Evolution of the Density of States Gap in a Disordered Superconductor

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We determine the effect of a random potential on the density of states $N(\omega)$ in the attractive Hubbard model. At weak coupling, disorder closes the gap concurrently with the destruction of superconductivity. At larger, but still intermediate coupling, a pseudogap in $N(\omega)$ remains beyond the point at which off-diagonal long range order vanishes. This change in the elementary excitations of the insulating phase corresponds to a crossover between Fermi and Bose insulators. [S0031-9007(98)07201-9]

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Analysis of the effect of randomness on the superconducting state has a long history [1], beginning with Anderson's observation [2] that in the presence of nonmagnetic disorder the Cooper wave function can be constructed by replacing $(k\uparrow, -k\downarrow)$ pairs by an appropriate combination of time reversed, but still extended, eigenstates. Recent theoretical work [3] has attempted to understand experiments [4] on the superconducting-insulator (SC-I) transition in thin films. Here, the superconducting phase is destroyed by strong disorder which localizes the electrons entirely. Numerical work [5] has focused on boson models in which coherence of the pair phase is the central issue, and the role of fluctuations in the pair amplitude is suppressed. Granular systems might be well described by such preformed Cooper pairs, and, furthermore, scaling arguments suggest universal conductivity might find a natural explanation within boson systems [3].

Despite the successes of numeric studies of interacting, disordered Bose systems, it is clear that explicit calculations for itinerant electron models, in which pairs can break apart, are essential. Experimentally, there is evidence for both SC-I transitions to a bosonic state [6] and to a fermionic state [7], distinguished by the existence or lack of an energy gap, respectively, in the insulating phase. There is currently considerable controversy regarding the meaning of the two insulating phases seen experimentally [8]. Theories implicating both bosons [9] and fermions [10] exist.

In this paper we describe the evolution of the single-particle density of states for the disordered, attractive Hubbard Hamiltonian, a model which can interpolate between Bose and Fermi limits. We show that increasing disorder destroys long range pairing correlations and drives a superconducting-insulator phase transition. However, the density of states $N(\omega)$ shows a gap which closes with the destruction of superconducting long range order for relatively weak couplings yet retains a gap beyond the critical disorder strength for larger couplings. Sweeps across the disorder-interaction phase diagram allow us to locate quantitatively the critical coupling strengths for gap and pair order formation in a set of representative cases. This is the first computation of the density of states in a finite dimensional disordered fermion model via the quantum Monte Carlo (QMC) and maximum entropy (ME) methods.

The attractive Hubbard Hamiltonian, in the presence of random site energies is

$$H = -t\sum_{\langle \mathbf{ij}\rangle\sigma}(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}) - \sum_{\mathbf{i}\sigma}(\mu - v_{\mathbf{i}})n_{\mathbf{i}\sigma} - |U|\sum_{\mathbf{i}}\left(n_{\mathbf{i}\uparrow} - \frac{1}{2}\right)\left(n_{\mathbf{i}\downarrow} - \frac{1}{2}\right). \quad (1)$$

Here $c_{\mathbf{i}\sigma}$ is a fermion destruction operator at site $\mathbf{i}$ with spin σ, $n_{\mathbf{i}\sigma} = c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma}$, and the chemical potential μ fixes the average density $\langle n\rangle$. The site energies $v_{\mathbf{i}}$ are independent random variables with a uniform distribution over $[-V/2, V/2]$. The interaction has been written in particle-hole symmetric form so that $\mu = 0$ corresponds to $\langle n\rangle = 1$ at all U and T when $V = 0$. The lattice sum $\langle \mathbf{ij}\rangle$ is over near neighbor sites on a two dimensional square lattice.

We solve for the equilibrium properties of this Hamiltonian using the determinant QMC method [11]. Previous numerical studies of the clean model have determined the phase diagram [12] by a finite-size scaling analysis of the equal time pair-pair correlation functions,

$$P_s(\mathbf{j}) = \frac{1}{N}\sum_{\mathbf{i}}\langle \Delta_{\mathbf{i}+\mathbf{j}}\Delta^{\dagger}_{\mathbf{i}}\rangle, \qquad \Delta^{\dagger}_{\mathbf{j}} = c^{\dagger}_{\uparrow\mathbf{j}}c^{\dagger}_{\downarrow\mathbf{j}}. \quad (2)$$

The phase diagram consists of a state with simultaneous charge density wave (CDW) and superconducting correlations at $T = 0$ and half filling, and a finite temperature Kosterlitz-Thouless transition (with a maximal $T_c \approx 0.1t$ for $|U| = 4t$) to a phase with power law decay of pairing correlations off half filling. In this paper we will study fillings $\langle n\rangle = 0.875$ for which strong CDW correlations are absent and the transition temperature to the SC phase is nearly maximal.

In Fig. 1 we show the suppression of long range correlations in $P_s(\mathbf{j})$ with increasing disorder strength. A finite-size scaling analysis of the structure factor determines the critical value $V_c = (3.25 \pm 0.2)t$ for the destruction of the superconducting state. V_c can also be identified by the superfluid density D_s and the conductivity [13]. These

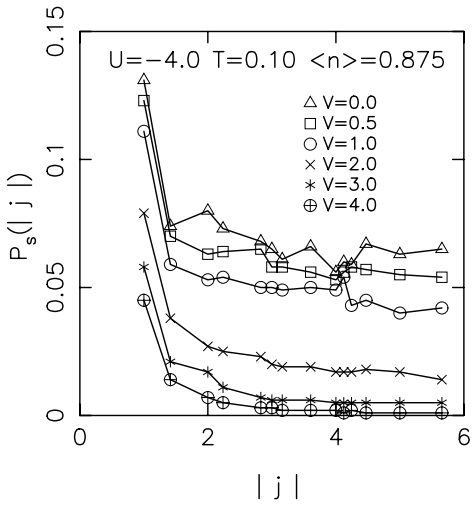

FIG. 1. The equal time pair correlation $P_s(\mathbf{j})$ is shown at $T = 0.10$ as a function of separation $\mathbf{j}$ for different degrees of disorder. $P_s(\mathbf{j})$ remains finite at large $\mathbf{j}$ for $V = 2.0$, but goes to zero rapidly with $\mathbf{j}$ at $V = 4.0$.

quantities give consistent values, $V_c = (3.2 \pm 0.7)t$ and $V_c = (3.5 \pm 0.5)t$, respectively, for the critical disorder.

The density of states is a quantity which, like the conductivity, is directly accessible experimentally. Its evaluation requires an inversion of the integral relation,

$$G(\tau) = \frac{1}{N} \sum_{\mathbf{p}} \langle c_{\mathbf{p}}(\tau) c_{\mathbf{p}}^{\dagger}(0) \rangle = \int_{-\infty}^{+\infty} d\omega \, \frac{e^{-\omega\tau} N(\omega)}{1 + e^{-\beta\omega}}, \tag{3}$$

between the density of states $N(\omega)$ and the imaginary time dependent Green's function $G(\tau)$. We do this using Bryan's method [14] and classic maximum entropy [15], using the full imaginary-time covariance matrix.

Although this approach is fairly well developed for clean systems, the inclusion of disorder raises a number of new questions of principle. The proper treatment of errors and correlations in the QMC data was the central achievement of the ME approach [16], and it is not obvious how additional fluctuations from disorder averaging will affect the procedure. Therefore, we have checked our calculation against analytic results both at weak and strong coupling. Besides verifying the numerics, the behavior in these two limits also presages the two distinct types of insulating behavior we see in the full model.

In the noninteracting limit we can diagonalize the Hamiltonian and obtain E_α, the single-particle eigenenergies, and thence $N(\omega) = \frac{1}{N} \sum_\alpha \delta(\omega - E_\alpha)$. In this limit the determinant QMC method computes the imaginary time fermion Green's function exactly. Tests of the ME approach in the clean case require that some noise be added to the exact $G(\tau)$ coming from the QMC [17]. In the random case, this *ad hoc* noise does not need to be added, since $G(\tau)$ already has error bars from disorder averaging. We find that the ME approach exactly tracks the disorder-induced broadening of $N(\omega)$ [18]. For small $|U|$ we expect disorder to broaden and eliminate the superconducting gap as well.

The strong-coupling, $t = 0$, limit also can be solved analytically. For a single site,

$$G(\tau) = \frac{e^{-\beta U/4} e^{-\tau\Delta_-} + e^{\beta(U/4+v_i)} e^{-\tau\Delta_+}}{2(e^{\beta U/4} \cosh \beta v_i + e^{-\beta U/4})},$$

$$N(\omega) = \frac{(1 + e^{-\beta\Delta_-}) e^{-\beta U/4}}{2(e^{\beta U/4} \cosh \beta v_i + e^{-\beta U/4})} \delta(\omega - \Delta_-) + \frac{(1 + e^{-\beta\Delta_+}) e^{\beta(U/4+v_i)}}{2(e^{\beta U/4} \cosh \beta v_i + e^{-\beta U/4})} \delta(\omega - \Delta_+). \tag{4}$$

Here $\Delta_\pm = \pm U/2 + v_i$. After disorder averaging, the two delta functions in the density of states $N(\omega)$ are broadened to two distributions centered about $\pm U/2$, each with width V. When $V = U$ these merge, and the gap in $N(\omega)$ at $\omega = 0$ is closed. However, the thermal factors greatly suppress $N(\omega)$ near $\omega = 0$. At $t = 0$ there is no long range pairing order, so that this "pseudogap" in the density of states reflects the tendency for on-site singlet formation. We have shown that our QMC + ME procedure accurately reproduces the analytic result Eq. (4) as a function of temperature, disorder strength, and interaction strength [18]. A central conclusion of our work is that this pseudogap behavior persists far from the strong-coupling limit as the hopping t is turned on.

We now study the crossover between these two possible types of effect of disorder on $N(\omega)$ in the full model. In Fig. 2 we show the evolution of $N(\omega)$ with increasing interaction strength $|U|$ at fixed disorder $V = 2t$. $N(\omega)$ evolves from its gapless, noninteracting form to possessing a well-formed gap at $|U| = 4t$. Similarly, in Fig. 3 we show the evolution of $N(\omega)$ with increasing disorder V, at fixed values of the interaction, $|U| = 4t$. In contrast to the noninteracting case where increasing V results in the expected broadening of $N(\omega)$, here the gap in $N(\omega)$ is remarkably robust. Note the values of V are well beyond the point where the superconducting-insulator transition has occurred, as indicated by the results in Fig. 1 and related measurements [13]. In the repulsive Hubbard model at the same value of U/t the gap in $N(\omega)$ requires that *long range* antiferromagnetic order be present, specifically, the correlation length ξ_{af} must exceed the lattice size [19]. In contrast, here we find that a gap in $N(\omega)$ persists despite the clear destruction of such long range order.

How can we interpret these results? In the weak-coupling limit, disorder broadens $N(\omega)$ at all energies. In particular, the superconducting gap in $N(\omega)$ is closed at the same point where disorder destroys the long range pair correlations. This closing of the gap is indicative of the predominance of fermionic elementary excitations in the insulating phase. In the strong-coupling limit, the density of states is not broadened by disorder near $\omega = 0$ and

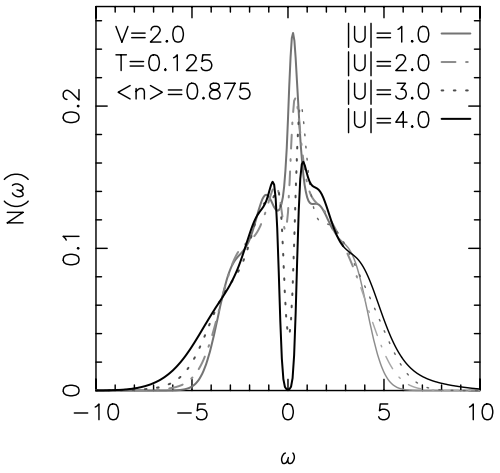

FIG. 2. The density of states $N(\omega)$ at $t = 1$, $T = 0.125$, $V = 2$, $|U| = 1, 2, 3, 4$ on an 8×8 lattice. For sufficiently small $|U|$, scattering by the disorder inhibits phase coherence and the superconducting gap is destroyed. A superconducting gap forms with increasing interaction strength U. A study of the pair correlations $P_s(\mathbf{j})$ indicates that gap formation occurs precisely with the onset of superconductivity.

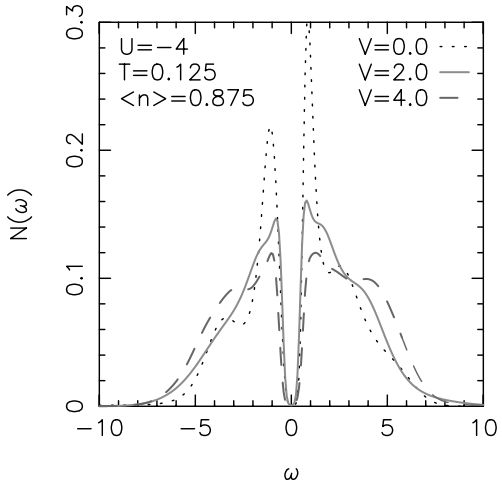

FIG. 3. The density of states $N(\omega)$ at $t = 1$, $U = -4$, $T = 0.125$, $V = 0.0$, 2.0, 4.0 on an 8×8 lattice. A study of the equal time pair correlation shows that for $V < V_c \approx 3.5$ the system is a superconductor. For $V \geq V_c$ the system is an insulator. The gap in $N(\omega)$ persists even after long range pair correlations, and superconductivity, are destroyed. Furthermore, there is no enhancement in $N(\omega)$ as one approaches V_c from either side, indicating that the system is not a Fermi liquid at the SC-BI transition.

a pseudogap survives. The results of Fig. 3 imply that already at a value of interaction strength $|U| = 4t$ which is only one-half the bandwidth, $W = 8t$, the superconducting gap is robust to disorder. In previous work [20], it was found that at $V = 0$ and $|U| = 4t$ the spin susceptibility exhibits a reduction at low temperatures, indicative of Bose-like behavior, despite the fact that the temperature dependence of the chemical potential $\mu(T)$ is still clearly that of a degenerate Fermi system. We conclude here that for an interaction strength as low as $|U| = 4t$, the density of states reflects Bose-like character at all V. As shown in Fig. 3, at either side of the critical disorder V_c for the destruction of long range order in this coupling regime, there are no indications of fermionic excitations in $N(\omega)$.

The phase diagram is shown in Fig. 4. For weak interactions, there is a SC-Fermi insulator (SC-FI) transition with disorder as seen in one class of experiments [7]. For a stronger, but nevertheless intermediate coupling, the phase diagram already exhibits the SC-Bose insulator (SC-BI) transition seen in another class of experiments [6]. The Bose and Fermi insulators are distinguished by the presence or absence, respectively, of local Cooper pairs. Such pairs reveal themselves in turn in gaps in quantities like $N(\omega)$ and the uniform spin susceptibility [13]. We have established the insulating character of the phase at intermediate couplings, $U = -3, -4, -6$ through a direct evaluation of the conductivity [13]. From Eq. (4) it follows that for small t the pseudogap in $N(\omega)$ opens even for very small $|U|/V$ at large β, indicating that the FI-BI crossover has the trajectory shown [18]. Theoretically, a universal resistivity is predicted by a bosonic treatment of the transition [9]. It has been suggested that the presence of fermions causes nonuniversal properties at the SC-I transition [21]. It is possible that the attractive Hubbard model will exhibit universal resistivity only in the Bose-insulator regime, though considerable further work needs to be done to settle this issue.

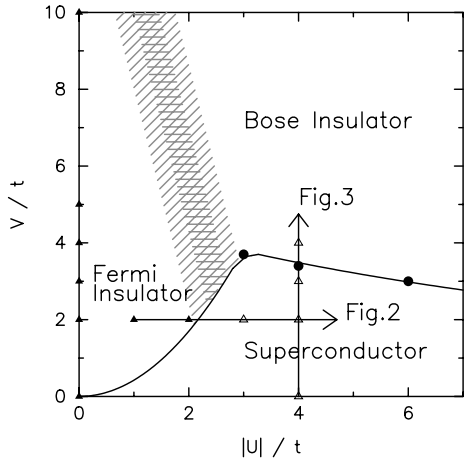

FIG. 4. Phase diagram as a function of disorder V/t and interaction strength $|U|/t$. The solid circles indicate the location of the entry into the superconducting phase as determined by our simulations. The remainder of the solid line indicates an estimate of the location of the boundary of the superconducting region. The arrows correspond to Figs. 2 and 3, open triangles indicate gapped regions while closed triangles indicate no gap in $N(\omega)$. In the superconducting regime the pair correlations have long range order and there is a gap in $N(\omega)$. In the insulating phases there is no pair long range order. The hatched region demarks schematically the crossover between the Bose and Fermi insulators.

The interplay of finite-size effects and the development of a gap in $N(\omega)$ is a subtle issue. As described above, in the case of the half-filled repulsive Hubbard model at $U = 4t$, an antiferromagnetic gap in $N(\omega)$ at finite temperature disappears when the lattice size is increased beyond the correlation length of antiferromagnetic order. We have studied this issue carefully by further evaluation of $N(\omega)$ on a range of lattices, and conclude that the gap we observe is a robust feature and not an artifact of finite lattice size. A crucial difference here from the case of the half filled repulsive model is that the antiferromagnetic transition takes place only at $T = 0$, whereas the superconducting transition off half filling in the attractive model takes place at finite temperature. It is also possible that further lowering of the temperature might result in the opening of a gap at small U [22]. However, it is clear that for the temperature range studied, that is, down to $\beta = 8$, the behavior of the density of states is qualitatively different for small and large $|U|$.

In conclusion, we have computed the density of states $N(\omega)$ in a disordered interacting fermion model with a combination of the QMC and ME methods. The disorder-induced broadening expected in the weak-coupling BCS limit is already absent by the time $|U| = 4t$, half the single-particle bandwidth $W = 8t$. Disorder closes the gap in the density of states for weak interactions but for stronger interactions has little effect on the gap well beyond the point where pair coherence vanishes and the system is insulating. At the coupling where a metallic state has been previously identified, the density of states suggests bosonic excitations on either side of the SC-I transition.

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