Destruction of superconductivity by impurities in the attractive Hubbard model

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We study the effect of $U=0$ impurities on the superconducting and thermodynamic properties of the attractive Hubbard model on a square lattice. Removal of the interaction on a critical fraction of $f_{\text{crit}} \approx 0.30$ of the sites results in the destruction of off-diagonal long-range order in the ground state. This critical fraction is roughly independent of filling in the range $0.75 < \rho < 1.00$, although our data suggest that f_{crit} might be somewhat larger below half filling than at $\rho = 1$. We also find that the two peak structure in the specific heat is present at f both below and above the value which destroys long-range pairing order. It is expected that the high-T peak associated with local pair formation should be robust, but apparently local pairing fluctuations are sufficient to generate a low-temperature peak.

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I. INTRODUCTION

The study of the interplay of disorder and interactions is one of the central problems in condensed-matter physics, and has been analyzed through a wide range of techniques.[1–7] Quantum Monte Carlo (QMC) is one approach[8] which has been applied only relatively recently, but now a number of investigations of the disordered, repulsive Hubbard model exist, both on finite lattices[9–13] and within dynamical mean-field theory where the momentum dependence of the self-energy is neglected.[14] Several interesting effects, including the possibility of the enhancement of $T_{\text{Néel}}$ by site disorder,[14] a Mott transition away from half filling,[15] and a change in the temperature dependence of the resistivity from insulating to metallic behavior when interactions are turned on,[16] have been predicted. These studies have also explored different types of disorder, including randomness in the chemical potential, hopping, Zeeman fields, and on-site interaction.[17] At half filling, some of these disorder types preserve particle-hole symmetry which has an important effect both on the behavior of the static (magnetic and charge) correlations,[9] and on the conductivity.[18]

The work described above concerns the interplay of randomness and *repulsive* interactions. Superconductor-insulator transitions provide a motivation to explore models with an effective *attractive* electron-electron interaction, since these interesting transitions are widely studied experimentally, especially in two dimensions.[19–22] However, QMC studies of models like the attractive Hubbard Hamiltonian with disorder are less numerous than for the repulsive case.[16,23] Previous work focused on locating the critical site disorder strength for the insulating transition and determining the value of the conductivity and its possible universality,[24] and on the interplay between the loss of phase coherence and the closing of the gap in the density of states.[25,26]

Another particularly interesting application of the attractive Hubbard model with disorder is the question of how inhomogeneities and pairing affect each other in high-temperature superconductors. The attractive Hubbard model is the simplest Hamiltonian where this interplay can be studied qualitatively.

Rather than looking at random chemical potentials, as in the previous work just described, here we will instead explore the effect of disordered interaction, specifically turning off the attraction on a fraction f of the sites in the $-U$ Hubbard model.[27] Such vacancies are analogous to nonmagnetic impurities in the repulsive Hubbard model, and, indeed, at half filling, the two problems are related by a particle-hole transformation. We determine the filling dependence of the critical impurity concentration for the destruction of superconductivity through measurements of the equal time pair correlations and the current-current correlations. We also study the effects of the disappearance of superconductivity on the specific heat. Without disorder, a high-temperature peak, associated with pair formation and a low-temperature one, associated with pair coherence, are present. With disorder, we show that the high-temperature peak is robust as superconductivity disappears, and the low-temperature one is weakened.

II. MODEL AND COMPUTATIONAL APPROACH

The attractive Hubbard Hamiltonian we study is

$$H = -t \sum_{\langle \mathbf{rr}'\rangle\sigma} (c^{\dagger}_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + c^{\dagger}_{\mathbf{r}'\sigma} c_{\mathbf{r}\sigma}) - \mu \sum_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma} - \sum_{\mathbf{r}} U(\mathbf{r}) \times \left(n_{\mathbf{r}\uparrow} - \frac{1}{2}\right)\left(n_{\mathbf{r}\downarrow} - \frac{1}{2}\right).$$

Here $c^{\dagger}_{\mathbf{r}\sigma}(c_{\mathbf{r}\sigma})$ are fermion creation (destruction) operators at site $\mathbf{r}$ with spin σ, and $n_{\mathbf{r}\sigma} = c^{\dagger}_{\mathbf{r}\sigma} c_{\mathbf{r}\sigma}$. We use the coefficient t of the kinetic energy term to set our energy scale (i.e., $t=1$). The kinetic energy lattice sum $\langle \mathbf{rr}'\rangle$ is over nearest-neighbor sites on a two-dimensional square lattice, and μ is the chemical potential. The on-site attraction $U(\mathbf{r})$ is chosen to take on the two values $U(\mathbf{r})=0$ and $U(\mathbf{r}) = -|U|$ with probabilities f

and $1-f$, respectively.[28] In this paper, we focus on a single interaction strength $|U|=4$. Notice that we have chosen a particle-hole symmetric form of the interaction. As a consequence, the energy level of a singly occupied vacancy site is higher by $|U|/2$ than a singly occupied site with nonzero interaction. We will report on results for the nonsymmetric form elsewhere.

We begin by briefly reviewing the physics of the pure attractive Hubbard model, $f=0$. At half filling, charge-density wave (CDW) and superconducting correlations are degenerate, and this symmetry of the order parameters drives the superconducting (and CDW) transition temperatures to zero. Doping breaks the symmetry in favor of pairing correlations, and there is now a Kosterlitz-Thouless transition to a superconducting state at finite temperature. It is well established that T_c rises rapidly with doping away from half filling, reaching a maximal value at $\rho=1\pm\delta$ with $\delta\approx 1/8$. T_c decreases gradually thereafter.[29,30] There is some debate as to the exact value of the maximal T_c, with estimates[31] in the range $0.05t<T_{c,\max}<0.2t$. The problem lies with the rather large system sizes needed to study Kosterlitz-Thouless transitions numerically, and hence to benchmark the accuracy of the approximate analytic calculations. Our focus here will not be on this finite temperature phase transition, but rather on the quantum phase transition out of the superconducting ground state which occurs through the introduction of a nonzero fraction f of vacancies.

To distinguish a superconducting phase, we first look for long-range structure in the equal time pair-pair correlation function,

$$c(\mathbf{r}) = \langle \Delta(\mathbf{r})\Delta^{\dagger}(0)\rangle,$$

$$\Delta^{\dagger}(\mathbf{r}) = c^{\dagger}_{\mathbf{r}\uparrow}c^{\dagger}_{\mathbf{r}\downarrow}.$$

This pair-pair correlation function can also be summed spatially to define the structure factor,

$$P_s = \sum_{\mathbf{r}} c(\mathbf{r}) = \sum_{\mathbf{r}} \langle \Delta(\mathbf{r})\Delta^{\dagger}(0)\rangle.$$

The finite-size scaling of P_s is described in the following section.

The current-current correlations probe the superfluid weight and provide an alternate means to detect the destruction of superconductivity.[32] We define

$$\Lambda_{xx}(\mathbf{r},\tau) = \langle j_x(\mathbf{r},\tau) j_x(0,0)\rangle,$$

$$j_x(\mathbf{r}\tau) = e^{H\tau}\left[it\sum_{\sigma} (c^{\dagger}_{\mathbf{r}+\hat{x},\sigma}c_{\mathbf{r},\sigma} - c^{\dagger}_{\mathbf{r},\sigma}c_{\mathbf{r}+\hat{x},\sigma})\right] e^{-H\tau}$$

and the Fourier transform in space and imaginary time,

$$\Lambda_{xx}(\mathbf{q},\omega_n) = \sum_{\mathbf{r}} \int_0^{\beta} d\tau e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\omega_n\tau}\Lambda_{xx}(\mathbf{r},\tau),$$

where $\omega_n = 2n\pi/\beta$.

The longitudinal part of the current-current correlation function satisfies the f-sum rule, which relates its value to the kinetic energy K_x,

$$\Lambda^{\mathrm{L}} \equiv \lim_{q_x\to 0}\Lambda_{xx}(q_x,q_y=0,\omega_n=0),$$

$$\Lambda^{\mathrm{L}} = K_x.$$

Here $K_x = \langle -t\Sigma_{\sigma}(c^{\dagger}_{\mathbf{r}+\hat{x},\sigma}c_{\mathbf{r},\sigma} + c^{\dagger}_{\mathbf{r},\sigma}c_{\mathbf{r}+\hat{x},\sigma})\rangle$. Meanwhile, in the superconducting state the transverse part,

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

can differ from the longitudinal part, the difference being the superfluid stiffness D_s,

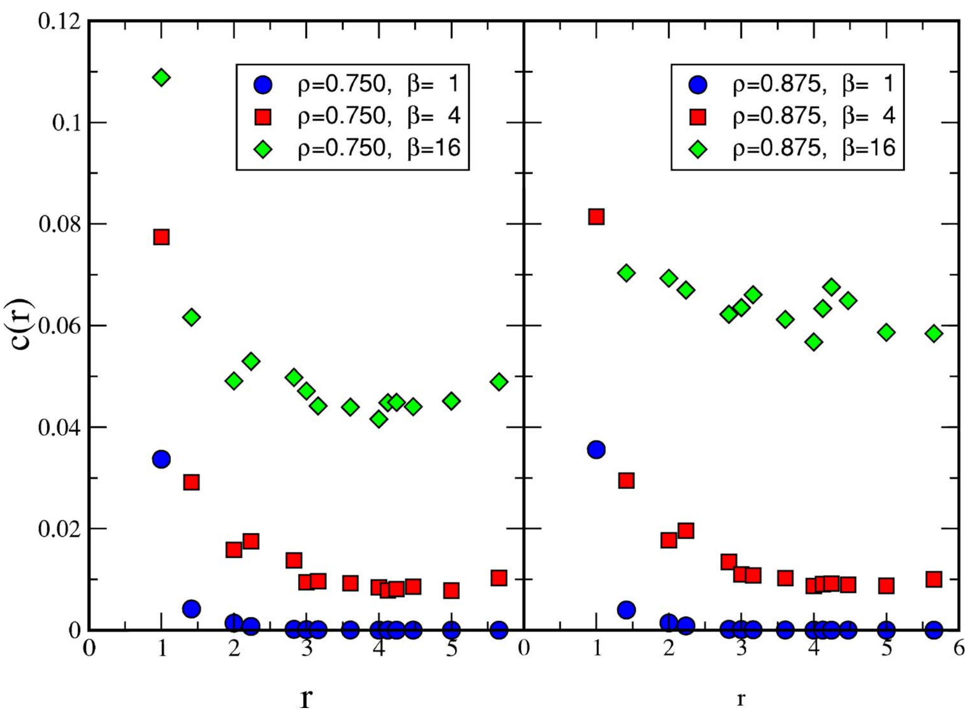

FIG. 1. (Color online) The equal-time pair correlation $c(\mathbf{r})$ is shown as a function of the separation $|\mathbf{r}|$ of the points of injection and removal of the pair. Here the lattice size is $N=8\times 8$, $f=1/16$, and the densities $\rho=0.750$ (left) and $\rho=0.875$ (right). Long-range correlations build up as the temperature is lowered, even though the attractive interactions have been somewhat diluted. Error bars are the size of the symbols. Scatter in the data is associated with the anisotropy in the correlations, which are not a function of the distance only.

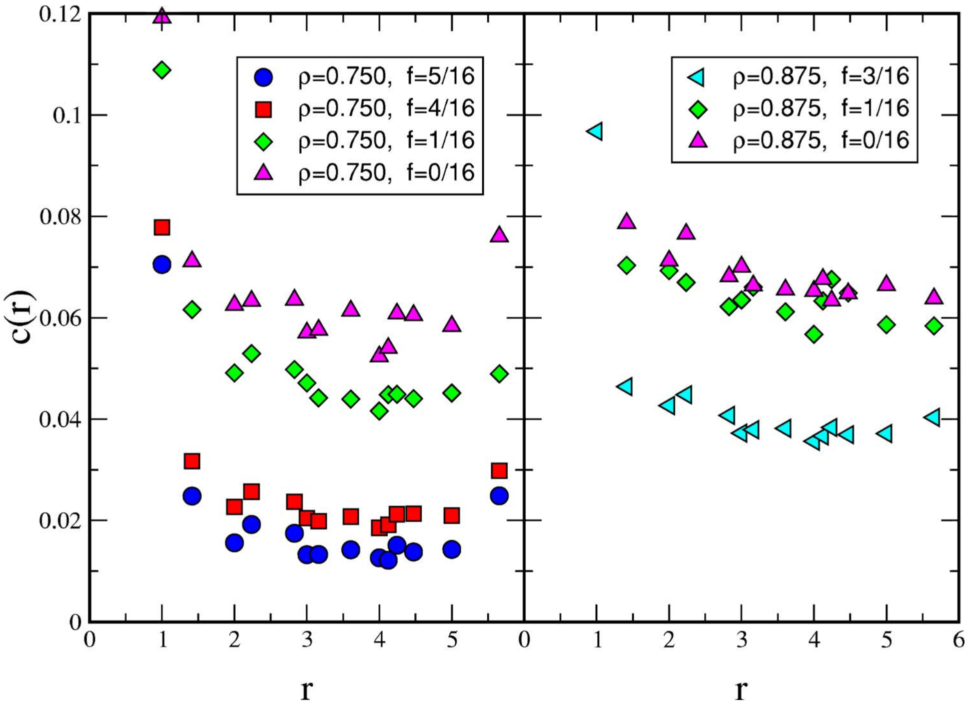

FIG. 2. (Color online) The equal time pair correlation $c(\mathbf{r})$ is shown as a function of the separation $|\mathbf{r}|$ of the points of injection and removal of the pair. Here the lattice size is $N=8\times 8$, the density $\rho=0.750$ (left), and the temperature $T=1/16$. Long-range correlations are decreased with increasing vacancy fraction f. Density $\rho=0.875$ is at right.

$$D_s/\pi = [\Lambda^{\mathrm{L}} - \Lambda^{\mathrm{T}}] = [K_x - \Lambda^{\mathrm{T}}].$$

Thus the current-current correlations provide an alternative, complementary method to the equal-time pair correlations for looking at the superconducting transition.

In order to evaluate these quantities, we use the determinant QMC method.[33] In this approach, we discretize the inverse temperature $\beta = L\Delta\tau$, and a path-integral expression is written down for the partition function Z. The electron-electron interactions are decoupled by the introduction of a Hubbard-Stratonovich field. The fermion degrees of freedom can then be integrated out analytically, leaving an expression for Z which involves an integral over the Hubbard-Stratonovich field, with an integrand which is the product of two determinants of matrices of dimension of the system size. We perform the integral stochastically. In the case of the attractive Hubbard model considered here, the traces over the spin-up and spin-down electrons are given by the determinant of the same matrix, the integrand is a perfect square, and hence there is no sign problem.

Observables are evaluated as the appropriate combinations of Green's functions which are given by matrix elements of the inverse of the matrix appearing as the integrand. Systematic errors in the pairing and current measurements associated with the discretization of β, with our choice of $\Delta\tau$, are typically smaller than the error bars associated with the statistical fluctuations for a single disorder realization and the error bars associated with sample-to-sample variations. The "Trotter errors" are discernable in the energy, but we have verified that they do not affect the qualitative behavior of the specific heat. Our procedure for measuring the specific heat is described in a subsequent section.

As remarked above, there is no "sign problem" for this attractive Hubbard model, so we can do computations at arbitrarily low temperature (large β). In practice, we find that for the parameter values and lattice sizes under consideration here the superconducting correlations reach their asymptotic ($T=0$) values when $T<1/12$ ($\beta>12$), though we collect data also at $T=1/16$ to check this conclusion. These temperatures are about one-hundredth of the bandwidth $W=8t$.

III. EQUAL-TIME PAIRING CORRELATIONS

We first show the spatial behavior of the pairing correlations $c(\mathbf{r})$. In Fig. 1, the vacancy fraction $f=1/16$ is fixed, and we see that long-range correlations in $c(\mathbf{r})$ develop as the temperature T is reduced. Results for two different densities $\rho=0.750$ and $\rho=0.875$ are given. The lattice size $N=8\times 8$. In Fig. 2 we fix $T=1/16$ and examine $c(\mathbf{r})$ for different f. As the vacancy rate increases, the long-range order vanishes.

These results can be analyzed more carefully by performing a finite-size scaling study of the pair structure factor P_s. If the pair correlations $c(\mathbf{r})$ extend over the entire lattice, P_s, which sums this quantity, will grow linearly with size. On the other hand, if the pair correlations are finite in range, P_s is independent of size. Figure 3 shows P_s as a function of β for different lattice sizes. In Fig. 3 we choose a small vacancy fraction $f=1/16$ (left panels) and see that at large β the pair structure factor increases significantly with lattice size. In the right panels of Fig. 3, at large vacancy fractions, $f=4/16$ and $f=5/16$, the pair structure factor grows much less rapidly with lattice size at low temperatures.

Figure 4 determines the critical vacancy fraction through a finite-size scaling analysis. As shown by Huse,[34] the spin-wave correction to the pair structure factor is expected to be proportional to the linear lattice size:

$$\frac{P_s}{L^2} = \Delta_0^2 + \frac{a}{L}, \tag{1}$$

where Δ_0 is the superconducting gap function at zero temperature, and $a(U,f)$ is independent of L. In Fig. 4 we plot

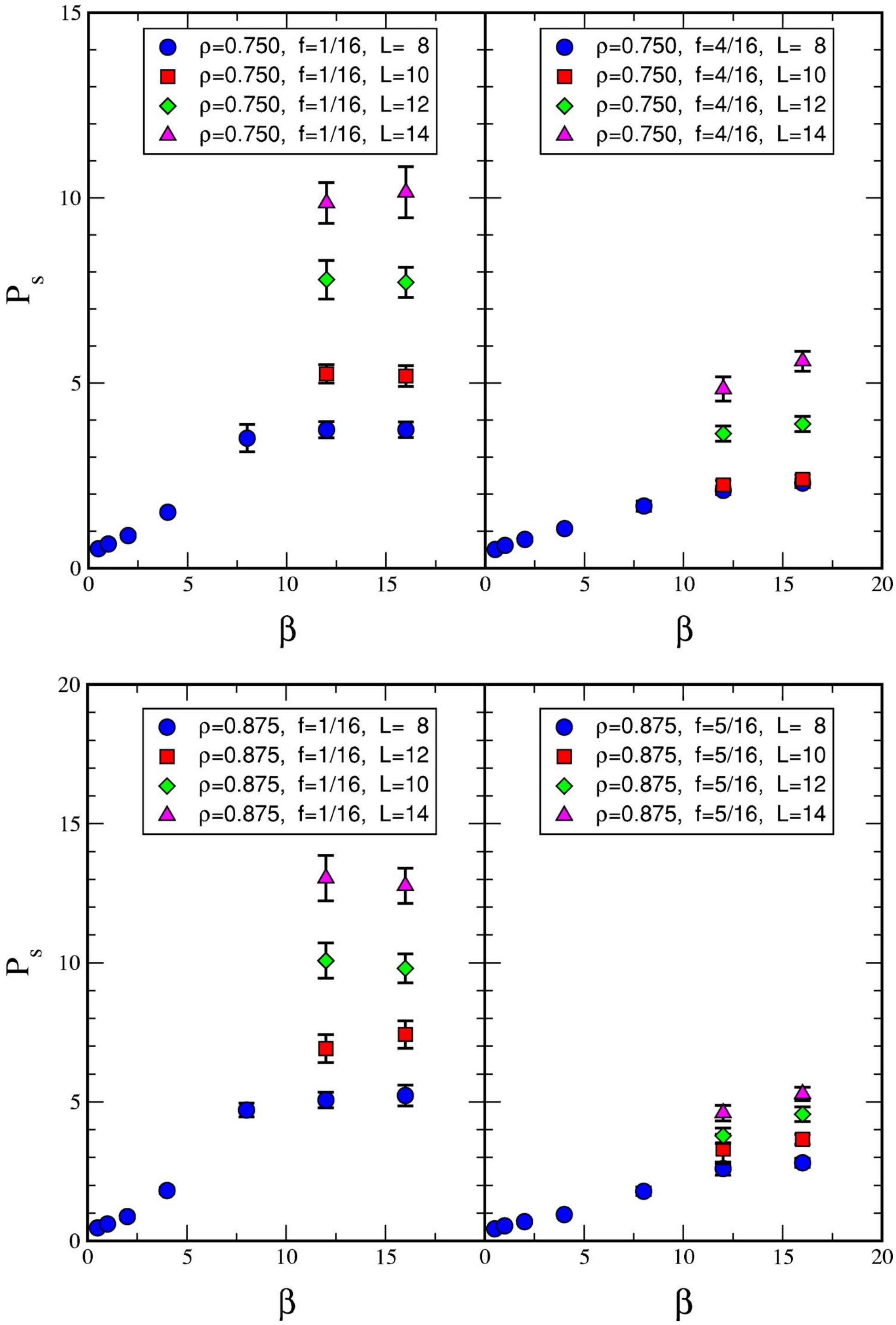

FIG. 3. (Color online) The equal-time pair structure factor P_s is shown as a function of inverse temperature β. In the upper-left panel, the density ρ=0.750, and dilution fraction f=1/16. P_s grows significantly with lattice size L^2 at low temperatures. The temperature at which data for the different lattice sizes separate indicates the point at which the coherence length $\xi(T)$ becomes comparable to the linear lattice size. The lower-left panel shows ρ=0.875, f=1/16, and the upper- and lower-right panels are ρ=0.750, f=4/16 and ρ=0.875, f=5/16, respectively.

the low-temperature value of P_s vs $1/\sqrt{N}$ for lattice sizes ranging from $N=8\times 8$ to $N=14\times 14$, and $\rho=0.750$, $\rho=0.875$, and $\rho=1.000$. At small f, there is the expected nearly linear behavior, extrapolating to a nonzero value in the thermodynamic limit.[35] As f increases, the nonzero extrapolation disappears. This figure contains one of the central results of this paper, namely the determination of the critical values of vacancy fraction f for the destruction of superconductivity. To within the resolution of these simulations, the critical dilution fraction $f_{\text{crit}}\approx 0.30$ for the destruction of superconductivity in the ground state is the same for fillings $\rho=0.750$ and $\rho=0.875$.

Half filling appears to behave somewhat differently. Disorder first enhances superconductivity, as seen by the crossing of the $f=0$ and $f=1/16$ lines in Fig. 4, before driving it to zero a bit sooner than for the doped cases. Impurity sites break the special superconducting and charge-density-wave degeneracy at $\rho=1$, thereby providing a possible reason for the initial enhancement.

It should be noted that the values of f_{crit} indicate that the transition is neither of the classical site-percolation types, for which $f_c^{\text{classical,site}}=0.41$, nor it is related to the quantum percolation one, for which $f_c^{\text{quantum,site}}=f_c^{\text{quantum,bond}}=0$, the latter

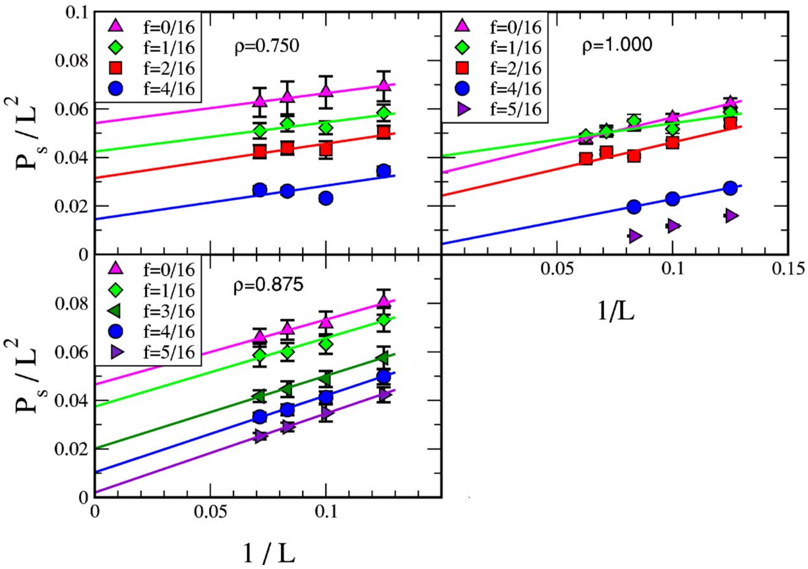

FIG. 4. (Color online) These finite-size scaling plots show the equal-time pair structure factor P_s at low temperature $T=1/16$ as a function of linear lattice size $1/L=1/\sqrt{N}$. Different curves are for different values of the vacancy fraction. For small f, P_s extrapolates to a nonzero value in the thermodynamic limit $1/L\to 0$. For larger f there is no longer a nonzero extrapolated value. The curves are upper-left panel $\rho=0.750$, lower-left panel $\rho=0.875$, and upper-right panel $\rho=1.000$. An interesting feature of the half filling data is the crossing of the $f=0$ and $f=1/16$ curves, indicating an initial enhancement of pairing by the impurity sites.

reflecting the fact that any disorder localizes tight-binding electrons.[36]

IV. CURRENT CORRELATIONS AND SUPERFLUID WEIGHT

These conclusions are confirmed by studying the current-current correlations. We first show, in the left panels of Fig. 5, that the longitudinal current-current correlation $\Lambda_{xx}(q_x,q_y=0,i\omega_n=0)$ extrapolates to the kinetic energy as $q_x\to 0$. This sum rule is satisfied in all parameter regimes, both small and large vacancy rate f, and both small and large temperatures T.

In contrast, the transverse response $\Lambda_{xx}(q_x=0,q_y,i\omega_n=0)$, given in the right-hand panels of Fig. 5, extrapolates to the kinetic energy with q_y only when the temperature is high at small f. As pairing correlations develop across the lattice with decreasing T (Fig. 1) the transverse response breaks away from the kinetic energy, indicating a nonzero superfluid weight D_s. At vacancy concentrations beyond the point at which superconductivity is destroyed, D_s remains zero with decreasing temperature.

In Fig. 6 we show the finite-size extrapolated values of P_s inferred from Fig. 4. These measurements give an indication of the location of $f_{\rm crit}$ in the thermodynamic limit. To within our numerical uncertainties, $f_{\rm crit}$ is the same for the fillings $\rho=0.750$ and $\rho=0.875$, and may be a bit less for $\rho=1.000$. In Fig. 6, for density $\rho=0.875$, we also show the low-temperature values of the superfluid fraction D_s obtained from Fig. 5. The two measurements, Δ_0 and D_s, give consistent results for $f_{\rm crit}$.

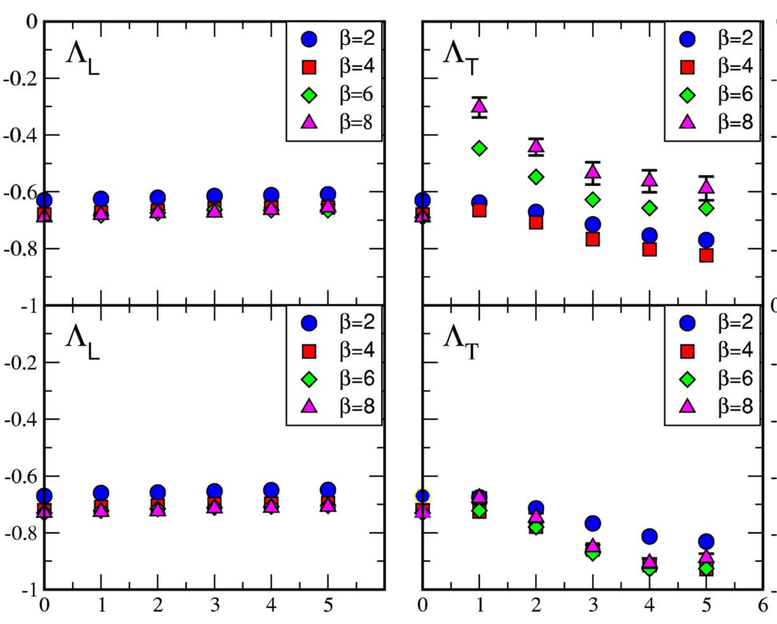

FIG. 5. (Color online) Left panels: Longitudinal current-current correlations $\Lambda_{xx}(q_x,q_y=0,i\omega_n=0)$ as a function of q_x. Here the density $\rho=0.875$. $\Lambda_{xx}(q_x,q_y=0,i\omega_n=0)$ extrapolates to the kinetic energy (symbols at $q=0$) for all temperatures and both fillings when $f=0.04$ (top), which is superconducting, and $f=0.32$ (bottom), which is not. Right panels: Transverse current-current correlations $\Lambda_{xx}(q_x=0,q_y,i\omega_n=0)$ extrapolate to the kinetic energy (solid square at $q_x=0$) at high temperature for $f=0.04$ (top), but break away at low T indicating the presence of a nonzero superfluid density. For $f=0.32$ (bottom) the dilution fraction exceeds $f_{\rm crit}$ so now at low temperature there is no superfluid density. All data are for 10×10 lattices.

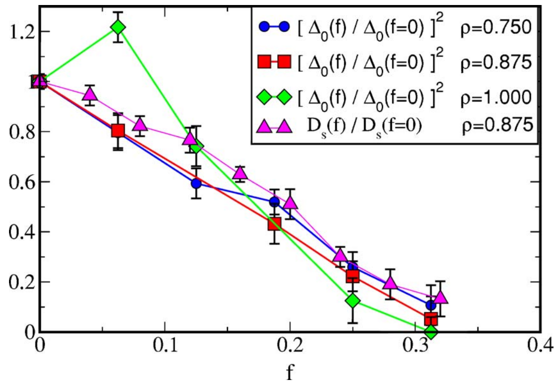

FIG. 6. (Color online) Values for the $L \to \infty$ pair structure factor versus vacancy fraction f at density $\rho=0.750$ (circles), $\rho=0.875$ (squares), and $\rho=1.000$ (diamonds). Also shown is the superfluid fraction D_s on a fixed 10×10 lattice size and $\beta=8$. Both measurements give a consistent estimate of $f_c \approx 0.30$.

V. SPECIFIC HEAT

At half filling, the specific heat of the repulsive (attractive) Hubbard Hamiltonians, in the absence of impurities, exhibits two features.[37–39] There is a peak associated with moment (pair) formation at high temperatures, $T \approx U/3$. At lower temperatures, $T \approx J/4 = t^2/U$, there is a second peak associated with magnetic ordering (pair coherence). Interestingly, in two dimensions, this two peak structure appears to survive even down to weak coupling where the two energy scales merge,[31] in contrast to the behavior in one dimension,[40–44] and in the paramagnetic phase in infinite dimensions.[45–47]

What happens to this behavior when disorder is introduced, specifically when $U=0$ sites are inserted, as in our present model? To address this question we compute the specific heat by fitting QMC data for $E_{\rm qmc}(T_n)$ to the functional form,

$$E_{\rm fit}(T) = E_{\rm fit}(0) + \sum_{l=1}^{M} c_l e^{-\beta l \Delta}.$$

The parameters Δ and c_l are selected to minimize

$$\chi^2 = \frac{1}{N_T} \sum_{n=1}^{N_T} \frac{[E_{\rm fit}(T_n) - E_{\rm qmc}(T_n)]^2}{[\delta E_{\rm qmc}(T_n)]^2}.$$

We choose a number of parameters M equal to about one-fourth of the QMC data points to allow a good fit to the data without overfitting. We check that different M around this value all provide comparable results.[48]

Figure 7 summarizes our results for the specific heat. At a vacancy fraction $f=0.40$, the high-temperature peak in the specific heat, which is associated with the formation of local pairs, is, as expected, somewhat broadened relative to the clean system ($f=0.00$), but remains otherwise robust. The low-temperature peak, associated with pair coherence, is much more substantially reduced, and shifted to lower T. However, it appears to remain present even for this value of f which is beyond $f_{\rm crit}$.

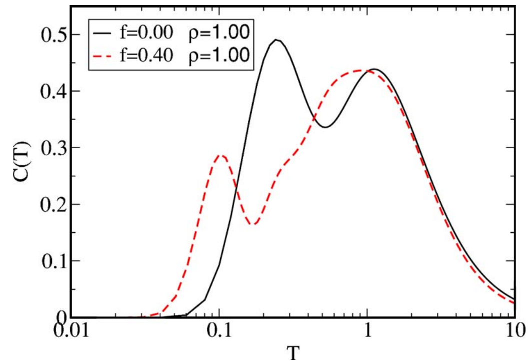

FIG. 7. (Color online) Specific heat of the attractive Hubbard model on $N=10\times 10$ lattices and density $\rho=1.000$ for $f=0.00$ (solid curve) and $f=0.40$ (dashed curve). The high-temperature peak indicates the temperature of local pair formation and is, as expected, not very much affected by the dilution of the attractive interaction on some of the sites. The low-T peak associated with pair coherence is substantially reduced by dilution, but appears to be present even at large f, where long-range order has been lost.

VI. CONCLUSIONS

In this paper we have looked at the destruction of the superconducting state in the attractive Hubbard model through the systematic inclusion of $U=0$ sites. A consistent picture emerges from an analysis of the pairing structure factor and the superfluid fraction, namely that pairing survives out to a dilution of about $3/10$ of the attractive sites, and that this value is not very dependent on the filling, although it may be somewhat increased away from half filling; this result is in marked contrast with data obtained within the coherent potential approximation,[27] which show a linear dependence of $f_{\rm crit}$ on the density. As the fraction f of $U=0$ sites is increased the high-temperature peak in $C(T)$, which signals local pair formation, remains relatively unchanged. The low-T peak which signals the establishment of pairing order gets pushed down. Although the inclusion of noninteracting sites might remind one of percolation, the transition here is not percolative. The critical value of f is neither that of classical site percolation nor of quantum percolation. Finally, we have shown that directly at half filling, pairing correlations are enhanced by the inclusion of vacancy sites. We attribute this effect to the breaking of degeneracy of the CDW and superconducting order in favor of pairing.

ACKNOWLEDGMENTS

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