Density of states and screening near the mobility edge

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Perturbation in the interaction strength is performed in the vicinity of the fixed point in the Anderson-localization problem. Logarithmic corrections to the single-particle density of states are found for all dimensionality $d \geq 2$. We also comment on the screening process near the mobility edge.

I. INTRODUCTION

The past few years have seen impressive progress in our understanding of the Anderson localization problem[1,2] as well as of the effects of electron-electron interaction in weakly disordered metals.[3,4] For noninteracting electrons the scaling description of the localization problem predicts a metal-insulator transition for dimensionality $d > 2$. However, interaction effects are expected to play important roles in the vicinity of the transition. McMillan[5] developed a description of the transition region based on extrapolation of the results of Ref. 1–4 to the critical region. However, a quantitative theory of the metal-insulation transition does not exist. As a first step towards the construction of such a theory, we explore in this paper the perturbation expansion in the interaction strength in the vicinity of the localization fixed point. We also comment on the treatment of screening by McMillan and emphasize the distinction between the single-particle density of states and the thermodynamic density of states $dn/d\mu$ which enters in the Thomas-Fermi screening expression. We point out several possible scenarios which the theory could take. Our discussion is heuristic and serves in the interim until a quantitative scaling theory is available for the interacting disordered problem.

II. DENSITY OF STATES NEAR THE MOBILITY EDGE

In this section we study a model problem of Fermions in a disordered medium interacting via a short-range, static potential $v(\vec{q})$. The question of screening in a Coulomb system will be discussed in the next section. The single-particle density of states at energy E measured relative to the Fermi energy is given by

$$N_1(E)=\frac{N_0}{1+d\Sigma/dE}\ , \tag{2.1}$$

where N_0 is the noninteracting density of states. In the formulation in terms of exact eigenstates $\Psi_m(\vec{r})$ of the disordered system,[6] the self-energy is given to lowest order in $v(q)$ by

$$\begin{aligned}\Sigma(E)&=\frac{1}{N_0}\sum_m [\delta(E-E_m)\Sigma_m]_{\text{av}}\\ &=-\frac{1}{N_0}\int_{-\infty}^{0} dE'\,d\vec{r}\,d\vec{r}\,'F(E,E',\vec{r},\vec{r}\,')\\ &\qquad\times v(\vec{r}-\vec{r}\,')\ ,\end{aligned} \tag{2.2}$$

where

$$\begin{aligned}F(E,E',\vec{r},\vec{r}\,')=\sum_{m,n}&[\delta(E-E_m)\delta(E'-E_n)\Psi_m^*(\vec{r})\\ &\times\Psi_n^*(\vec{r}\,')\Psi_m(\vec{r}\,')\Psi_n(\vec{r})]_{\text{av}}\end{aligned} \tag{2.3}$$

and the square brackets with subscript "av" denote impurity averaging. Quite generally, F can be related to the density-density response function

$$\begin{aligned}A(q,\omega)=\int_{-\infty}^{\infty}& dt\,d\vec{r}\,d\vec{r}\,'e^{i\omega t}e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}\\ &\times\langle[\rho(\vec{r},t),\rho(\vec{r}\,',0)]\rangle\end{aligned} \tag{2.4}$$

by

$$A(q,\omega)=\omega\int F(\omega,\vec{r})e^{i\vec{q}\cdot\vec{r}}d\vec{r}\ , \tag{2.5}$$

so that

$$\frac{d\Sigma}{dE}=\frac{1}{N_0}\int d\vec{q}\,\frac{v(q)A(q,\omega)}{\omega}\ . \tag{2.6}$$

In an earlier work[6] $A(q,\omega)$ was computed in the weak-impurity-scattering limit, so that

$$A(q,\omega)=\frac{dn}{d\mu}\frac{\omega Dq^2}{\omega^2+(Dq^2)^2} \tag{2.7}$$

and $\ln\omega$ and $\omega^{1/2}$ corrections to the density of states were found in two and three dimensions, respectively.[3,4] We now extend this treatment to the strongly disordered region by assuming that the noninteracting disordered system is describable by a one-parameter scaling theory.[1] In a one-parameter theory there is only one critical exponent ν for the correlation length ξ,

$$\xi=\left|\frac{t-t^*}{t}\right|^{-\nu}, \tag{2.8}$$

where $t=g^{-1}$ and the dimensionless scaling variable is

$$g=G/(e^2/\hbar), \tag{2.9}$$

which is the conductance G in units of $e^2/\hbar$. This means that all physical quantities scale according to their natural dimensions and the critical exponent η becomes trival, i.e.,[2,7,8]

$$\eta=2-d. \tag{2.10}$$

(Unfortunately, our η has a different meaning from McMillan's η as well as from the η of Gefen and Imry.[9])

Accordingly, even in the critical region the density-density correlation function can be written as

$$A(q,\omega)=\frac{dn}{d\mu}\frac{\omega D(q,\omega)q^2}{\omega^2+[D(q,\omega)q^2]^2}, \tag{2.11}$$

where the diffusion constant becomes q and ω dependent. The full scaling behavior of $D(q,\omega)$ is discussed in detail elsewhere.[10,11] Here we just present a heuristic discussion on the limiting cases. It is convenient to introduce

$$\sigma(q,\omega)=\frac{dn}{d\mu}D(q,\omega). \tag{2.12}$$

In the $q,\omega\to 0$ limit this is the Einstein relation. Note that what enters in Eq. (2.12) is the thermodynamic density of states $dn/d\mu$ and not the single-particle density of states N_1. This is clear from considering σ and D as the current response to a potential and density gradient, respectively. This distinction is important when interaction is taken into account, because N_1 contains a singularity near the Fermi energy whereas $dn/d\mu$ is a smooth function of density or disorder. Gefen and Imry[9] have written down Eq. (2.12) with N_1, which I believe to be in error.

The assumption of one-parameter scaling implies that $\sigma(q,\omega)$ obeys the following scaling relation:

$$\sigma(q,\omega)=g^*\xi^{2-d}F(x,y), \tag{2.13}$$

where g^* is the fixed-point conductance and F is a dimensionless function of two dimensionless variables,

$$x=i\omega\frac{dn}{d\mu}\xi^d \tag{2.14}$$

and

$$y=\xi q. \tag{2.15}$$

For x,y smaller than unity we are outside of the critical region and $F\approx 1$. This gives the by now familiar result

$$\sigma=g^*\xi^{2-d}. \tag{2.16}$$

For $y\gg 1$, i.e., on a length scale $L\ll\xi$, we are in the critical region. The conductivity or diffusion constant is scale dependent,[1] $\sigma\sim g^*L^{2-d}$. We now consider the static limit of Eq. (2.13) where F is a function of y only. In the critical region $\xi\to\infty$ and σ must be independent of ξ. This implies that $F\sim y^{d-2}$ and

$$\sigma(q,0)=Ag^*q^{d-2}, \tag{2.17}$$

where A is a numerical constant that cannot be determined by the scaling arguments. The q dependence of Eq. (2.17) conforms with the conventional definition of η in terms of the density-density response function and agrees with Eq. (2.10).

We are now ready to evaluate $d\Sigma/dE$ using Eqs. (2.6) and (2.11). We note that the important region of integration is

$$D(q,\omega)q^2>\omega, \tag{2.18}$$

which is the static limit. D is a function of q only and we have the following limits:

$$D(q)q^2=\begin{cases}D_\xi q^2, & q\xi\ll 1 & (2.19a)\\ \alpha q^d, & q\xi\gg 1, & (2.19b)\end{cases}$$

where

$$D_\xi=(dn/d\mu)^{-1}g^*\xi^{2-d} \tag{2.20}$$

is simply a restatement of Eq. (2.16) and where

$$\alpha=Ag^*/(dn/d\mu). \tag{2.21}$$

The integral in Eq. (2.6) can be evaluated approximately by decomposition into two sections:

$$\frac{d\Sigma}{dE}=I_1+I_2, \tag{2.22}$$

where

$$I_1=S_d\int_0^{\xi^{-1}}dq\,q^{d-1}\frac{v(0)D_\xi q^2}{E^2+(D_\xi q^2)^2} \tag{2.23}$$

and

$$I_2=S_d\int_{\xi^{-1}}^{l^{-1}} dq\, q^{d-1}\frac{v(0)\alpha q^d}{E^2+(\alpha q^d)^2} \qquad (2.24)$$

The factor $S_d=2\pi^{d/2}/\Gamma(d/2)$ is the angular integration constant and we have used the fact that for the noninteracting system $dn/d\mu=N_0$. We have also taken the $q\to 0$ limit in $v(q)$ because the singularity of the intergrand occurs for small q. Evaluation of Eq. (2.24) gives

$$I_2=-\frac{v(0)}{\alpha}\frac{S_d}{d}\frac{1}{2}\ln\left[\left[\frac{E}{\alpha l^{-d}}\right]^2+\left[\frac{\xi}{l}\right]^{-2d}\right]. \qquad (2.25)$$

The most interesting feature of this result is that we obtain logarithmic singular for all dimensions greater than 2.

It is useful to introduce the crossover frequency

$$\bar{E}=\alpha\xi^{-d}. \qquad (2.26)$$

We now evaluate I_1 in two limits. For $E\gg\bar{E}$ we obtain

$$I_1\approx v(0)\frac{S_d}{\alpha}\left[\frac{\bar{E}}{E}\right]^2, \qquad (2.27)$$

which is negligible compared with I_2 in this limit. For $E\ll\bar{E}$ we obtain

$$I_1=\frac{v(0)S_d}{(d-2)D_\xi^{d/2}}(\bar{E}^{(d-2)/2}-E^{(d-2)/2}). \qquad (2.28)$$

For $d=3$ this is the old $E^{1/2}$ result, but with D replaced by D_ξ.

To summarize, in lowest order in $v(0)$ the density of states is given by

$$N_1=N_0\Big/\left[1-\frac{v(0)}{\alpha}\frac{S_d}{d}\ln(E\tau)\right] \qquad (2.29)$$

for $E\gg\bar{E}$. We have used the fact that for $k_F l\approx 1$,

$$\alpha l^{-d}\approx\alpha k_F^{d-1}l^{-1}\approx v_F l^{-1}\approx\tau^{-1}$$

up to a numerical constant, where τ is the elastic scattering time. For $E\ll\bar{E}$, we have in three dimensions

$$N_1=N_0/\{1+v(0)S_d[D_\xi^{-3/2}(\bar{E}^{1/2}-E^{1/2})-\alpha^{-1}\ln(l/\xi)]\}. \qquad (2.30)$$

Thus for small E the correction initially begins as $E^{1/2}$ and changes over to $\ln E$ for $E>\bar{E}$. Furthermore, $\bar{E}$ approaches zero near the mobility edge and N_1 goes to zero at the mobility edge in all dimensions greater than two. Clearly we only have the first term in the perturbation theory in v and Eqs. (2.29) and (2.30) are valid only when the corrections are small. However, the perturbation theory should provide the correct qualitative features.

III. SCREENING

For Coulomb interaction, the screened potential in three dimensions is given in the weak-scattering limit as[6]

$$v_s(q,w)=\frac{4\pi e^2}{q^2}\frac{Dq^2-i\omega}{Dk^2-i\omega}, \qquad (3.1)$$

where

$$k^2=4\pi e^2 dn/d\mu \qquad (3.2)$$

is the Thomas-Fermi screening constant. For noninteracting systems Eq. (3.1) continues to hold near the mobility edge, as long as D is replaced by $D(q,\omega)$. The crossover from static to dynamic screening is given by

$$\omega\approx D(q,\omega)q^2. \qquad (3.3)$$

Near the mobility edge D approaches zero and the region of static screening shrinks to zero. However, in the static limit the screening length is still given by Eq. (3.2). We expect Eq. (3.2) to continue to hold even for interacting system, because in the static limit the electron density has time to readjust and screen in the Thomas-Fermi manner. Note that it is $dn/d\mu$ that enters Eq. (3.2) and not the single-particle density of states N_1. We note that $dn/d\mu$ does not contain any singularity; singularities such as those in N_1 are tied to the Fermi energy. McMillian has used Eq. (3.1) and (3.2) to describe screening, but he used N_1 instead of $dn/d\mu$ in Eq. (3.2). The vanishing of N_1 at the mobility edge then leads to a divergence of the screening length. The same approach was adopted recently by Gefen and Imry.[9] We believe that the use of N_1 in Eq. (3.2) is in error and the development that follows from that is suspect. Along the same line the relation between the conductivity and diffusion constant $\sigma=(dn/d\mu)D$ follows from very general grounds by considering current responses to density or potential gradients. The single-particle density of states N_1 should not replace $dn/d\mu$ in the static limit in the way it was done in Ref. 9. Our conjecture that Eqs. (3.1) and (3.2) continue to hold for an interacting system can be tested by perturbation theory in $v(q)$. This calculation is in progress.

Without the use of N_1 in Eq. (3.2) the scaling equations for the conductance g and for the interaction constant decouple. Thus no conclusion can be drawn about the nature of the new fixed point. Our first-order perturbation calculation in $v(q)$ shows that the interaction is a marginal variable in all dimensions $d > 2$ in that it produces a logarithmic correction. Three possibilities remain: (i) The noninteracting fixed point is stable, (ii) a new stable fixed point emerges, and (iii) we have a line of fixed points with variable exponents. Possibility (i) seems unlikely while possibility (iii) is most intriguing. These possibilities can be distinguished only by going to higher order in $v(q)$. Presumably the logarithmic series in Eq. (2.29) will exponentiate and

$$N_1 \propto E^{\gamma} \tag{3.4}$$

for $E \gg \bar{E}$. If a new stable fixed point arises [case (ii)], γ will be a universal constant whereas for a line of fixed points [case (iii)], γ will depend on $v(0)$. Hopefully these possibilities can be distinguished by detailed calculations.

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[1]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).

[2]F. Wegner, Z. Phys. B 35, 207 (1979).

[3]B. L. Altshuler and A. G. Aronov, Zh. Eksp. Teor. Fiz. 77, 2028 (1979) [Sov. Phys.—JETP 50, 968 (1979)].

[4]B. L. Altshuler, A. G. Aronov, and P. A. Lee, Phys. Rev. Lett. 44, 1288 (1980).

[5]W. L. McMillan, Phys. Rev. B 24, 2739 (1981).

[6]E. Abrahams, P. W. Anderson, P. A. Lee, and T. V. Ramakishnan, Phys. Rev. B 24, 6783 (1981).

[7]A. J. McKane and M. Stone, Ann. of Phys. (NY) 131, 36 (1981).

[8]S. Hikami, Phys. Rev. B 24, 2671 (1981).

[9]Y. Gefen and Y. Imry (unpublished).

[10]E. Abrahams and P. A. Lee (unpublished).

[11]See also Y. Imry, Y. Gefen, and D. J. Bergman (unpublished) for a heuristic discussion.