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Self-consistent theory of Anderson localization for the tight-binding model with site-diagonal disorder

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We present a self-consistent theory of the frequency-dependent conductivity with no adjustable parameters for a tight-binding model with random energy levels, using the locator expansion. The resulting phase diagram and the conductivity and localization length as a function of energy and disorder are in quantitative agreement with results of numerical diagonalization of finite-size systems. The results demonstrate for the first time that quantum interference effects are responsible for localization over the complete energy range, including the band edges.

Just about 30 years ago Anderson[1] introduced the notion of localization of a quantum particle in a random potential. The importance of the idea was recognized by Mott[2] and by Thouless,[3] who extended and refined the concept and explored its application to electron transport in solids. It took about 20 yrs until it was realized that the Anderson transition is in fact a continuous phase transition characterized by a diverging length, critical exponents, and an order parameter.[3-5] The precise form of the scaling at the localization transition, in particular whether more than one scaling parameter is required in the strong-coupling regime, is presently a matter of controversy.[6-10] In the framework of our theory one-parameter scaling is an inescapable consequence unless there exist as yet undiscovered singularities of a new type in terms of perturbation theory omitted in our approximation. In the following, we will take one-parameter scaling theory for granted at least in a certain vicinity of the transition, if not the critical regime itself. The question then remaining is how to connect the critical regime with the parameters of the Hamiltonian in a quantitative way. It is this question to which the present paper attempts to provide a comprehensive answer.

Early attempts to establish this relation led to the formulation of self-consistent theories,[11,12] which indeed yielded scaling in agreement[11] with field-theoretic treatments[4,13] up to three-loop order in the ε expansion. While this was encouraging, these theories were not yet fully renormalized, e.g., in that the coupling constant and the density of states entering the self-consistent equation were only evaluated in weak coupling. A qualitative renormalization of the self-consistent theory (SCT) using the analogy to single-particle localization in an average potential well was attempted by Economou and co-workers.[14,15]

In this paper we calculate the parameters of the SCT for a random tight-binding model in single-site approximation using a formulation based on the locator expansion.[16] The resulting conductivity and localization length will be compared with numerical diagonalization results for finite systems.

We consider the Hamiltonian

$$H=\sum_{n,m}\varepsilon_{nm}\,|n\rangle\langle m|+\sum_{n}V_n\,|n\rangle\langle n|\,, \tag{1}$$

with random site energies V_n distributed according to probability $P(V)$ and transition amplitudes ε_{nm} for a hopping process from site m to site n ($\varepsilon_{nn}=0$). In later evaluations we use a rectangular distribution

$$P(V)=(1/W)\Theta[(W/2)-|V|]\,,$$

where Θ is the step function.

Our aim is to sum infinite classes of perturbation theory for the conductivity in terms of the disorder such that the most divergent terms are taken into account in a self-consistent and scale-invariant way.[11] It is useful to phrase the perturbation expansion in terms of a locator expansion,[17,18] a simple locator being defined as the atomic on-site Green's function $g_n^{R/A}(E)=1/(E-V_n\pm i\eta)$ with $\eta\to 0$, and the hopping-matrix element ε_{nm}. The single-particle Green's function, e.g., is expanded as

$$G_{nm}(E)=g_n\left[\delta_{nm}+\varepsilon_{nm}g_m+\sum_l\varepsilon_{nl}g_l\varepsilon_{lm}g_m+\ldots\right].$$

Each contribution may be represented by a diagram consisting of propagator lines for ε_{nm} and locator lines ending at a point designating a given site. Averaging over the energy-level distribution $P(V)$ introduces a well-known difficulty:[18] Locators in the expansion which happen to be at the same site have to be averaged coherently (indicated by locator lines attached to the same point). Therefore, in any expansion in terms of averaged locators, lattice sums are restricted to sites which do not appear elsewhere in a

diagram. This inconvenience is handled by extending the sums over all lattice sites, and correcting for the added terms by subtracting "multiple-occupancy corrections" (MOC). For a given diagram MOC's are constructed by breaking off locator lines from common sites in all possible ways and subtracting these terms from the original diagram. Note that MOC diagrams may, in turn, require MOC's (next generation) if they happen to have multiple locator lines at any site. The problem is not peculiar to locator expansions but also arises in an extended state formulation on the lattice.

The approximation we are going to be using for calculating quantities which behave noncritically at the Anderson transition is the single-site approximation or coherent-potential approximation (CPA).[19,20] It may be viewed as the first term in a cluster expansion and is expected to become exact in the limit of large lattice coordination numbers.[21] For the averaged one-particle Green's function it amounts to summing up all diagrams of G with noncrossing locator lines and the corresponding MOC's. The resulting averaged Green's function (in momentum space)

$$G_p(E)=[1/\sigma_0(E)-\varepsilon_p]^{-1}$$

is found from the self-consistency condition

$$\left\langle \frac{g_0-\sigma_0}{1-(g_0-\sigma_0)U_0} \right\rangle = 0 , \tag{2}$$

where the angular brackets denote the impurity average and $U_0=\sum_p U_p$, with

$$U_p=\varepsilon_p+\varepsilon_p G_p \varepsilon_p=(G_p/\sigma_0-1)/\sigma_0$$

the renormalized hopping matrix. For simplicity, we consider nearest-neighbor hopping on a d-dimensional simple cubic lattice (lattice constant a) for which $\varepsilon_p=2\varepsilon\sum_{i=1}^{d}\times\cos p_i a$. Note that the self-energy $\Sigma(E)=E-1/\sigma_0(E)$ is momentum independent in CPA.

The frequency-dependent conductivity $\sigma(\omega)$ or, equivalently, the coefficient of diffusion $D(\omega)=\sigma(\omega)/[e^2N(E_F)]$ may be extracted[11] from the behavior of the density relaxation function

$$\phi(q,\omega)=2\pi i N(E_F)/[\omega+iD(\omega)q^2]$$

in the limit $\omega,q\to 0$ [$N(E)=\pi^{-1}\sum_p \mathrm{Im}G_p^A(E)$ is the density of states]. Here $\phi(q,\omega)=\sum_{\mathbf{p}}\phi_{\mathbf{p}}(q,\omega)$ and

$$\phi_{\mathbf{p}'}=\sum_{\mathbf{p}}\langle G^R_{p+p'_+}(E+\omega)G^A_{p'_-p_-}(E)\rangle ,$$

where $\mathbf{p}_\pm=\mathbf{p}\pm\mathbf{q}/2$ and $\mathbf{p}'_\pm=\mathbf{p}'\pm\mathbf{q}/2$ and $R(A)$ refers to the retarded (advanced) Green's function. The vertex function $\phi_{\mathbf{p}}(q,\omega)$ obeys the integral equation[16]

$$(G^{R^{-1}}_{p_+}-G^{A^{-1}}_{p_-})\sigma_0^R\sigma_0^A\phi_p(q) = (G^A_{p_-}-G^R_{p_-})\left[\tilde{\gamma}_p+\sum_{p'}\gamma_{pp'}\varepsilon_{p'_+}\varepsilon_{p'_-}\phi_{p'}\right] , \tag{3}$$

with $\gamma_{pp'}$ the irreducible vertex function and $\tilde{\gamma}_p=\sum_{p'}[\gamma_{pp'}-(\text{MOC at final locator point})]$.

In the hydrodynamic limit $\omega,q\to 0$, (3) may be solved for the density relaxation function $\phi=\sum_{\mathbf{p}}\phi_{\mathbf{p}}$ and the longitudinal current relaxation function $\phi_j=\sum_{\mathbf{p}}(\mathbf{v}_p\cdot\hat{\mathbf{q}})\phi_p$ (where $\mathbf{v}_p=\nabla_p\varepsilon_p$ is the particle velocity) using the projection

$$\phi_p(q,\omega)=A_p\phi(q,\omega)+B_p(q)\phi_j(q,\omega)+\Delta\phi_p ,$$

with A and B to be determined below. The term $\Delta\phi_p$ is less divergent than ϕ and ϕ_j for $q,\omega\to 0$ and may be dropped. Multiplying (3) by one and $\mathbf{v}_p\cdot\hat{\mathbf{q}}$, respectively, and summing on $\mathbf{p}$, one derives the continuity equation and the momentum relaxation equation[16]

$$\begin{aligned} &\omega\phi-q\phi_j=2\pi i N(E)+0(\omega) , \\ &qL\phi+M\phi_j=qR , \end{aligned} \tag{4}$$

where L, M, and R may be approximated by their $q\to 0$ limiting value. It follows that the diffusion coefficient is given by $D(\omega)=-iL(\omega)/M(\omega)$. Here $M(\omega)$ is a generalized current relaxation rate, given by a momentum average of the irreducible vertex $\gamma_{pp'}$, and L is a single-particle quantity.

In single-site approximation $\gamma_{pp'}$ is given by a renormalized locator pair γ_0 consisting of the series of all possible bare locator "stars" with renormalized propagators U_0 plus all noncrossing MOC's:[16]

$$\gamma_0(\omega)=\frac{\sigma_0^A-\sigma_0^R-\omega\sigma_0^R\sigma_0^A}{\omega(1+U_0^R\sigma_0^R+U_0^A\sigma_0^A)+U_0^A-U_0^R} . \tag{5}$$

The corresponding quantity without MOC's at the outermost legs is[16]

$$\tilde{\gamma}_0(\omega)=\frac{G_0^A-G_0^R}{\sigma_0^A-\sigma_0^R-\omega\sigma_0^R\sigma_0^A}\gamma_0(\omega) . \tag{6}$$

By summing the ladder diagrams with γ_0 as the irreducible vertex, one finds

$$\Gamma_L(\mathbf{q},\omega)=\frac{2i(\mathrm{Im}\sigma_0^A)^2/\mathrm{Im}G_0^A}{\omega+iD_0q^2}, \text{ for } \omega,q\to 0 , \tag{7}$$

which has the correct diffusion pole structure, with D_0, the bare diffusion constant, given by

$$D_0=[\pi N(E_F)]^{-1}\sum_p(\mathbf{v}_p\cdot\hat{\mathbf{q}})^2(\mathrm{Im}G_p^A)^2 . \tag{8}$$

Quantum localization is caused by the coherent backscattering of electrons in a random potential. In perturbation theory this is expressed by an infrared divergence of the sum of maximally crossed diagrams:[5] $\Lambda_{pp'}(\mathbf{q},\omega)=\Gamma_L(\mathbf{p}+\mathbf{p}',\omega)$. These diagrams contribute infrared divergent terms to the irreducible vertex $\gamma_{pp'}$, which renormalize the diffusion coefficient to smaller values. This in turn affects the diffusion pole and hence $\Lambda_{pp'}$, and feeds back into $\Lambda_{pp'}$. The fully renormalized $\gamma_{pp'}$, may be determined following Ref. 10, where it was shown that the most divergent diagrams of $\gamma_{pp'}$ at the Anderson transition may be summed up to give the density relaxation function with two legs interchanged, i.e., $\phi(\mathbf{p}+\mathbf{p}')$. The selection of the set of "maximally crossed" diagrams for $\gamma_{pp'}$ including all possible internal parts is the principal approximation of the present theory. To proceed, we have to account for the fact that the diagrams for ϕ do not have MOC's at the two outermost locator points, whereas $\gamma_{pp'}$ does have those. This introduces a correction factor C_i for

each diagram of $\phi(\mathbf{p}+\mathbf{p}')$, which depends on the structure of the outermost locator averages, i.e., whether two or more locators are connected. In the latter case the locator star may reach into the interior of the diagram, which would generally lead to a momentum-dependent correction factor. We have not been able to sum these contributions directly. The same difficulty arises in calculating the projector coefficients A_p and $B_p(q)$.

Fortunately, one can make use of a symmetry property of the locator expansion,[22] which greatly simplifies the calculation of the C_i's. We consider a shift of the zero of energy such that $\varepsilon_p \to \varepsilon_p + E_0$ and $E \to E + E_0$. All observable quantities must be invariant under this transformation, e.g., $G_p(E)$ and $D(\omega)$, whereas $\sigma_0^{-1} \to \sigma_0^{-1} + E_0$ and $\gamma_0, \tilde{\gamma}_0$ are not. We may use the freedom to choose E_0 to our advantage. It turns out that in the limit $E_0 \to \infty$ all expressions simplify because the momentum dependence gets suppressed. In particular, it may be shown that the correction factors C_i for multilegged locator stars discussed above vanish as $1/E_0$ compared to the locator pair. Thus, only locator pairs have to be kept, which introduces a momentum independent C, determined to be $\lim_{E_0 \to \infty} (\gamma_0/\tilde{\gamma}_0)^2$.

As a result, one obtains a self-consistency relation for the diffusion coefficient

$$D(\omega) = D_0 + \gamma \sum_{\mathbf{p},\mathbf{p}'} (\mathbf{v}_p \cdot \hat{\mathbf{q}}) \frac{\mathrm{Im} G_p^A (\mathrm{Im} G_{p'}^A)^2}{(p+p')^2 - i\omega/D(\omega)} (\mathbf{v}_{p'} \cdot \hat{\mathbf{q}}) , \tag{9}$$

where $\gamma = 2\mathrm{Im}(\Sigma^A)/[\pi^2 N^2(E) D_0]$.

We have evaluated (9) numerically by employing the exact numerical solution of the single-particle CPA equation. The momentum integrals in (9) were further approximated by using the isotropic energy-momentum relation defined by

$$N_0(\varepsilon_p) = 4\pi p^2 |dp/d\varepsilon_p| / (2\pi)^d ,$$

with the model bare density of states

$$N_0(E) = N_d (B/2)[1 - (2E/B)^2]^{-1+d/2}$$

for $d = 1,2,3$ and $N_1 = 1/\pi$, $N_2 = \frac{1}{2}$, $N_3 = 2/\pi$. Here $B = 2Z\varepsilon$ is the bare bandwidth for Z nearest-neighbor sites in the lattice. The results are consistent with one-parameter scaling theory as discussed in Refs. 11, 16, and 23. A two-parameter scaling theory as suggested by certain perturbation-theory arguments[7] and by renormalization-group calculations[8] would require the existence of a different kind of infrared singular contribution in the irreducible vertex part $\gamma_{pp'}$, which we have not been able to identify so far. In particular, all states are found to be localized and $D(\omega) = -i\omega\xi^2$ in $d = 1,2$ with ξ the localization length. In $d = 3$ we find a metal-insulator phase transition along a line in the W-E plane shown in Fig. 1. In Fig. 2 the localization length is plotted for given energy $E = 0$ as a function of disorder in dimensions $d = 1,2,3$. Also shown are the results of a numerical diagonalization for a quasi-one-dimensional finite system assuming scaling behavior in the transverse directions.[24,25] Excellent agreement is found in the complete energy range. Near the band edge, the phase boundary is seen to bend outward, following the density of states. This behavior is simply due to the fact that for energy E near the band edge the

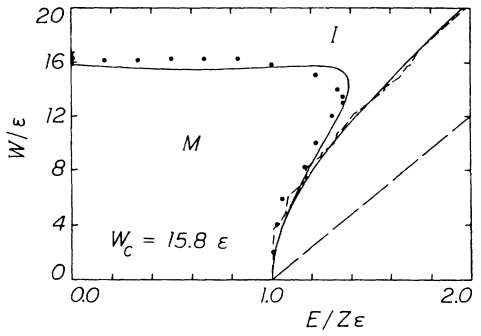

FIG. 1. Phase diagram showing metallic (M) and insulating (I) regions for the box-shaped level distribution in $d = 3$. Phase boundary according to Eq. (9) (solid line) and Ref. 23 (full circles, error bar indicated for $E = 0$: $\pm 0.5\varepsilon$). Also shown is the band edge as determined in CPA (solid line) and numerically in Ref. 23 (short-dashed line) and the exact upper bound (long-dashed line).

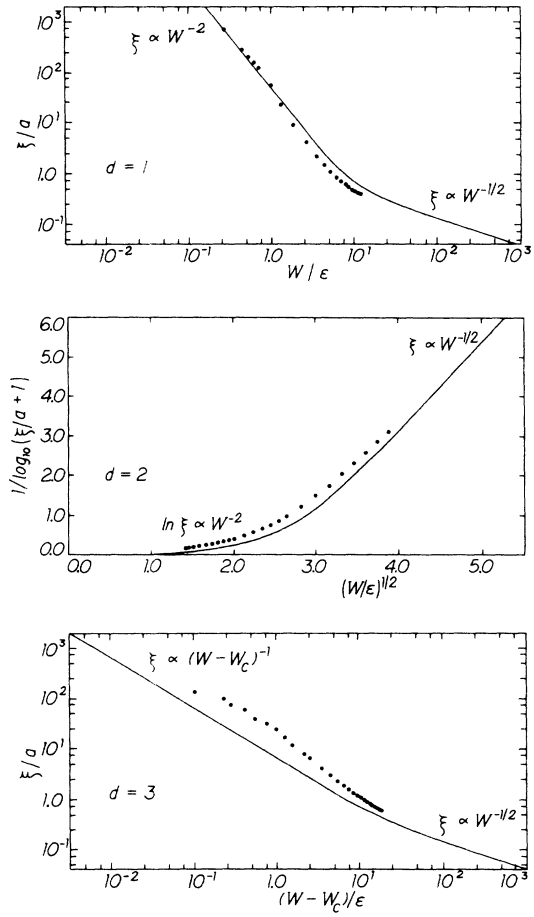

FIG. 2. Localization length ξ in units of the lattice spacing as a function of disorder in dimensions $d = 1,2,3$ for half-band filling, calculated from Eq. (9) (solid lines) and according to Ref. 23 (solid circles). Asymptotic power laws for weak and strong localization are indicated.

density of states and hence, the effective hopping probability increases with increasing disorder.[26] Indeed, the phase boundary follows the band edge [determined numerically in Ref. 25 as the energy where $N(E)=2.5\times10^{-3}N(0)$] in the limit of small W in both the numerical and our analytical results. The quantum interference effect, which is believed to cause localization in the band center, is seen to be responsible for localization near the band edges as well, in contrast to the conjecture put forward in Ref. 25 that near the band edges potential localization may be dominant. The regime of potential localization may be estimated to be well outside the CPA band.[22] Also, the so-called "classical localization" mechanism proposed by Götze and co-workers[12] and not included in our theory does not appear to be important. The localization length ξ obtained from (9) and plotted in Fig. 2, is in excellent agreement with the numerical results for $d=1$ and $d=2$, but in good agreement only for $d=3$. Whether the remaining discrepancy is due to the single-site approximation (CPA) being not quite adequate and the approximation adopted in deriving the SCT being insufficient, or else the numerical extrapolation procedure being less convergent in higher dimensions remains to be seen. The obvious trend is for the CPA to become more reliable and for the numerical finite-size scaling used in Ref. 25 to be more slowly convergent in higher dimensions ($d=2,3$). Also indicated in Fig. 2 are the asymptotic power laws in $W(d=1,2,3)$ as obtained analytically from (9). For strong coupling ($W\rightarrow\infty$), the localization length decreases as $W^{-1/2}$. The results of Ref. 25 appear to follow this law, although for $d=1$ and particularly for $d=3$, the data do not extend sufficiently far into the strong-coupling region.

In conclusion, we have derived a quantitative theory of Anderson localization within the limitations of the SCT for a tight-binding model with arbitrary site-diagonal disorder in any dimension. The dc conductivity and localization length calculated for the box-shaped distribution and nearest-neighbor hopping are in very good agreement with "exact" numerical results for finite-size systems considering that the theory has no adjustable parameters. A detailed discussion and further results for the frequency-dependent conductivity and other level distributions will be given elsewhere.

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