattering limit. We can extend it to the strong disorder case by substituting[4] D_0 in the denominator of the right-hand side of Eq. (1) by $D(\omega)$. Thus we have a self-consistent equation for $D(\omega)$. For extended states and in the limit $\omega \to 0$ the self-consistent equation is identical with Eq. (1) because both $\omega/D(\omega)$ and ω/D_0 approach zero. However, for localized states, $\omega/D(\omega)$, in contrast to ω/D_0, does not go to zero. To see this, consider the polarizability $\alpha(\omega)$, which is defined by $\sigma(\omega) = -i\omega\alpha(\omega)$ and (for an insulator) is finite[5] in the $\omega \to 0$ limit. Note that $-i\omega/D(\omega)$ has the dimension of an inverse length square denoted by ξ^{-2}. It was argued[4] that ξ is the localization length. This proposal is supported by numerical results[5] for $\sigma(\omega)$ for a one-dimensional disordered system; we found that these results are not inconsistent with ξ being the localization length. Therefore we replace $-i\omega/D(\omega)$ by ξ^{-2} in the denominator of the integral in Eq. (1) and for $\omega \to 0$ obtain that

$$\sigma_0 = \frac{2e^2}{(2\pi)^d \pi\hbar} \int \frac{d\vec{q}}{q^2 + \xi^{-2}} \quad . \tag{2}$$

The most general way to treat the problem of a bound state in a potential well is by employing Green's-function techniques.[6] Consider the Hamiltonian $H = H_0 + V$, where H_0 is its unperturbed part and V is the potential well. Let us define the operator $G(E) \equiv (E-H)^{-1}$; when $E = E_b$, where E_b is a bound discrete level, G blows up. Thus the bound levels, if any, will appear as poles of $G(E)$. The operator $G(E)$ can be expressed as

$$G(E) = (E - H_0 - V)^{-1} = \{(E-H_0)[1-(E-H_0)^{-1}V]\}^{-1}$$
$$= (1 - G_0 V)^{-1} G_0 \quad ,$$

where $G_0(E) \equiv (E-H_0)^{-1}$. The easiest case for an explicit determination of E_b is when H_0 is a tight-binding Hamiltonian with one orbital $|l\rangle$ for each lattice site l and when $V = -|l\rangle |V_0| \langle l|$. Then it is straightforward to show[6] that E_b will be solution of the equation

$$-\langle l|G_0(E_b)|l\rangle |V_0| = 1 \quad . \tag{3}$$

By introducing the eigenstates of H_0, $\{|k\rangle\}$, we can reexpress G_0 as

$$G_0(E) = (E-H_0)^{-1} = \sum |k\rangle\langle k|(E-E_k)^{-1} \quad .$$

The summation over k can be transformed to an integration over k. The eigenvalues E_k near the lower band edge E_l have a quadratic dependence on k, $E_k = E_l + \hbar^2 k^2/2m^*$ and $E_b = E_l - \hbar^2 k_b^2/2m^*$, so that we can recast Eq. (3) as follows[6]:

$$\frac{1}{\Omega |V_0|} = \frac{1}{(2\pi)^d} \frac{2m^*}{\hbar^2} \int \frac{d\vec{k}}{k^2 + k_b^2} , \tag{4}$$

where k_b is the inverse of the localization length of the bound state, and Ω is the volume of the primitive lattice cell. An appropriate upper cutoff is needed in Eq. (4) [as well as in Eq. (2)] to account for the fact that the quadratic dependence on k (or q) is valid only for small k (or q). An equation of the same form as Eq. (4) determines the bound state for the continuous case.[6] Note that Eq. (4), which solves the problem of finding the bound levels in an external potential V, is mathematically equivalent to Eq. (2) [with the replacement $(\Omega |V_0|)^{-1} = \pi m \sigma_0 / e^2 \hbar$] which describes the localization problem. It must be pointed out that Eq. (4) always gives a bound state,[6] even for weak $|V_0|$, provided that $d \leq 2$. The same is true for the localization problem described by Eq. (2), i.e., all states are localized, even for very weak disorder, provided that $d \leq 2$.

The formal equivalence of Eqs. (2) and (4) strongly suggests that there may be a direct physical connection between the problem of localization in disordered systems and that of a bound level in a single potential well. If such a connection could be established, it would definitely contribute to our understanding of the localization mechanism in disordered media. A possible way (which we currently explore) for establishing the physical equivalence of the two problems is by employing Edward's[7] path integral formulation.[8] The latter may allow the rigorous mapping of the localization problem to that of a bound level in a self-consistently determined potential well. Then it may be possible to connect this effective potential well to the quantity σ_0, establishing thus the desired equivalence.

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