Density of states and critical resistivity of strongly disordered systems

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Recently we proposed that the anomalous diffusion at short length scales associated with localization is responsible for the unusual sensitivity of the high-T_c superconductors to disorder. We showed that the Coulomb pseudopotential in superconductors is a universal function of ρ/ρ_c, where ρ is the resistivity and ρ_c is a critical resistivity characteristic of the system, and obtained relatively small values of ρ_c from the experimental T_c-vs-ρ curves. In the present paper we show that in the strong-disorder region in three dimensions the density of states is also a universal function of the same parameter, so that in the absence of any microscopic calculation of ρ_c, a comparison of the density of states and T_c as function of disorder provides a crucial test of the theory. We find very good agreement with existing data on granular Al. We also find that the density of states has a logarithmic energy dependence in this region, a result independently obtained by Lee. In addition, we make quantitative predictions about where and when to expect this logarithmic correction to be important, and comment on why it has not been observed yet.

I. INTRODUCTION

According to the scaling theory of localization[1] the conductance g of a system of size L is described by a universal function $\beta(g)=d\ \mathrm{lng}/d\mathrm{ln}L$. For large g, $\beta(g)$ can be expanded in powers of $1/g$ where the leading correction comes from the so-called "maximally crossed" diagrams and to a reasonably good approximation it can be assumed to be given by $\beta(g)=1-g_c/g$ in three dimensions (3D) even near the critical conductance g_c. The conductivity $\sigma(L)=g(L)/L$ is then given by $\sigma(L)=\sigma+g_c/L$ where $\sigma=\sigma(\infty)$ is the macroscopic conductivity, so that up to a length scale $L_s=\rho g_c$ determined by the disorder of the system characterized by its resistivity ρ, the conductivity and hence the diffusion coefficient goes roughly as l/L, where l is the mean free path. For strong enough disorder, $L_s \gg l$, this region of scale-dependent diffusion associated with localization becomes significant. We have recently shown[2] that this anomalous diffusion at short length scales gives rise to a highly retarded Coulomb interaction which in turn increases the Coulomb pseudopotential in a strongly disordered superconductor considerably. We proposed that this phenomenon is responsible for the unusual sensitivity of the high-T_c superconductors to disorder.

In the present paper we calculate the change in the density of states as a function of disorder due to the scale-dependent diffusion associated with localization.[1,2] We find that in the strong-disorder regime the density of states is a universal function of ρ/ρ_c where ρ is the resistivity and $\rho_c=l/g_c$ is the critical resistivity characteristic of the system. A microscopic calculation of ρ_c for strongly interacting systems is not yet possible, and values obtained for ρ_c by fitting the T_c-vs-ρ curves of high-T_c superconductors were found[2] to be relatively small compared to the estimated free-electron value,[1] $\sim 10^{-3}\ \Omega\,\mathrm{cm}$ (for $l \sim 5$ Å). Several suggestions were made in Ref. 2 regarding the cause of this renormalization, and our expression (12) for the density of states as a function of ρ/ρ_c provides an independent way of estimating this important localization parameter from tunneling experiments, and hence is a crucial test of the theory. We also find that the well-known $\sqrt{E}$ dependence in 3D for small energy E relative to the Fermi energy crosses over to a logarithmic energy dependence for larger E in the strong-disorder regime. This result has been independently obtained by Lee.[3] In addition, our explicit resistivity dependence allows us to make quantitative predictions about the degree of disorder and the crossover energy beyond which this logarithmic behavior should be observable.

II. DENSITY OF STATES

In terms of the exact eigenstate $\psi_i(\vec{r})$ of the disordered system, the impurity-averaged self-energy $\Sigma(E)$ of an electron of energy E is given by[4]

$$\Sigma(E)=-\int_{-\infty}^{0} dE'\,F(E,E';\vec{r},\vec{r}')v(\vec{r}-\vec{r}')\ , \quad (1)$$

where

$$F(E,E';\vec{r},\vec{r}')=\sum_{i,j}\delta(E-E_i)\delta(E'-E_j)\times\psi_i^*(\vec{r})\psi_j^*(\vec{r}')\psi_i(\vec{r}')\psi_j(\vec{r}) , \tag{2}$$

and $v(\vec{r}-\vec{r}')$ is the Coulomb interaction. Assuming that $F(E,E';\vec{r},\vec{r}')$ can be expected to have the form $F(E-E';\vec{r}-\vec{r}')$, quite generally, Eq. (1) for the self-energy becomes

$$\Sigma(E)=-\int_{-\infty}^{0}dE'\int d\vec{r}\,d\vec{r}'\,dt\,e^{i(E-E')t}\times|\phi(\vec{r},\vec{r}',t)|^2 v(\vec{r}-\vec{r}') , \tag{3}$$

where the quantity

$$|\phi(\vec{r},\vec{r}',t)|^2=\sum_{ij}\psi_i^*(\vec{r})\psi_j^*(\vec{r}')\times\psi_i(\vec{r}')\psi_j(\vec{r})e^{-i(E_i-E_j)t} \tag{4}$$

can be identified either with the density-density correlation function[4] with frequency $\omega=E_i-E_j$, or simply with the probability function of a wave packet[5]

$$\phi(\vec{r}-\vec{r};t)=\sum_i\psi_i^*(\vec{r})\psi_i(\vec{r})e^{-iE_it}$$

set up at $\vec{r}=\vec{r}'$ at $t=0$. In either case it can be expected to have a diffusive behavior given by

$$|\phi(\vec{r},\vec{r}'t)|^2=e^{-|\vec{r}-\vec{r}'|^2/4Dt}/Q(t) , \tag{5}$$

where $Q(t)$ is the normalization factor and D is the diffusion coefficient. Finally, the short-range Coulomb interaction $v(\vec{r}-\vec{r}')$ can be approximated by a δ function $V_c\delta(\vec{r}-\vec{r}')$ without much loss in generality. So the Coulomb self-energy becomes

$$\Sigma(E)=-N_0V_c\int_{-\infty}^{0}dE'\int dt\,e^{i(E-E')t}/Q(t) . \tag{6}$$

The change in the density of states will be given by

$$\delta N(E)=\frac{\partial\Sigma(E)}{\partial E} .$$

As noted in Ref. 2, a scale-dependent diffusion coefficient forces the normalization factor $Q(t)$ to behave very differently at short time scales. However, to calculate the change in the density of states we need a smooth function for $D(r)$ in contrast to the nonsmooth function used there. Here we use the following function for $D(r)$ which has all the appropriate limits, namely $D(r)=D_0l/L_s$, $r\gg L_s$, $D(r)=D_0l/r$, $r\ll L_s$, and $D(r)=D_0$ for $L_s=l$ for all $r>l$:

$$D(r)=D_0\frac{l}{L_s}\left[1+\frac{L_s-l}{r}\right] . \tag{7}$$

The normalization factor $Q(t)$ is then determined by demanding

$$1=\int_0^l d\vec{r}\,\delta(\vec{r}-V_Ft)+\frac{4\pi}{Q(t)}\int_l^\infty dr\,r^2e^{-r^2/4D(r)t} . \tag{8}$$

The integral

$$I=\int_l^\infty dr\,r^2\exp\left[-\frac{r^3}{4D_0lt(L_s-l+r)/L_s}\right] \tag{9}$$

of Eq. (8) can be reduced to

$$I=\frac{2}{3}\left[\frac{zr}{L_s-l}-\gamma(t)\right]e^{-z/\gamma(t)}\Bigg|_{z_0}^{\infty}+\frac{1}{\gamma(t)}\int_{z_0}^\infty dz\,zf(cz)e^{-z/\gamma(t)} , \tag{10}$$

where

$$z=r^3(L_s-l)/2(L_s-l+r) ,$$

$$\gamma(t)=2D_0lt(L_s-l)/L_s ,$$

$$z_0=z(r=l),\quad c=[2/3(L_s-l)]^3 ,$$

and

$$yf(y)=y^{4/3}[(1+\sqrt{1-y})^{1/3}+(1-\sqrt{1-y})^{1/3}] .$$

It turns out that without much error we can use the large-y limit for $yf(y)$ for all y, and set the lower limit of the integral equal to zero. In this simple limit we obtain a continuous function for $Q(t)$,

$$Q(t)\simeq 4\pi\left[2D_0lt\frac{L_s-l}{L_s}+\Gamma(\tfrac{5}{2})(4D_0lt/L_s)^{3/2}\right] . \tag{11}$$

Thus the anomalous term linear in t becomes dominating at short time scales given by $t<(L_s/l)^3\tau/3\pi$ for $L_s\gg l$.

It is now straightforward to calculate the change in the density of states. We get

$$\frac{\delta N(E)}{N_0}=a\ln(1+\sqrt{E\tau/b}) , \tag{12}$$

where

$$a=(3\pi/2)(\mu_0/p_F^2l^2)/(1-\rho_c/\rho) ,$$

$$b=3\pi(\rho_c/\rho)^3/(1-\rho_c/\rho)^2 ,$$

$\rho_c = l/g_c$, and $\mu_0 = N_0 V_c$. Note that Eq. (12) is valid only for $\rho > \rho_c$ where localization effects start becoming important. For weaker disorder where there is no anomalous diffusion region, $L_s = l$, and we must set $\rho = \rho_c$.

We now examine the following various limiting cases of expression (12) for $\delta N(E)/N_0$.

(i) Weak disorder: In this region, $p_F l \gg 1$. There is no localization effect ($L_s = l$) and resistivity is determined by the mean free path of the system. This is the Altshuler-Aronov region.[6] In this region, Eq. (12) becomes $\delta N(E)/N_0 \simeq \sqrt{E/\Delta}$ where

$$\Delta = (8E_F/3\pi\mu_0^2)(p_F l)^3$$

so that $\Delta \sim 1/\rho^3$.

(ii) Intermediate disorder: In this region, the mean free path is already of the order of the lattice spacing and cannot change any further, $p_F l \sim 2$. On the other hand, effects associated with localization just start to become important, i.e., $\rho \gtrsim \rho_c$ in this region. As long as ρ_c/ρ remains comparable to 1, b remains large compared to 1 and we can expand the logarithm. To leading order in $\sqrt{E\tau/b}$, we again have $\delta N(E)/N_0 \simeq \sqrt{E/\Delta}$ where now

$$\Delta = (8E_F/3\pi\mu_0^2)(p_F l)^3(\rho_c/\rho)^3 .$$

Note that $p_F l$ is now a constant with further increase in disorder but Δ still goes as $1/\rho^3$.

(iii) Strong disorder: This is the region where $\rho \gg \rho_c$ so that $b \ll 1$. However, sufficiently close to the Fermi energy one always has a range of E for which $\sqrt{E\tau/b} \ll 1$, and so we always get $\sqrt{E}$ behavior for small enough E. For a given disorder (fixed a and b), the density of states $N(E)$ crosses over from $\sqrt{E}$ dependence to logarithmic dependence on E in accordance with Lee. The crossover occurs around

$$E\tau = 3\pi(\rho_c/\rho)^3/(1-\rho_c/\rho)^2 .$$

For the $A15$ compounds and the rare-earth borides with high superconducting transition temperature,[2] ρ/ρ_c can easily be ~ 5 so that $E\tau$ (crossover) ~ 0.1. However, a logarithmic energy dependence, or at least a deviation from $\sqrt{E}$ dependence, should be evident even much before $E\tau \sim 0.1$. Thus, tunneling experiments on these systems, if done over a wide range of bias voltages, should be able to determine the importance of the effects of nonclassical diffusion associated with localization. Note that the density of states is a universal function of ρ/ρ_c. It was found in Ref. 2 that the superconducting transition temperature T_c of a strongly disordered superconductor is also a function of the same parameter. Since there is only one unknown quantity ρ_c, experimental results on $N(E)$ will be an independent crucial test for the validity of the theory of universal degradation of T_c proposed in Ref. 2.

III. CRITICAL RESISTIVITY: GRANULAR ALUMINUM

Dynes and Garno[7] measured the tunneling density of states $N(E)$ as a function of energy E in granular Al. They seem to find a $\sqrt{E}$ dependence for all the samples they studied. However, the range of bias voltage probed for their most disordered sample, e.g., is only $\sim 10^{-3}$ V, in which a logarithmic dependence may be difficult to distinguish from a $\sqrt{E}$ dependence. It is, however, interesting to note that for $\rho \gtrsim \rho_c$ the density of states has the form

$$N(E) \sim N_0\{1+[E/\Delta(\rho)]^{1/2}\} ,$$

so that we can compare our $\Delta(\rho=\rho_c)$ with their data and estimate ρ_c for granular Al. [Note that Δ is defined by $\delta N(E)/N_0 = \sqrt{E/\Delta}$ so that according to our results it can be defined only for $\rho \gtrsim \rho_c$ where it goes as $1/\rho^3$ and their plot of $\Delta(\rho)$ vs ρ cannot be meaningfully compared for $\rho \gg \rho_c$.] From our expression for Δ in the region $p_F l \sim 2$, $\rho \gtrsim \rho_c$ [region (ii)], and using $\tau^{-1} \sim E_F \sim 3$ eV we get $\Delta(\rho=\rho_c) \sim 2\times 10^2$ eV. There is no experimental point corresponding to values of $\Delta > 10$ eV, but a $1/\rho^3$ line through the nearest available points gives as a rough estimate a value of $\rho_c \gtrsim 10^{-4}$ Ω cm. This is the point where localization effects start becoming important and according to Ref. 2 should be reflected in the superconducting transition temperature T_c-versus-resistivity measurements. In particular the theory predicts that the superconducting T_c should decrease in a universal fashion with increasing resistivity starting from $\rho = \rho_c$. It is found indeed that the initial increase in T_c with resistivity in granular Al is arrested at $\rho \sim 10^{-4}$ Ω cm and for $\rho > 10^{-3}$ Ω cm, T_c decreases with increasing ρ in the universal fashion proposed. Considering the crude approximations used, this agreement is quite remarkable. Note that the mechanism for the initial increase in T_c is not yet known; the present analysis shows that the decrease is due to localization effects, the plateau being probably due to competition between the two mechanisms.

IV. CONCLUSION

In conclusion, we have calculated the change in the density of states as a function of disorder. It is a universal function of ρ/ρ_c and provides an independent way of estimating the localization parameter ρ_c. This provides a crucial test for the theory of universal degradation of superconducting T_c we pro-

posed in an earlier paper. The existing data on granular Al yields good agreement with our theory. We should mention here that ρ_c for granular Al turns out to be close to the free-electron estimate. Tunneling data on, e.g., the $A15$ compounds (which are expected to have much smaller ρ_c), would be very interesting to compare with. Also the crossover to a logarithmic energy dependence should be observable in both granular Al and the $A15$ materials.

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