Dielectric anomalies near the Anderson metal-insulator transition

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The linear-response expressions for the dielectric constant and conductivity as functions of wave number and frequency are evaluated near the localization metal-insulator transition for noninteracting quasiparticles. New behavior is found in the microscopic range. The static dielectric constant from the insulating side is found to diverge with twice the exponent characterizing the vanishing of the conductivity from the metallic side. The dynamic structure factor follows easily from our expressions and we suggest that it can be measured, in principle, using high-frequency electromagnetic radiation.

The ability of a metal to screen the Coulomb interaction totally at large distances is an important characteristic of the conducting state of matter. This is related to the wave-vector ($\vec{q}$)-dependent static dielectric constant $\epsilon(\vec{q},\omega=0)$ (Ref. 1) diverging as q^{-2} when $q\to 0$. In the insulating phase, however, $\lim_{q\to 0}\epsilon(\vec{q},0)\equiv\epsilon_0$ is finite. Near a continuous metal-insulator transition, one would thus expect a diverging ϵ_0 from the insulating side. This is shown here to be the case for the localization, disorder-induced transition, according to the scaling theory[2] for it. Interesting and unusual frequency dependence of both $\epsilon(\vec{q},\omega)$ and conductivity $\sigma(\vec{q},\omega)$ may therefore also be expected, resulting in rather exotic optical properties. In fact, such anomalies are known to exist[3] near the percolation threshold in a metal-insulator macroscopic composite.

In this Brief Report we establish the critical behavior of $\epsilon(\vec{q},\omega)$ and $\sigma(\vec{q},\omega)$ near the localization transition for a degenerate fermion system in a self-consistent potential for frequencies much smaller than the inverse elastic relaxation time. Important differences exist between this case and that of the macroscopic composite. These may allow an experimental discrimination between a genuine localization transition and the one dominated by large scale inhomogeneities, which result in percolation-type behavior. We also present results for $\sigma(\vec{q},\omega)$ and $\epsilon(\vec{q},\omega)$ in the "microscopic" range, relevant for higher frequencies (or temperatures) and smaller wavelengths, where different power laws are obtained. From the theoretical point of view, the understanding of the correlation function[4] related to the dielectric response[5] may help in elucidating the physical meaning of the order parameter associated with localization. Understanding the screening is also crucial in order to incorporate properly the electron-electron Coulomb interaction effects,[6] of relevance in real physical systems. In fact, similar phenomena may well occur near the Mott-Hubbard metal-insulator transition caused by the interactions[7] even without disorder. Interesting speculations related to this have been made by Toulouse.[8] Recent experiments on doped Si (Ref. 9) are in a good agreement with the scaling laws obtained here. We shall consider in this paper only the three-dimensional case where a mobility edge is believed to exist.

A simple scaling-type argument[10] giving heuristically the scaling law relating the diverging ϵ_0 from the insulating side to the vanishing $\sigma(0,0)$ from the metallic side follows by considering Fig. 1. Here, the static dielectric constant $\epsilon(\vec{q},0)$ is schematically depicted as a function of q for the metallic and insulat-

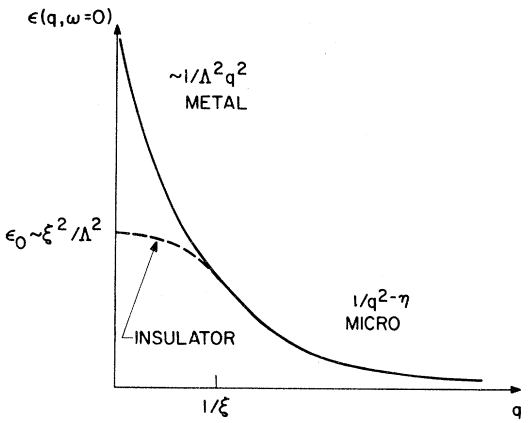

FIG. 1. The static dielectric constant $\epsilon(q,0)$, as a function of q (schematic). For $q\gg 1/\xi$, both the metal and the insulator are expected to have a dielectric constant $\sim A/q^{2-\eta}$ where A is a constant. For $q\ll 1/\xi$ the metal should show screening [$\epsilon(q,0)\sim q^{-2}$] while for the insulator, $\lim_{q\to 0}\epsilon(q,0)$ is a finite constant ϵ_0.

ing phases in both the "microscopic" $q \gg 1/\xi$ and the macroscopic $q \ll 1/\xi$ ranges.[11] In the former range the two phases are indistinguishable, displaying in general a $q^{2-\eta}$ behavior of ϵ, where η is the usual critical exponent associated with the anomalous dimension of ϵ. In the latter range the metallic phase is expected to display screening $\epsilon(\vec{q},0)=1/\Lambda^2 q^2$, where Λ is the screening length, while the insulating phase is expected to have an $\epsilon(\vec{q},0)$ tending to a finite limit ϵ_0, as $q \to 0$. Since as $q \to 1/\xi$ from below the dielectric functions for both phases should be similar, and because $\epsilon(\vec{q},0)$ does not change much for $q < 1/\xi$ in the insulator, it follows that the order of magnitude of ϵ_0 should be

$$\epsilon_0 \sim \xi^2/\Lambda^2 \sim \xi^{2-\eta}\,, \tag{1}$$

(one has $\Lambda^2 \sim \xi^\eta$ by matching the two above forms at $q \sim 1/\xi$), i.e., it diverges with $(2-\eta)$ times the exponent characterizing the vanishing[2,12] of $\sigma(0,0)$ (given by $\sim e^2/\hbar\xi$) when the transition is approached from the metallic phase. This relation, with $\eta \cong 0$, is consistent with the experimental results of Ref. 9. The same exponent ratio becomes on the order of $0.3-0.5$ for the macroscopic composite case.[3] One may feel that this difference in the ratio is large enough to make the two cases experimentally distinguishable. The approximate calculations reported here for noninteracting quasiparticles support the picture of Fig. 1 and Eq. (1) and turn out to produce a value of $\eta=0$ so that the above exponent ratio is exactly *2*. The total frequency-dependent $\epsilon(\vec{q},\omega)$ and $\sigma(\vec{q},\omega)$ are given. Our expressions enable one to easily obtain the dynamic structure factor $S(\vec{q},\omega)$ for the disordered system—a quantity which is, in principle, measurable. Recently, McMillan[13b] constructed a scaling theory[2,12(a)] with Coulomb interaction effects. Near the fixed points *with interactions*, he finds (1) with $0<\eta<2$ (his η is 3 minus ours). Our results are near the *no interaction* fixed point and can be obtained from Ref. 13(b) by putting $\eta=0$ (or McMillan's η to be 3). However, we obtain full screening throughout the metallic phase and at the transition. We believe that out treatment clarifies the relations between diffusion and screening in the various regimes.

We start from the linear-response formula[1] for the complex dielectric function

$$\tilde{\epsilon}(\vec{q},\omega)=\epsilon(\vec{q},\omega)+(4\pi i/\omega)\sigma(\vec{q},\omega),$$

which is exact for noninteracting fermions

$$\tilde{\epsilon}(\vec{q},\omega)=1-\lim_{\eta\to 0}\frac{4\pi e^2}{Vq^2}\int dE_i N(E_i)\int dE_f N(E_f)\,|\langle f|e^{i\vec{q}\cdot\vec{r}}|i\rangle|^2\frac{f(E_i)-f(E_f)}{E_i-E_f+\hbar\omega+i\eta}, \tag{2}$$

where V is the volume of the system, $N(E)$ the density of states per unit energy whose variation with E for small E will be neglected [later we denote $n(E)\equiv N(E)/V$], $f(E)$ is the Fermi function, E is measured from the Fermi energy and $|i\rangle$ and $|f\rangle$ are exact single-particle states. Following suggestions in Refs. 6(c) and 13 one can derive a relation between the matrix elements in Eq. (2) and a dynamic structure factor[14] $S_0(\vec{q},\omega)$, for quantum diffusion, defined in the following way. At $t=0$ the particle is started with a wave packet around the origin which is much narrower than ξ in space and is also of minimal width in energy. Then

$$S_0(\vec{q},\omega)=\sum_{i,f}p_i\,|\langle f|e^{i\vec{q}\cdot\vec{r}}|i\rangle|^2\delta(E_f-E_i-\hbar\omega)$$
$$=\int dt\, e^{i\omega t}F(\vec{q},t), \tag{3}$$

where, for a Gaussian distribution (in a semiclassical approximation), which should hold after many elastic collisions,

$$F(q,t)=\exp[-\tfrac{1}{2}q^2\langle r(t)^2\rangle]\,, \tag{4}$$

and p_i are the weights of the initial states $|i\rangle$. Assuming that for the narrow range of E_i considered, the matrix elements squared depend only on energy differences, we find

$$|\langle f|e^{i\vec{q}\cdot\vec{r}}|i\rangle|^2=S_0(q,\omega)/N(0),\quad \omega=E_f-E_i\,, \tag{5}$$

and $\hbar$ is taken as 1. Using (2) and (5) we immediately find

$$\sigma(\vec{q},\omega)=\frac{\pi\omega^2e^2}{q^2}n(0)S_0(\vec{q},\omega)$$
$$\left[\underset{q<<1/\xi}{\to}\frac{e^2n(0)D\omega^2}{(Dq^2)^2+\omega^2}\ \text{or}\ \frac{\sigma(0,0)\omega^2}{(Dq^2)^2+\omega^2}\right], \tag{6}$$

where to get the last expression we used the Einstein relation between D and σ and the linear increase $\langle r^2\rangle=2Dt$ for macroscopic times. From this it follows[14(b)] by (4) that

$$S_0(\vec{q},\omega)=Dq^2/\pi[(Dq^2)^2+\omega^2]\,.$$

Here D is the macroscopic diffusion constant which, within the scaling theory,[2] vanishes like ξ^{-1} when localization is approached from the conducting side. For $q \ll 1/\xi$ the macroscopic expressions are sufficient [see Figs. 2(a) and 2(b)]. This is valid for the conducting phase, where the macroscopic D is finite. It is now straightforward to obtain the real part corresponding to Eq. (6) of the dielectric constant,

$$\epsilon(\vec{q},\omega)=1+\frac{4\pi n(0)e^2DDq^2}{(Dq^2)^2+\omega^2}\,. \tag{7}$$

These expressions,[6(c)] valid at low frequencies, yield the optical properties of the conductor for $q \ll 1/\xi$.

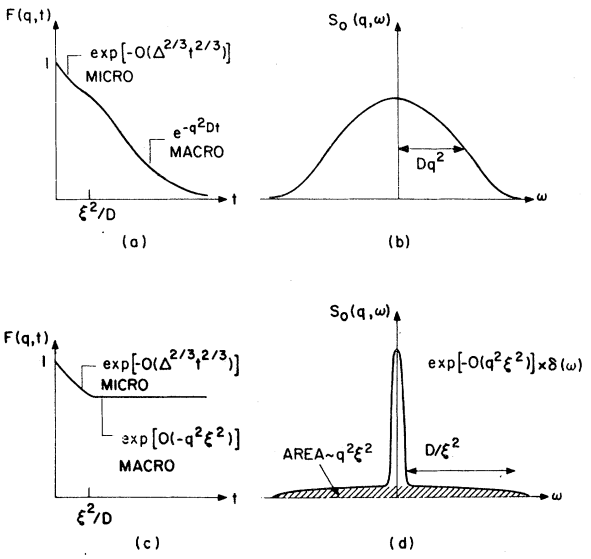

FIG. 2. Schematics of $F(q,t)$ and $S_0(q,\omega)$ in the metallic and insulating phases for $q \ll 1/\xi$: (a) $F(q,t)$ for the metal, changes around $t \sim \xi^2/D$ from $\exp[-O(\Delta^{2/3}t^{2/3})]$ to $\exp(-q^2Dt)$; (b) $S_0(q,\omega)$ for the metal, a Lorentzian of width Dq^2; (c) $F(q,t)$ for the insulator, saturates at $\exp[-O(q^2\xi^2)]$ for $t > \xi^2/D$; (d) $S_0(q,\omega)$ for the insulator, consists of a dominant $\delta(\omega)$ part and a broad background of weight $O(q^2\xi^2)$. Here D is the macroscopic diffusion constant for the metal at the same ξ.

We would now like to extend them to the microscopic ($q \gg 1/\xi$) range and to the insulating phase.

Let us start with $\omega = 0$ to simplify the calculation, and take $Dq^2 \ll kT \ll E_f$ (assuming a degenerate Fermi system). Essentially similar results hold also at the $T \to 0$ limit. The Fermi function is now smooth on the relevant range of $(E_f - E_i)$ and one may replace $[f(E_f) - f(E_i)]/[E_f - E_i]$ by $f'(E_i)$ to get

$$\epsilon(\vec{q},0) = 1 + \frac{4\pi e^2}{q^2} n(0) P \int_{-\infty}^{\infty} S_0(\vec{q},\omega)\, d\omega \ . \quad (8)$$

$S_0(\vec{q},\omega)$ satisfies the sum rule $\int S_0(\vec{q},\omega)\, d\omega = F(\vec{q},0) = 1$. Thus $\epsilon(\vec{q},0) = 1 + 1/\Lambda^2 q^2$, where $\Lambda = [4\pi e^2 n(0)]^{-1/2}$ is the Thomas-Fermi screening length. (Notice that in this picture we ignore the electron-electron interactions. Inclusion of these interactions[13(b)] induces a change in the density of states and the screening length may thus be different.) This is valid in the whole metallic range, including the macroscopic and microscopic domains (i.e., $\eta = 0$). The situation in the insulating phase is different, however. The wave packet at $T = 0$ consists only of states that are localized near the origin and thus can never escape from a volume of the order of ξ^3, so that as $t \to \infty$, $r^2(t) \to O(\xi^2)$. From this and the microscopic range, discussed later, follow the schematic forms of $F(\vec{q},t)$ and $S_0(\vec{q},\omega)$ for the insulator depicted in Figs. 2(c) and 2(d). The localization thus endows $S_0(\vec{q},\omega)$ with a $\delta(\omega)$ part which is dominant for $q \ll 1/\xi$. It does not contribute to the principal part of Eq. (8) and only the small smooth background of area $O(q^2\xi^2)$ contributes. Thus, for the insulating phase, for $q \ll 1/\xi$, $\epsilon(\vec{q},0) \sim \xi^2/\Lambda^2$ in agreement with the heuristic expectation of Eq. (1). The background part [Fig. 2(d)] of $S_0(\vec{q},\omega)$ was also estimated explicitly. Using Eq. (6) we obtain an expression for the conductivity in the insulating phase for $q \ll 1/\xi$. We interpolate between the low- ($\omega \ll D/\xi^2$) and high- [$\omega \gg D/\xi^2$, similar to Eq. (10) below] frequency regimes:

$$\sigma(\vec{q},\omega) \sim \frac{\omega^2 e^2 n(0)(D\xi)^{2/3}}{A_1\omega^{5/3} + A_2(D/\xi^2)^{5/3}} \ , \quad (9)$$

where here and in the following expressions A_i ($i = 1,2,\ldots,$) stand for numerical coefficients of order unity. At low frequencies[15] the leading term is

$$\sigma(\vec{q},\omega) \sim \sigma_m(0,0)[\omega/(D/\xi^2)]^2 \ ,$$

where $\sigma_m(0,0)$ is the metallic conductivity at the same $\xi(\sim e^2/\hbar\xi)$. This divergence of the coefficient of ω^2 in $\sigma(\omega)$ as the transition is approached was first obtained by Wegner.[12(b)] The dielectric constant in the insulating regime is likewise given by

$$\epsilon(q,\omega) = 1 + 4\pi e^2 n(0) \frac{(D\xi)^{2/3}}{A_3\omega^{2/3} + A_4(D/\xi^2)^{2/3}} \ .$$

We now focus our attention on the microscopic behavior for $t < \xi^2/D$, which dominates what happens at $q > 1/\xi$ and/or $\omega > D/\xi^2$. According to the scaling theory[2,16] the diffusion constant $D(L)$ is length-scale (L) dependent, and, in fact, it is proportional to $1/L$ for $L \ll \xi$. It thus follows[16] that $\langle r^2(t)\rangle \sim t^{2/3}$, and $F(q,t) = \exp[-(\Delta t)^{2/3}]$ where $\Delta \sim D\xi q^3$, D again being the macroscopic diffusion constant. It is now possible only to evaluate $S_0(\vec{q},\omega)$ for $\omega \ll \Delta$ and $\omega \gg \Delta$, a convenient interpolation formula being

$$S_0(q,\omega) = \frac{A_5\Delta^{2/3}}{A_6\Delta^{5/3} + \omega^{5/3}} \ . \quad (10)$$

This yields from (6) the conductivity in the microscopic (both metal and insulator!) range.[17] For $\omega \sim \tau_{\rm in}^{-1}$ and $q \sim l_{\rm in}^{-1}$, where $l_{\rm in}^3 \sim D\xi\tau_{\rm in}$, this agrees with the dc conductivity in the microscopic range previously discussed,[16] and has important consequences as far as the temperature dependence of the low-frequency conductivity is concerned. One can also evaluate $\epsilon(\vec{q},\omega)$ in this range, which yields again an interpolation form

$$\epsilon(\vec{q},\omega) = 1 + \frac{4\pi e^2 n(0)}{q^2} \frac{A_7\Delta^{2/3}}{A_8\omega^{2/3} + \Delta^{2/3}} \ . \quad (11)$$

The static $\epsilon(\vec{q},0)$ can be evaluated at $T = 0$, which again yields $\epsilon(\vec{q},0) = 1 + 1/q^2\Lambda^2$.

To summarize: The linear-response expressions for $\epsilon(\vec{q},\omega)$ and $\sigma(\vec{q},\omega)$ can be evaluated around the localization transition. In particular, the static dielectric constant for the insulator is shown to diverge, for noninteracting quasiparticles, with an exponent twice that characterizing the vanishing of the conductivity from the metallic side, a result which is quite different from the macroscopic composite case. New expressions and power laws are found in the microscopic range. All these quantities appear to satisfy a sort of dynamic scaling[5(a)] which will be discussed, along with the detailed optical properties elsewhere.

Finally, it is straightforward to evaluate from our expressions and well-known general relationships the physical dynamic structure factor $S(\vec{q},\omega)$ for the degenerate disordered Fermi system [which is, of course, different from the hypothetical $S_0(\vec{q},\omega)$ used here]. We would like to suggest that this can be measured, in principle, by scattering high-frequency electromagnetic radiation to which the system is relatively transparent. For low-density conductors such as In_2O_{3-x}, this includes visible light.[18] This may prove to be a further useful way to probe the details of these systems.

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