Superconductor-insulator transition in a disordered electronic system

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We study an electronic model of a two-dimensional s-wave superconductor in a random potential using quantum Monte Carlo simulations. The superfluid density and the strength of the delta function in the optical conductivity are found to vanish beyond a critical disorder. We calculate the temperature-dependent resistivity $\rho_{\rm dc}(T)$ for a highly disordered interacting Fermi system. Using this we identify the nonsuperconducting state as an insulator. [S0163-1829(96)51830-8]

The problem of the effect of strong disorder on superconductivity and of the resulting superconductor(SC)-insulator(I) transition in low-dimensional systems has been studied experimentally for a number of years.[1] Theoretically, the problem is challenging because of the complicated interplay between interactions and disorder.[2] Within mean-field theory,[3] superconductivity persists essentially all the way to the site localized limit due to an inadequate description of the disorder-induced fluctuations of the local order parameter. Much of the recent theoretical effort has focused on the dirty boson problem[4] which is expected to capture the essential physics of these fluctuations. The boson models which are argued to describe universal properties in the vicinity of the SC-I transition are also more amenable to analytical[4] and numerical[5,6] studies. However, if one is interested in characterizing the phases, and testing the universality of the conductance at the transition, one has to go back to a description in terms of the electronic degrees of freedom.

As a first step in this direction we use quantum Monte Carlo (QMC) simulations to study the simplest fermionic problem—the attractive Hubbard model with onsite disorder—which can have superconducting, insulating, and (possibly) metallic phases. Our main results are the following.

(1) At low temperatures, we calculate the superfluid stiffness D_s, a measure of the Meissner effect, and the charge stiffness D, related to the infinite conductivity. We find that $D_s = D$, and that both decrease with increasing disorder V. Beyond a critical V_c the system becomes nonsuperconducting.

(2) We use a simple analytic continuation method to extract the T-dependent dc resistivity $\rho_{\rm dc}(T)$ from QMC data. This method is argued to be valid for disordered systems, and independent checks on its validity are presented.

(3) We find that for $V > V_c$ the system shows insulating behavior with $d\rho_{\rm dc}/dT < 0$.

(4) The resistivity as a function of T and V is also used to independently estimate the critical disorder V_c, which is in good agreement with that obtained from D_s.

(5) Our results are consistent with a direct SC-I transition in two dimensions (2D), without an intervening metallic phase.

Our model is defined by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \sum_{i\sigma} (\mu - v_i) n_{i\sigma} - |U| \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

We set $t=1$ and measure all energies in units of t. Here $c_{i\sigma}$ is a fermion destruction operator at site i with spin σ, $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$, and the chemical potential μ fixes the average density $\langle n \rangle$. The site energies v_i are independent random variables with a uniform distribution over $[-V, V]$. The lattice sum $\langle ij \rangle$ is over near neighbor sites on a two-dimensional square lattice. Note that this model focuses on the localization induced by the disorder; it does not, however, incorporate the disorder-dependence of the effective electron-electron interaction.[2]

QMC simulations have played an important role in the study of model (1) in the absence of disorder ($V=0$): in elucidating its phase diagram[7] and its anomalous normal state behavior.[8] Here we use the same QMC technique,[9] to study the disordered case, which is still free of the the fermion sign problem.

We shall focus on various quantities obtained from the current-current correlation function Λ.[10] The (paramagnetic piece of the) current operator is defined as

$$j_x(\mathbf{l}\tau) = e^{H\tau} \left(it \sum_\sigma (c^\dagger_{\mathbf{l}+\hat{x},\sigma} c_{\mathbf{l},\sigma} - c^\dagger_{\mathbf{l},\sigma} c_{\mathbf{l}+\hat{x},\sigma}) \right) e^{-H\tau}. \quad (2)$$

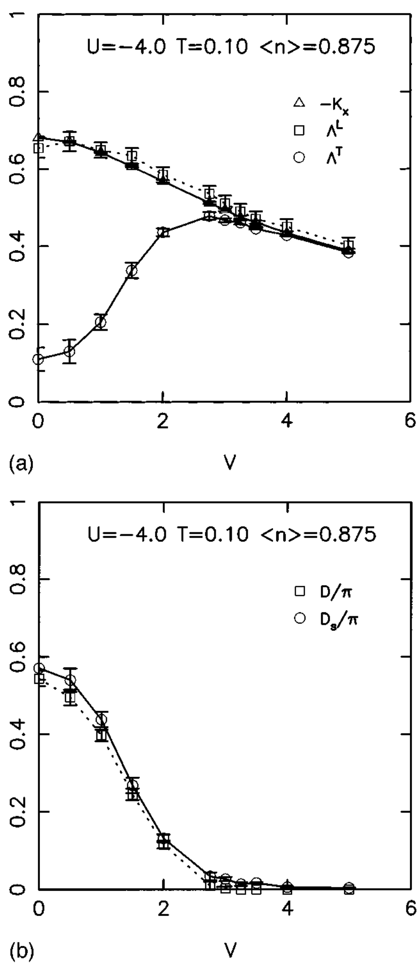

FIG. 1. (a) The kinetic energy, $-K_x$, and transverse and longitudinal current-current correlation functions, Λ^T and Λ^L, are shown as a function of disorder V. Λ^L tracks $-K_x$ as required by gauge invariance. The difference between Λ^T and $-K_x$ signals a nonzero superfluid density [see Eq. (5)]. (b) The superfluid density D_s and charge stiffness D (a measure of infinite dc conductivity) as a function of disorder V. $D_s = D$ for all V.

The *impurity averaged* Λ_{xx} is then given by

$$\Lambda_{xx}(\mathbf{q}; i\omega_n) = \sum_{\mathbf{l}} \int_0^\beta d\tau \langle j_x(\mathbf{l},\tau) j_x(0,0)\rangle e^{i\mathbf{q}\cdot\mathbf{l}} e^{-i\omega_n\tau}, \quad (3)$$

where $\omega_n = 2n\pi/\beta$, and $\langle \cdots \rangle$ denotes a thermal average at a temperature $T=\beta^{-1}$ for a given realization of disorder *and* an average over an ensemble of such realizations.

Gauge invariance requires that the longitudinal part of Λ satisfy the equality[10,11]

$$\Lambda^{\mathrm{L}} \equiv \lim_{q_x\to 0} \Lambda_{xx}(q_x, q_y=0; i\omega_n=0) = -K_x, \quad (4)$$

where $K_x = \langle -t\Sigma_\sigma (c^\dagger_{\mathbf{l}+\hat{\mathbf{x}},\sigma} c_{\mathbf{l},\sigma} + c^\dagger_{\mathbf{l},\sigma} c_{\mathbf{l}+\hat{\mathbf{x}},\sigma})\rangle$, the kinetic energy in the x direction, represents the diamagnetic part of the response. We have verified this equality as a nontrivial check on our numerics; see Fig. 1(a).

The superfluid stiffness D_s is obtained from the transverse current-current correlation function[10,11]

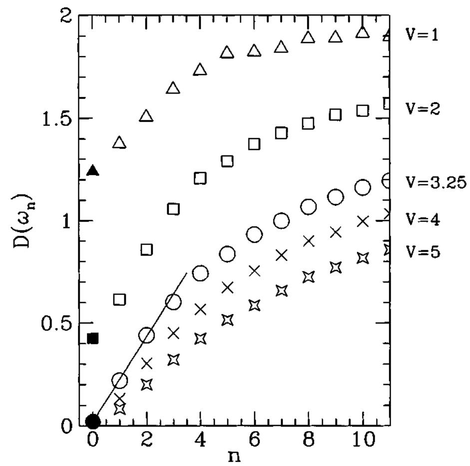

FIG. 2. $D(\omega_n)$ as a function of $n = \omega_n/2\pi T > 0$, for fixed $T=0.1$ and various disorder strengths. The extrapolated value $D(\omega_n \to 0)$ is shown as a solid symbol at $n=0$. For small V this extrapolation yields a nonzero D indicating a SC. For the metallic system $V=3.25(\simeq V_c)$ we obtain σ_{dc} from the slope at small n; see text.

$$\Lambda^T \equiv \lim_{q_y\to 0} \Lambda_{xx}(q_x=0, q_y; i\omega_n=0),$$

$$D_s = \pi[-K_x - \Lambda^T]. \quad (5)$$

Results[12] for Λ^T, Λ^L, and $-K_x$ are plotted in Fig. 1(a) for $U=-4$, $T=0.10$, and $\langle n\rangle = 0.875$ as a function of V. Λ^T is estimated by using a linear extrapolation of the two smallest q_y values. In Fig. 1(b) we plot D_s, which decreases monotonically with disorder. There is a critical value V_c beyond which $D_s=0$ and the system becomes nonsuperconducting. Note that D_s and D (to be defined below) were measured at T low enough that measurements of $\langle c_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c^\dagger_{j\downarrow}\rangle$ confirm that the pairing correlations are well formed across the entire lattice.

We now turn to the conductivity $\mathrm{Re}\sigma(\omega) = D\delta(\omega) + \sigma_{\mathrm{reg}}(\omega)$. The first term represents the infinite dc conductivity of a superconductor, with the charge stiffness (Ref. 10) $D = \pi[-K_x - \lim_{\omega\to 0} \mathrm{Re}\Lambda_{xx}(\mathbf{q}=0; \omega + i0^+)]$. The regular part of the conductivity is given by $\sigma_{\mathrm{reg}}(\omega) = \mathrm{Im}\Lambda(\mathbf{q}=0;\omega)/\omega$, where $\Lambda(\mathbf{q};\omega+i0^+) = \mathrm{Re}\Lambda(\mathbf{q};\omega) + i\mathrm{Im}\Lambda(\mathbf{q};\omega)$, omitting the xx subscripts for simplicity. To study the dc limit we will use two independent methods. We first use the Matsubara correlation function

$$D(\omega_n) = \pi[-K_x - \Lambda_{xx}(\mathbf{q}=0, i\omega_n)], \quad (6)$$

shown in Fig. 2. From the spectral representation for $\Lambda(i\omega_n)$ and the sum rule $\int_0^\infty d\omega\, \mathrm{Re}\sigma(\omega) = \pi(-K_x)/2$ we obtain

$$D(\omega_n) = D + 2\omega_n^2 \int_0^\infty d\omega\, \sigma_{\mathrm{reg}}(\omega)/[\omega^2 + \omega_n^2]. \quad (7)$$

It follows that $D(\omega_n)$ increases monotonically with n from $D(\omega_n \to 0) = D$ to $D(\omega_n\to\infty) = \pi(-K_x)$ (not shown in Fig. 2 but verified in the data).

From the extrapolation $D(\omega_n\to 0)$ we get a nonvanishing D, and hence infinite dc conductivity for low disorder

($V<V_c$) superconducting systems; see Fig. 2. The V dependence of D is shown in Fig. 1(b), and within the accuracy of our numerics, we find that $D=D_s$ for all disorder strengths. For $V>V_c$, we find $D=0$. Note that, in contrast to nonrandom systems (Ref. 10), D at $T=0$ cannot be used to characterize the nonsuperconducting state for $V\geqslant V_c$ since neither dirty metals nor insulators have a δ function in $\sigma(\omega)$.

We must therefore find a way to extract the T-dependent resistivity to distinguish a metal from an insulator. From the fluctuation-dissipation theorem we obtain

$$\Lambda_{xx}(\mathbf{q};\tau)=\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\,\frac{\exp(-\omega\tau)}{[1-\exp(-\beta\omega)]}\mathrm{Im}\Lambda_{xx}(\mathbf{q};\omega), \quad (8)$$

for $0\leqslant\tau\leqslant\beta$. To obtain Im$\Lambda$ from $\Lambda(\mathbf{q};\tau)$, which is computed in the QMC, requires a numerical inversion of the Laplace transform. We instead use a technique[8] valid for $T\ll\Omega$, where Ω is the scale on which ImΛ deviates from its low frequency behavior (Im$\Lambda\simeq\omega\sigma_{\rm dc}$). Provided $T\ll\Omega$, Eq. (8) simplifies to

$$\Lambda_{xx}(\mathbf{q}=0;\tau=\beta/2)=\pi\sigma_{\rm dc}/\beta^2, \quad (9)$$

which yields the dc conductivity. We note that this simplification may *not* be valid for nonrandom systems: e.g., for a Fermi liquid the scale $\Omega\simeq 1/\tau_{\rm e-e}\sim N(0)T^2$ so one can never satisfy $T\ll\Omega$ at low T. However, for the highly disordered state that we study, we expect the scale Ω to be set by the disorder V and to be T independent, so that Eq. (9) is valid. We will present below additional consistency checks of this approximation.

In Fig. 3(a) we plot the dc resistivity $\rho_{\rm dc}=1/\sigma_{\rm dc}$ as a function of temperature for various degrees of disorder. We use units where $e^2=\hbar=1$ so that the quantum of resistivity $\rho_Q=h/(4e^2)=\pi/2$. For small disorder we see that $\rho_{\rm dc}$ decreases with lowering T; with increasing disorder the T dependence is altered qualitatively: for large V we see that $d\rho_{\rm dc}/dT<0$, strongly suggestive of insulating behavior ($\rho_{\rm dc}=\infty$ at $T=0$).

To see where this transition takes place it is useful to replot the data of Fig. 3(a) as $\rho_{\rm dc}$ as a function of the disorder strength V for different temperatures. This is done in Fig. 3(b); from the crossing point of the various curves we estimate the critical disorder V_c separating the SC from the insulator. We note that our results for $\rho_{\rm dc}(T)$ [and $D(\omega_n)$ discussed below] for $|U|=3,4,6$ are consistent with a direct SC-I transition in 2D, without an intermediate metallic phase.[13]

The curves in Fig. 3 are remarkably similar to those found in the experimental literature,[1] and represent the first QMC calculations of the T-dependent resistivity in a disordered, interacting fermi system.

In the SC state the form of Re$\sigma(\omega)$ changes due to the appearance of $D\delta(\omega)$ below T_c, and Eq. (9) is not applicable. Thus it cannot be used to see that the low disorder systems in Fig. 3(a) do indeed go superconducting at lower temperatures. To see the SC behavior explicitly, we recall the $D(\omega_n)$ analysis presented above, which works best at low T since it involves an $\omega_n\to 0$ extrapolation. As seen from the results of Figs. 1(b) and 2 the low disorder systems ($V<3$) clearly show a nonzero D indicative of infinite dc conductivity.

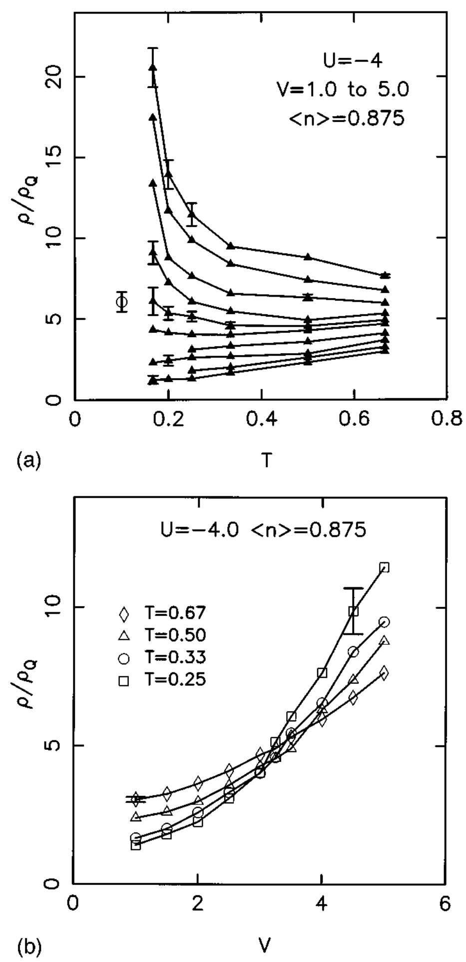

FIG. 3. (a) dc resistivity, obtained from Eq. (9), as a function of temperature, with disorder strength $V=1$ (lowest curve), 1.5, 2, 2.5, 3, 3.25, 3.5, 4, 4.5, and 5 (top curve). The point at $T=0.10$, for $V=3.25\simeq V_c$, is obtained from $D(\omega_n)$; see Fig. 2. (b) $\rho_{\rm dc}$ as a function of disorder V for various temperatures T. Representative error bars are shown.

As an independent check on the results of Eq. (9) we estimate the conductivity of the metal (with $V=V_c$), separating the SC from the insulator, from the small ω_n behavior of $D(\omega_n)$. The metal has a finite dc conductivity Re$\sigma(\omega\to 0)=\sigma_{\rm dc}$, which leads to $D(\omega_n)=\pi\sigma_{\rm dc}|\omega_n|$ for $\omega_n\to 0$, using Eq. (7). Thus the slope of $D(\omega_n)$ at small ω_n may be used to estimate the conductivity; see Fig. 2 where the best linear fit to the points at $n=1,2,3$ is shown. The value of $\rho_{\rm dc}=\sigma_{\rm dc}^{-1}$ obtained using this method, at $T=0.10$ for $V=3.25(\simeq V_c)$, is shown in Fig. 3(a). This low T estimate is in excellent agreement with the results of Eq. (9) at higher temperatures.

It is also worth emphasizing the consistency of results obtained from different observables. The critical V_c may be estimated in several independent ways. Low temperature estimates of V_c obtained from the vanishing of D_s (Ref. 14) and of D are clearly identical [see Fig. 1(b)]. In addition, $D(\omega_n)$ is consistent with metallic behavior, i.e., a linear approach to the origin, only for $V\simeq V_c$; the SC systems have a nonzero intercept D and the insulators do not approach the origin linearly. Another estimate of V_c comes from the higher temperature crossing plots [see Fig. 3(b)].

On the 8×8 systems studied, we find excellent agreement between these methods. For instance, for $|U|=3$, $V_c=3.5\pm0.7$ (from D_s) and $V_c=3.8\pm0.5$ (from ρ_{dc}); while for $|U|=4$, $V_c=3.2\pm0.7$ (from D_s) and $V_c=3.5\pm0.5$ (from ρ_{dc}).

We can also estimate the resistance at V_c using Eq. (9) and independently from the slope of $D(\omega_n)$, both of which give very similar results. We find $\rho(V_c)/\rho_Q=4.1\pm1.3$ (for $|U|=3$); 5.2 ± 1.5 (for $|U|=4$); and 8.3 ± 2.0 (for $|U|=6$). The finite lattice estimate of $\rho(V_c)$ appears to depend on the strength of the attractive interaction $|U|$ (as a function of which one expects a crossover from a fermionic to a bosonic regime in this model; for the nonrandom models, see Ref. 8). The dirty boson model predicts[15] that $\rho(V_c)$ is universal, while the experiments[1] show sample and material dependence, with some indications[1(d)] that the fermionic quasiparticles are responsible for the nonuniversality of this quantity.

A finite-size scaling analysis of QMC data can clearly answer the question of universality of $\rho(V_c)$, and is currently being pursued. What we have shown here is that reliable low-temperature calculations in a disordered, interacting fermion model are feasible in the vicinity of a quantum critical point, and one can determine experimentally interesting quantities such as the superfluid density and T-dependent dc resistivity.

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[12] We have run on 8×8 lattices with a discretization of β of $\Delta\tau=1/8$. We have averaged over 10–20 disorder realizations, doing 200–800 equilibration sweeps followed by 1000–5000 measurement sweeps for each realization. The error bars in all the figures are determined by the sample-to-sample variations (due to disorder); the statistical fluctuations (from the QMC) are smaller by a factor of about 5.

[13] For $|U|=0$, the scaling theory of Anderson localization shows that there is no metallic phase in 2D (Ref. 2) For $|U|\to\infty$, there are general arguments against the existence of a Bose metal at $T=0$ in any dimension; see A. J. Leggett, Physica Fennica **8**, 125 (1971). Thus, *if* there is a metallic phase in the 2D model, it can only be at intermediate $|U|$ where the QMC should be most reliable. Note that the model of Eq. (1) would very likely have a metallic phase for small $|U|$ in 3D.

[14] Since $D_s\simeq(V-V_c)^\zeta$ with (Ref. 4) $\zeta=z\nu>1$, we expect V_c to lie in the small D_s tail in Fig. 1(b).

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