Self-consistent scaling theory of the metal-insulator transition in disordered systems

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We propose a self-consistent description of the diffusion of electrons dressed by the Coulomb exchange interactions in a disordered system, as the metal-insulator transition is approached from the metallic side. The critical anomalies of the single-particle density of states and dielectric function are evaluated each in terms of the other. New scaling laws between the critical behaviors of these quantities as well as the diffusion constant and the frequency-dependent conductivity are obtained. It is argued that the density of states which appears in the expressions for the conductivity and the dielectric function becomes the anomalous one for frequencies higher than some relaxation rate of the many-body system.

The transition at very low temperatures of a conductor to an insulator[1-4] as a function of increasing disorder is qualitatively understood for noninteracting electrons on the basis of the scaling theory[5] of Anderson localization[6] (see, however, Ref. 7). This transition is caused by the mobility edge, E_m, crossing the Fermi energy, E_F. However, the effects of electron-electron interactions become important near the transition and modify it markedly. It has recently become clear[8-10] that these interactions play a much more important role in disordered conductors than in pure ones. Since the interactions can by themselves precipitate a Mott-Hubbard[1] type metal-insulator transition even in ordered systems, it is not surprising that they should become relevant near the disorder-induced transition as well. In fact, the interaction-induced single electron density of states (DOS), $n(E)$, anomalies[11-14] have been experimentally found to increase as the system approaches the transition from the metallic side, an effect which appears to be the precursor of the Coulomb gap[15,16] below the transition [$n(E_F)=0$ at the transition and in the insulating phase].

Guided by these observations, McMillan[17] has recently constructed a heuristic renormalization-group (RG) theory of the metal-insulator transition with both localization and exchange interaction being relevant. He has obtained a second-order transition with a dc conductivity, σ, that vanishes continuously as the transition is approached from the metallic side. McMillan's pioneering theory has also yielded the above-mentioned DOS anomalies as well as the divergence of the static dielectric constant, ϵ, as the transition is approached from the insulating side. Specific relationships among the critical exponents characterizing these critical anomalies were derived as well as the temperature and frequency dependence of σ. In this note we treat this problem differently and in a more simple-minded fashion. While the static (equilibrium) DOS, $\partial n/\partial\mu$, is not expected to behave singularly, we propose that above a certain frequency one crosses over to a regime where the ω-dependent single-particle DOS determines the physical properties of the system. This DOS is expected to become singular as the transition is approached. We obtain new and *different* relations among the critical exponents. We hope that our results will be checked by experiments as well as by more detailed theoretical computations. The latter are also necessary in order to obtain numerical values for the two independent exponents of this scaling theory, which our approach does not yield. We argue that our scaling relations rely on general enough arguments so that they have to be obeyed by more detailed theories as well as by real systems.

We start by observing that in the case of noninteracting electrons, where the DOS is noncritical—one can get the critical behavior of both the conductivity and dielectric constant[18-20] from the scaling theory of localization and linear-response theory. In the presence of interactions a critical behavior of the DOS may arise from the exchange correction to the self-energy.[10,17,21] We also treat only the exchange corrections to the self-energy, which should be augmented by the Hartree as well as by higher-order terms in a more complete theory. We follow McMillan[17] in assuming that the critical modified DOS also appears in the conductivity and diffusion constant and enters the linear-response expressions. This should be valid for frequencies above some characteristic rate of the system ω_x.[22] We have put these modifications into the theory, by evaluating the renormalized DOS and dielectric function self-consistently each in terms of the other.

The dependence of the effective energy-level separation on the time scale is analogous to the well-known Franck-Condon effect. Similar effects are expected to occur in other many-body systems.[23]

In the metallic phase the system has a finite macroscopic diffusion constant D which should vanish when the transition is approached with some as yet unknown power, x, of[5] ξ,

$$D \sim \xi^{-x} \ . \tag{1}$$

The divergence of ξ in terms of the experimental control parameter (e.g., the difference[2-4] from the critical concentration) is given in terms of another unknown critical exponent ν, which will not enter into our arguments that will describe everything in terms of powers of ξ. As the transition is approached, the behavior of the static quantities [e.g., the q-dependent dielectric constant $\epsilon(q)$ or $\sigma(q)$] is essentially the same as for noninteracting electrons, since the static screening length $\Lambda_s^2=(4\pi e^2 dn/d\mu)^{-1}$ is a nondiverging quantity. For frequencies $\omega>\omega_x$ one should rather use the critical "dynamical" density of states $n(\omega)$.

Hereafter we assume that[22] $\omega_x<\bar{E}$ [where $\bar{E}\sim D/\xi^2$ is the crossover frequency from the macroscopic to the microscopic (critical) regime[18-20]], which means that at the frequency $\bar{E}$, the effective DOS is the dynamical one. It is

straightforward to consider other scenarios as well (e.g., $\omega_x > \bar{E}$).

As the transition is approached, the behavior of the dielectric constant (for $\omega \gtrsim \omega_x$) as a function of the wave number q is schematically given for small q in Fig. 1. For macroscopic q, $q << 1/\xi$, the metal should screen the Coulomb interactions and therefore $\epsilon(q) \cong 1/q^2\Lambda_d^2$. In contrast with the case of noninteracting electrons,[20] Λ_d should also diverge as the transition is approached, as discussed below. In the microscopic regime, $q >> 1/\xi$, $\epsilon \sim 1/q^{2-\eta}$, where η is the critical exponent associated with the correlation function which is related to the dielectric constant. The coefficient in front of $q^{\eta-2}$ is noncritical.[18] By matching the above two forms at $q \sim 1/\xi$ we obtain for the divergence of Λ_d

$$\Lambda_d \sim \xi^{\eta/2} \ . \tag{2}$$

Note that it follows from Fig. 1 that ϵ diverges like $\xi^{2-\eta}$ as the transition is approached from the insulating side. We assume $\eta \leq 2$. In the limiting case $\eta = 2$ one would obtain $\Lambda_d \sim \xi$, which, however, does *not* necessarily follow from our picture. Note also that our η which conforms to the accepted critical phenomena notation, is equal to $3 - \eta_M$, where η_M is McMillan's η. From the Thomas-Fermi screening theory in the metallic phase (which one would expect to hold in the macroscopic metallic range, as was actually demonstrated in Ref. 20), one finds that Λ_d^2 is proportional to the inverse of the single-particle DOS at the Fermi energy, $n(0)$; thus,

$$n(0) \sim \xi^{-\eta} \ . \tag{3}$$

It now follows from the Einstein relation that the critical vanishing of the low-frequency ($\omega_x \leq \omega < D/\xi^2$) conductivity is given by

$$\sigma \sim \xi^{-x-\eta} \ . \tag{4}$$

The single-particle DOS in the metallic phase near the transition (where energies are measured from the Fermi energy) is schematically depicted in Fig. 2 where $\bar{E} \sim \xi^{-(2+x)}$ (this, incidentally, establishes the dynamic critical exponent z). In the macroscopic range ($E << \bar{E}$), $n(E)$ is given by

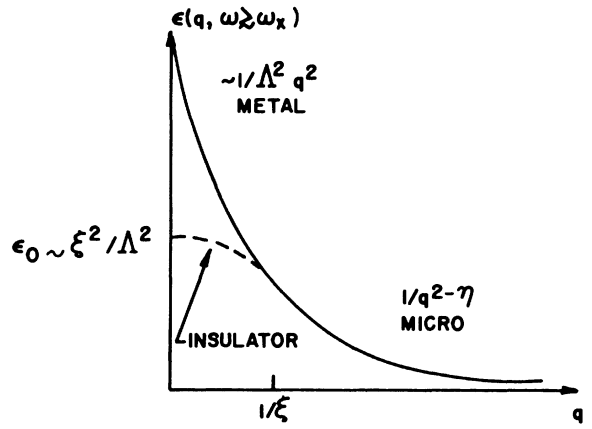

FIG. 1. $\epsilon(q, \omega \gtrsim \omega_x)$ in the metallic phase (full line) and in the insulating phase (dashed line)—schematic. For $q >> 1/\xi$, $\epsilon(q)$ is given by a noncritical constant divided by $q^{2-\eta}$. For $q << 1/\xi$, $\epsilon(q) \sim 1/q^2\Lambda_d^2$, where Λ_d is the metallic dynamic screening length, in the metal and $\epsilon(q) \to \xi^2/\Lambda_d^2 \sim \xi^{2-\eta}$ in the insulator.

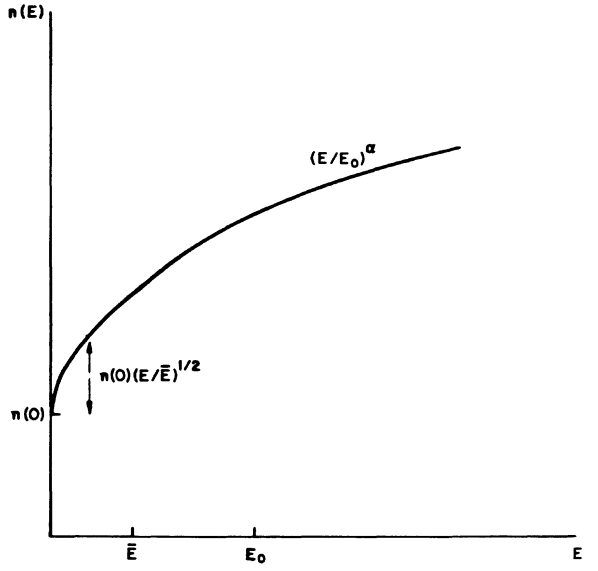

FIG. 2. Schematics of the density of states (in units of the unperturbed one) vs energy (measured from E_F). For $E << \bar{E}$, $n(E) = n(0)[1 + \text{const}(E/\bar{E})^{1/2}]$, and for $E >> \bar{E}$, $n(E) \sim (E/E_0)^{\alpha}$.

$n(0)$ plus a small energy-dependent correction which will be evaluated later. For $E > \bar{E}$, the microscopic range, $n(E)$ is proportional to some power of E [we measure $n(E)$ in units of the unperturbed density of states $n_0(0)$, so the coefficient in Eq. (5) is of order unity]:

$$n(E) \cong (E/E_0)^{\alpha} \ , \tag{5}$$

where α is another critical exponent and E_0 is a (noncritical) scale energy. Of course, at the transition $\bar{E} = 0$ and (5) is valid for every (small) E. Matching (5) with (3) at $\bar{E}$ yields one relation among the critical exponents

$$\alpha = \eta/(2+x) \ . \tag{6}$$

To make further progress we have to analyze the diffusion of a single electron thrown into the electronic sea, on the microscopic scale, $L << \xi$. Since here $D(L)$ depends upon L, the mean-square displacement $\langle x^2 \rangle$, of a wave packet started locally from the origin[10,12,20,21] at $t = 0$, grows with the diffusion constant[24] $D(L \sim (\langle x^2 \rangle)^{1/2})$. Assuming that $D(L)$ is proportional to a power of L for $L << \xi$ and matching with Eq. (1), we find that $D(L) \sim D(L/\xi)^{-x}$ for $L << \xi$. It thus follows that $\langle x^2 \rangle$ grows like $t^{2/(2+x)}$ in the microscopic range. From this we can obtain the dynamic structure factor for the electron,[20,21] by Fourier transforming $\exp[-O(q^2 t^{2/(2+x)})]$ and constructing an interpolation formula between the large and small ω limits

$$S_0(q, \omega) \sim \frac{q^2}{\omega^{(4+x)/(2+x)} + \text{const} q^{4+x}} \ . \tag{7}$$

S_0 can be used to evaluate the wave vector and frequency dependence of both the dielectric constant and the conductivity, in terms of the squares of the matrix elements of e^{iqx} between the eigenstates for the diffusing electron moving in the field of the others. The squares of these matrix elements[10,17,20,21] are proportional to $S_0(q, \omega)$ and to the inverse of $n(\omega)$ (ω is equal to the difference in energy between the initial and final states). We thus find at the

transition, or for $\omega > \bar{E}/\hbar$ (and for $q \to 0$)

$$\sigma(\omega) \sim \omega^{1+\alpha-2/(2+x)} \sim \omega^{(\eta+x)/(2+x)} \ . \tag{8}$$

This (as well as the preceding formulas) generalizes the noninteracting electrons result $\omega^{1/3}$ (where $\alpha = 0$ and $x = 1$). Equation (6) was used to obtain the second equality. Equation (8) is immediately seen to match with the dc result Eq. (4) at $\omega \sim \bar{E}/\hbar$. To obtain the dc conductivity at finite temperatures one replaces ω by the inverse inelastic (or phase breaking) time.

One can now immediately evaluate the correction to the DOS, due to the exchange self-energy $\Sigma(E)$, which is thought to give the main single-particle DOS anomaly in the disordered conductor[17,21]

$$\Sigma(E) \sim \int_{E' < E_F} dE'\, n(E') \int d^3q\, q^{-\eta} \frac{S_0(q, (E-E')/\hbar)}{n((E-E')/\hbar)} \ . \tag{9}$$

This yields correctly $n(0)$ of Eq. (3) with a small "macroscopic" correction of the order of $n(0)(E/\bar{E})^{1/2}$ for $E << \bar{E}$ (see Fig. 2) and the form (5) for $E >> \bar{E}$, with $E_0 \sim D\xi l^{-3}$ (l being the relevant microscopic length, e.g., the elastic mean free path) with

$$\alpha = \frac{x+\eta-1}{2+x} \ , \tag{10}$$

which together with Eq. (6) yields

$$x = 1 \ . \tag{11}$$

This is one of our main results and may also be obtained by requiring that E_0 is not critical. This means physically that in terms of ξ the vanishing of D in the interacting system is identical to that of both σ and D in the noninteracting system. However, in the interacting system, σ picks up a factor $\xi^{-\eta}$ due to the DOS correction (for $\omega_x < \omega < \bar{E}/\hbar$).

We have checked the full q and ω dependencies of both σ and ϵ. Everything is consistent with the picture presented so far. For example, the behavior of Fig. 1 is recovered for $\epsilon(q, \omega \gtrsim \omega_x)$ and the appropriate behavior for $\sigma(q, \omega > \omega_x)$ can also be obtained. A quantity of interest for the optical properties of the disordered conductor is $\epsilon(\omega, q = 0)$. We find for $\omega >> \bar{E}/\hbar$

$$\epsilon(\omega) \sim \omega^{\alpha-2/3} \ , \tag{12}$$

which is, of course, valid for all frequencies at the transition.

It is also interesting to notice that under our assumptions one might expect that near the transition the frequency-dependent conductivity should cross over from its static value to a much lower dynamical value [i.e., one should take into account the critical $n(\omega)$ when ω becomes larger than ω_x]. This is true in principle for other quantities as well.

An important question is how close does the transition have to be approached in order for the above interaction effects to be felt. The condition for this is that the depression of the DOS be significant so that the increase in Λ has to be taken into account self-consistently. This is not the case in the weak localization case where only a small $\sqrt{E}$ anomaly is obtained[12-14] due to exchange interactions even in the simplest localization picture. Once the scale energy E_0 is much larger than the crossover energy, $\bar{E}$, the microscopic $(E/E_0)^{\eta/3}$ behavior and a strong DOS anomaly will occur. This happens when $\xi >> l$.

To summarize, by using the renormalized density of states and dielectric function self-consistently, we have constructed a scaling theory of the approach to the transition from the metallic side. The exponents α, η, and x, in terms of which all the critical behaviors of the relevant physical quantities are given, satisfy the relationships

$$x = 1; \ \alpha = \eta/3 \ . \tag{13}$$

Thus, everything is determined by η (or by η and ν in terms of the physical parameters). Our relationships are different from those obtained from the pioneering approximate RG calculation by McMillan.[17] In particular, the results for $\sigma(\omega)$ and $\epsilon(\omega)$ are new. We are currently considering the insulating phase where the Hartree terms are of decisive importance[15,16,25] as well as the two-dimensional case. These terms may also be relevant for low-density conductors close to the transition. Measurements of the temperature and frequency dependence of σ and ϵ near the transition,[2] as well as of the critical behavior of the DOS[11-13] should yield stringent tests on our relationships as well as specific determinations of the values of η and ν. Of special interest are the optical properties in the far-infrared range resulting from this theory.

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