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Quasiparticle gap in a two-dimensional Kosterlitz-Thouless superconductor

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The negative-U Hubbard model, doped away from half filling, is believed to undergo a Kosterlitz-Thouless transition into a superconducting state with power-law pair-field correlations. We have used numerical simulation techniques to calculate the temperature dependence of the spin susceptibility and the single-particle density of states. These quantities show that a gap in the single-particle spectrum develops for a two-dimensional layer in the Kosterlitz-Thouless state.

The two-dimensional negative-U Hubbard model provides perhaps the simplest many-body description of a single layer which can become superconducting. For a half-filled band (one electron per site), the degeneracy of the charge-density-wave (CDW) phase and the superconducting phase drives the transition temperature to zero. However, when the system is doped away from half filling, the CDW correlations are suppressed and the system is believed to undergo a Kosterlitz-Thouless[1] transition into a superconducting state with power-law pair-field correlations.[2,3] Here we examine the nature of this state as determined from numerical simulations of the spin susceptibility $\chi(T)$ and the single-particle density of states $N(\omega)$.

The Hubbard model we have studied has a near-neighbor hopping t and a negative on-site U interaction:

$$H=-t\sum_{\substack{\langle \mathbf{ij}\rangle\\ s}}(c_{\mathbf{i}s}^{\dagger}c_{\mathbf{j}s}+c_{\mathbf{j}s}^{\dagger}c_{\mathbf{i}s})+U\sum_{\mathbf{i}}n_{\mathbf{i}\uparrow}n_{\mathbf{i}\downarrow}-\mu\sum_{\mathbf{i}s}n_{\mathbf{i}s}\,. \tag{1}$$

Here $c_{\mathbf{i}s}^{\dagger}$ creates an electron of spin s on the ith site of the lattice, $\langle \mathbf{ij}\rangle$ are near neighbors on a two-dimensional square lattice, and $n_{\mathbf{i}s}=c_{\mathbf{i}s}^{\dagger}c_{\mathbf{i}s}$. The numerical simulations[4] reported here were carried out for an 8×8 periodic lattice. Qualitatively similar results were obtained for 4×4 and 6×6 lattices and at different densities. The chemical potential was set such that the average site occupation was $\langle n\rangle=0.87$. This corresponds to having of order 8 holes (56 electrons) on the 64-site lattice.[5] The on-site interaction, for most of the results reported here, was taken as $U/t=-4$, corresponding in magnitude to half the bandwidth of $8t$.

The onset of superconductivity was monitored by studying the equal-time pair-field correlation function

$$C(l)=\langle\Delta_{\mathbf{i}+l}\Delta_{\mathbf{i}}^{\dagger}\rangle\,, \tag{2}$$

with $\Delta_{\mathbf{i}}^{\dagger}=c_{\mathbf{i}\uparrow}^{\dagger}c_{\mathbf{i}\downarrow}^{\dagger}$. The open squares in Fig. 1 show the Monte Carlo data for $C(4,4)$ corresponding to the largest possible separation on an 8×8 lattice. From a finite-size scaling analysis,[3] the Kosterlitz-Thouless transition temperature (T_{KT}) of the infinite two-dimensional lattice was estimated to be of order $0.1t$ for $U/t=-4$ and $\langle n\rangle=0.87$. On an 8×8 lattice, the pairing correlations extend over the finite-size lattice at higher temperatures than this, as seen from the rapid growth of $C(4,4)$ for temperatures less than $0.2t$ in Fig. 1(a).

The spin susceptibility

$$\chi=\lim_{\mathbf{q}\to0}\frac{1}{N}\sum_{l}e^{i\mathbf{q}\cdot l}\int_0^{\beta}d\tau\langle[n_{\mathbf{i}+l,\uparrow}(\tau)-n_{\mathbf{i}+l,\downarrow}(\tau)][n_{\mathbf{i},\uparrow}(0)-n_{\mathbf{i},\downarrow}(0)]\rangle \tag{3}$$

is denoted by the solid squares in Fig. 1. For $U/t=-4$, Fig. 1(a), at temperatures well above the T_{KT}, χ approaches a constant Pauli-like behavior with χ approximately equal to the single-particle density of states $N(\mu)$ at the Fermi energy. As the system is cooled and pairing fluctuations developed, χ begins to decrease. As the system enters the Kosterlitz-Thouless phase and correlations extend across the 8×8 lattice $C(4,4)$ rises and χ decreases dramatically indicating the opening of a superconducting gap. Figure 1(b) shows a similar behavior for $U/t=-6$. Note that in this case, the deviation in χ begins at a higher temperature and the value of χ at temperature well above T_{KT} is smaller than for $U/t=-4$. This reduction of the high-temperature susceptibility reflects the decrease in the local moment[6] due to the increase in double site occupation $\langle n_{\mathbf{i}\uparrow}n_{\mathbf{i}\downarrow}\rangle$ at temperature less than $|U|$.

In order to further explore the nature of the two-dimensional superconducting state and the existence of a gap in the quasiparticle spectrum, we have calculated the single-particle density of states

$$N(\omega)=\frac{1}{N}\sum_{p}A(p,\omega)\,. \tag{4}$$

Here $A(p,\omega)$ is the single-particle spectral weight, which we have determined from the Monte Carlo data for the single-particle Green's function

$$G(p,\tau)=-\langle Tc_p(\tau)c_p^{\dagger}(0)\rangle$$

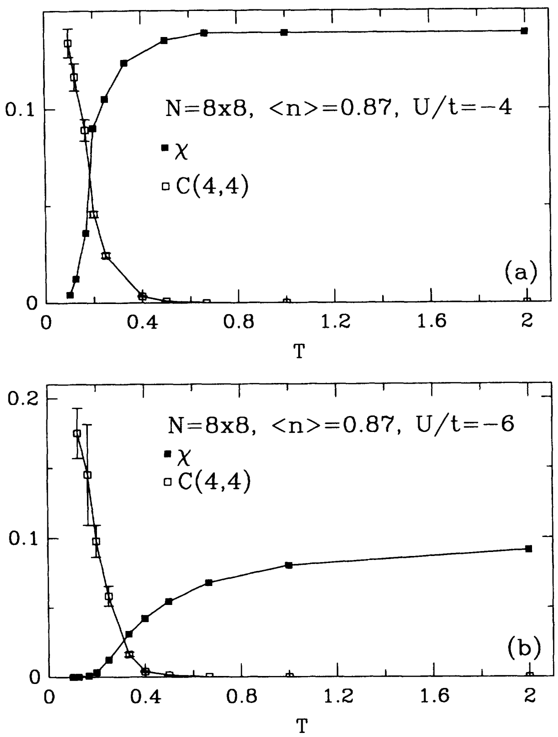

FIG. 1. (a) The magnetic spin susceptibility $\chi(T)$ (solid squares) vs temperature T for an 8×8 lattice with $U=-4t$ and $\langle n\rangle=0.87$. The open squares denote the pair-field correlation function $C(4,4)$ at the point of maximum spatial separation on this lattice size; (b) same as (a) for $U=-6t$.

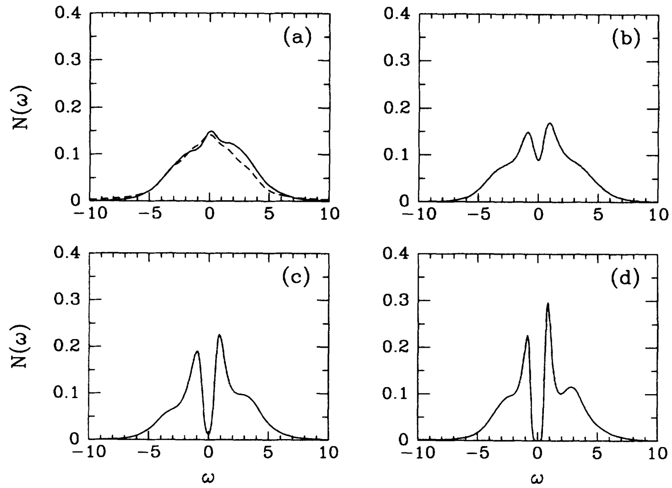

FIG. 2. The single-particle (single-spin) density of states $N(\omega)$ vs ω for $U=-4$, $t=1$, and $\langle n\rangle=0.87$ at different temperatures. Here ω is measured relative to the chemical potential μ, which is -0.15 at low temperatures. (a) $\beta=2$, the dashed curve is the density of states for the noninteracting system (with Lorentzian broadening $\Gamma=1t$) and both curves show the Van Hove peak; (b) $\beta=4$, here the gap begins to develop; (c) $\beta=6$; (d) $\beta=8$, here the gap is well developed on the 8×8 lattice; the asymmetry reflects the Van Hove peak.

by inverting the integral relation[7]

$$G(p,\tau>0)=-\int_{-\infty}^{\infty}d\omega A(p,\omega)\frac{e^{-\tau\omega}}{1+e^{-\beta\omega}}. \tag{5}$$

This has recently been discussed for the positive-U Hubbard model,[8] and we have used similar techniques (including use of moments) to obtain the results shown in Figs. 2(a)–2(d).

The density of states of the noninteracting infinite lattice extends from $-4t$ to $4t$, with a Van Hove logarithmic singularity at $\omega=0$. With $U=0$, the density of states $N(\omega)$ for an 8×8 lattice with a Lorentzian broadening of 1.0 is shown as the dashed curve in Fig. 2(a). The Lorentzian broadening has been added to facilitate comparison with the Monte Carlo results that always are broadened due to the effects of statistical errors.[8] The solid curve is $N(\omega)$, computed from the Monte Carlo values for $G(p,\tau)$, with $U=-4t$ evaluated at a high temperature, $\beta t=2$. At this high temperature, the single-particle density of states of the interacting system is similar to that for the noninteracting system. However, as shown in Figs. 2(b)–2(d), as the temperature is lowered and the superconducting pair-field correlations develop, a gap opens in $N(\omega)$. Note that this gap is centered about $\mu=-0.15$. The asymmetry reflects the Van Hove peak in the noninteracting density of states. At low temperatures, the gap Δ is of order U/t. Figure 2(d) is in very good agreement with exact diagonalization results.[9]

To summarize, we have studied the temperature dependence of the spin susceptibility and the single-particle density of states. At temperatures less than $|U|$, the size of the local site moment depends upon $|U|$, decreasing as $|U|$ increases. Note that this higher temperature reduction in χ increases with $|U|$ even though at values of $|U|\gtrsim 8t$ the Kosterlitz-Thouless transition temperature decreases with increasing $|U|^2$. As the Kosterlitz-Thouless transition temperature is approached, the pair-field correlation length rapidly increases, exceeding the lattice size, and below this temperature $\chi(T)$ decreases rapidly to zero, indicating a quasiparticle gap has opened. Indeed, in this same temperature region we found a gap opened in the single-particle density of states $N(\omega)$. At low temperatures this gap in $N(\omega)$ is well developed in agreement with exact results at zero temperature.[9] Thus the two-dimensional negative-U Hubbard model, doped away from half filling, exhibits a gap in its quasiparticle properties in the Kosterlitz-Thouless state.

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[5]At half filling, i.e., $\langle n\rangle = 1$, due to the mapping of the attractive Hubbard model into the repulsive one the density of states looks the same for both models. We reproduced the $U > 0$ results (see Ref. 8) to check our code. We also obtained results for different fillings but their qualitative behavior is similar to the one for $\langle n\rangle = 0.87$ presented in this paper.

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