Coupled electrons and pair fluctuations in two dimensions: a transition to superconductivity in a conserving approximation

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Abstract

We report on a fully self-consistent determination of a phase transition to a superconducting state in a conserving approximation. The transition temperature calculated for a two-dimensional Hubbard model with an attractive interaction in the fluctuation exchange approximation agrees with quantum Monte Carlo calculations. The temperature dependences of the superfluid density and of the specific heat near $T_c$ indicate that the phase transition in this model of coupled collective degrees of freedom and electronic degrees of freedom is consistent with neither mean-field theory, Gaussian fluctuations about a mean field order parameter, nor unbinding Kosterlitz-Thouless vortices.
The quasi two-dimensional nature of copper-oxide superconductors has focused considerable attention on the role of fluctuations associated directly with superconductivity \[1\]. In a strictly two-dimensional superconductor \[2\], thermal fluctuations of the order parameter preclude a finite temperature phase transition to a state with long-range order \[3, 4\]. A Kosterlitz-Thouless transition may occur between two ‘disordered’ phases, with the low temperature phase characterized by a finite superfluid density and correlation functions that decay algebraically with distance \[5\]. Should fluctuations be important for the copper-oxide superconductors, their effects would be most apparent in the normal state where weak three-dimensional coupling does not substantially influence the essentially two-dimensional character of electronic properties. Fluctuations of the superconducting order parameter may explain the pseudogap in the normal-state single-particle excitation spectrum as well as the anomalous temperature dependences observed for transport and thermodynamic properties in the normal state \[1, 6\].

Figure 1: Internal energy (diamonds) and free energy (squares) as a function of the threaded flux calculated in the FEA for a 2D Hubbard model on a \(32 \times 32\) lattice with \(U = -4\) and \(n = 0.75\) for a temperature above (open) and below (filled) the superconducting transition. The energy and free energy are measured with respect to their zero-flux values. Below the superfluid transition, an energy barrier at \(\phi_B/\phi_o = 0.25\) appears for both \(E\) and \(F\) for the single period shown.

To explore the role of Cooper-pair fluctuations, we focus on the evolution of the
superconducting state with decreasing temperature in the fluctuation exchange approximation (FEA) \[7\], a conserving approximation \[8\] beyond mean field theory. The FEA and the Hubbard Hamiltonian \[9\] with an attractive interaction constitute a minimal model of coupled quasiparticles and s-wave Cooper-pair fluctuations. We report the first observation of a phase transition in the full FEA. The FEA superconducting phase transition occurs at a temperature in excellent agreement with quantum Monte Carlo (QMC) calculations.

We probe superconductivity by calculating the internal energy \(E\) and free energy \(F\) as a function of magnetic flux \(\phi_B\) threading the periodic lattice. Byers and Yang \[10, 11\] argued that off-diagonal long range order makes \(E(\phi_B)\) periodic in \(\phi_B\) with period \(\phi_0/2 = hc/2e\). Scalapino, White, and Zhang \[12\] subsequently showed that the superfluid density determines the curvature of \(F(\phi_B)\) near \(\phi_B = 0\),

\[F(\phi_B) \approx F(0) + \frac{1}{2} D_s(T) \left( \frac{\phi_B}{\phi_0} \right)^2 + \cdots,\]

where \(D_s(T)/2\pi^2\) is the superfluid density in units where the hopping is \(t = 1\) (see below). Similarly, the energy \(E(\phi_B)\) satisfies

\[E(\phi_B) \approx E(0) + \frac{1}{2} \left[ D_s - T \frac{dD_s}{dT} \right] \left( \frac{\phi_B}{\phi_0} \right)^2 + \cdots,\]

which has been used to argue for a KT transition from Monte Carlo calculations on small lattices. Explicit quantum Monte Carlo calculations of \(E(\phi_B)\) as a function of temperature for the two-dimensional attractive Hubbard model show a low-temperature superfluid state \[13, 14\] consistent with the onset of algebraic pair correlations \[15, 16\].

Fig. 1 illustrates one of our central results: \(E(\phi_B)\) and \(F(\phi_B)\) are flat at high temperature, but at low temperatures become periodic with period \(\phi_0/2\) and barrier at \(\phi_0/4\), indicating the formation of a low-temperature superconducting state \[17\].

We consider a Hubbard model on an \(L \times L\) lattice with periodic boundary conditions. In an applied magnetic flux \(\phi_B\), the Hubbard Hamiltonian is,

\[H(\phi_B) = -t \sum_{r,\sigma} \left[ \exp \left( \frac{2\pi i \phi_B}{\phi_0 L} \right) c_{r,\sigma}^\dagger c_{r+\hat{x},\sigma} + h.c. \right] -t \sum_{r,\sigma} \left[ c_{r,\sigma}^\dagger c_{r+\hat{y},\sigma} + h.c. \right] + U \sum_{r,\sigma} n_{r,\uparrow} n_{r,\downarrow},\]

where \(-t\) is the nearest-neighbor hopping matrix element and \(U (< 0)\) is an on-site (attractive) interaction.

We calculate the grand thermodynamic potential \(\Omega\), from the (self-consistent) self-energy \(\Sigma\) and propagator \(G\) using the Luttinger-Ward formula \[18\],

\[\Omega (T, \mu, \phi_B) = -2 \text{Tr} \left[ \Sigma G + \ln(-G^{-1}_0 + \Sigma) \right] + \Phi[G],\]
where $\Phi[G]$ generates the skeleton diagram expansion for the self-energy,

$$\Sigma(k, \varepsilon_n) = \frac{1}{2} \frac{\delta \Phi[G]}{\delta G(k, \varepsilon_n)},$$

(5)

which, together with Dyson’s equation, provides closed equations for $G$ and $\Sigma$.

Complete expressions for $\Phi_{FEA}[G]$ and $\Sigma_{FEA}[G]$ appear elsewhere\[19\]. The FEA for $\Sigma$ contains exchanged spin, density, and Cooper-pair fluctuations \[20\]. The contribution from Cooper-pair fluctuations is $\Sigma_{pp}(\mathbf{r}, \tau) = T_{pp}(\mathbf{r}, \tau) G(\mathbf{-r}, -\tau)$, where

$$T_{pp}(\mathbf{q}, \omega_m) = \frac{U^3 \chi_{pp}^2(\mathbf{q}, \omega_m)}{1 + U \chi_{pp}(\mathbf{q}, \omega_m)}$$

(6)

is an effective non-local and retarded interaction generated by repeated interactions of $s$-wave pairs, and $\chi_{pp}(\mathbf{r}, \tau) = G(\mathbf{r}, \tau) G(\mathbf{-r}, -\tau)$ is the particle-particle bubble. We do not explicitly break gauge symmetry, and hence no anomalous one-particle propagators enter our calculations, but off-diagonal order (of arbitrary spin or orbital symmetry) can still appear spontaneously in our two-particle propagators, because the functional $\Phi$ is explicitly of infinite order in $U$.

The thermodynamic description of a superfluid transition requires reliable calculations of small differences in internal energies and free energies for different $\phi_B$. These are calculated from $G$, $\Sigma$, and $\Omega$,

$$E(\phi_B) = \frac{1}{2} \text{Tr} \left[ \{2\epsilon_k + \Sigma\} G \right],$$

(7)

$$F(\phi_B) = \Omega + \mu n,$$

(8)

where $\epsilon_k$ is the bare dispersion relation, and as in Eq. 4, all quantities on the right-hand side of Eqs. 7 and 8, including $\epsilon_k$, are functions of $\phi_B$. We use a Fourier-transform-based parallel algorithm to solve self-consistently the FEA equations \[21, 22\]. Contributions to convolution sums from high-frequency tails, essential for accurate calculations of thermodynamic properties, are included analytically.

Calculating $D_s(T)$ from Eq. (1) using the fully self-consistent propagators and free energy is equivalent to obtaining $D_s(T)$ from the full conserving FEA current-current correlation function; hence our observation of superconductivity is not inconsistent with previous work that did not see evidence for superconductivity in an approximate FEA response function \[23\].

The energy shown in Fig. 1 was calculated for a $32 \times 32$ lattice with $U = -4$ and a density $n = 0.75$ \[17\]. Fig. 2 shows the temperature evolution of the energy barrier $\Delta_s E = E(\phi_o/4) - E(0)$ for small lattices in comparison with QMC results \[13\] and mean field theory (MFT). Our results for $n = 1.0$ show no evidence for superconductivity, consistent with QMC calculations and theoretical expectations.
The negative values for $\Delta_\phi E$ in both the QMC and FEA and the downturn at low-$T$ in the FEA are apparently finite-size effects. For $n = 0.75$, the results from FEA and QMC agree surprisingly well, but the increase with lattice size in the maximum of $\Delta_\phi E$, interpreted as a signature of a KT transition in the QMC results, is significantly smaller in the FEA.

![Graph showing temperature-dependent energy barriers $\Delta_\phi E$ for $U = -4$ calculated in the FEA (filled diamonds) shown in comparison with the quantum Monte Carlo data of Ref. 11 (open circles) for lattices of the same size, and $\Delta_\phi E$ calculated in mean-field theory (open squares). The FEA shows a finite barrier (indicating superfluidity) for $n = 0.75$ (left column) and a transition temperature well below the mean-field theory value of $\approx 0.7$ and in good agreement with the transition temperature $\approx 0.1$ obtained in quantum Monte Carlo calculations for lattices of the same size. Like the quantum Monte Carlo calculations, we find no evidence for superfluidity in the FEA for $n = 1$.](image)

The QMC calculations focussed on $\Delta_\phi E$, the barrier at $\phi_0/4$, because these calculations have significant noise and the response is largest for this $\phi_B$. In our calcu-
lations, numerical noise is much smaller and we are able to use smaller values of the flux to estimate the superfluid density and its temperature derivative from Eqs. (1) and (2). The top panel of Fig. (3) shows our estimates of $D_s(T)$ and $dD_s(T)/dT$ for a $32 \times 32$ lattice obtained with a flux of $\phi_B/\phi_0 = 0.1$; errors due to higher-order terms in Eqs. (1) and (2) are expected to be less than $2.5\%$.

The slowly increasing $D_s(T)$ with decreasing temperature does not suggest the form $D_s \propto \Theta(T_K - T)$ expected for the vortex-driven transition of Kosterlitz and Thouless. (bottom) The onset of superfluidity is evidently associated with a near-instability of the particle-particle fluctuation T-matrix as signaled by the approach of $-U\chi_{pp}(q=0, \omega_m=0)$ to unity.

The behavior of $D_s(T)$ shown in Fig. (4) differs from expectations for both a mean-field transition ($D_s \propto T_c - T$ below $T_c$ in the thermodynamic limit) and for a KT transition ($D_s$ is discontinuous at $T_c$ in the thermodynamic limit). On a $64 \times 64$
lattice, the rise in $D_s(T)$ occurs at slightly lower temperature, but $D_s(T)$ is otherwise very similar to the result shown for a $32 \times 32$ lattice.

The bottom panel in Fig. 3 shows that the superfluid transition occurs as $T_{pp}$ approaches an instability, i.e. as $U\chi_{pp}$ approaches $-1$. The $T$-matrix is not the self-consistent pair-susceptibility for the FEA and a near instability does not in general signal a phase transition. In this case, extrapolation of $-U\chi_{pp} (q = 0, \omega_m = 0)$ for $T \approx 0.25$ to unity yields a temperature in good agreement with that for the onset of energy-barrier formation.

![Figure 4](image.png)

Figure 4: Specific heat as a function of temperature for a $32 \times 32$ site 2D Hubbard lattice (diamonds) with $U = -4$ and $n = 0.75$. The temperature of the peak in the specific heat correlates with the transition temperature. Also shown is the specific heat for a $64 \times 64$ lattice (open circles) for the same density and interaction strength.

A prominent peak appears in the specific heat as shown in Fig. 4. The peak is not consistent with MFT, which predicts a jump in the specific heat, nor with Gaussian fluctuations about a mean-field order parameter. In the latter case
fluctuations round the corners of the jump in reasonably narrow critical region. The specific heat is also not consistent with expectations for a KT transition, which shows a peak above $T_c$ from the entropy associated with unbinding topological vortices. Comparison of the specific heat and entropy shown for $32 \times 32$ and $64 \times 64$ lattices indicates that finite-size effects in the results shown for these quantities are small.

The superconducting transition we observe in the FEA is apparently neither a simple mean-field transition nor a KT transition, unless the FEA results for $D_s(T)$ contain unusual finite-size effects that die very slowly with increasing lattice size. Our tentative explanation is that the anomalous temperature dependence we observe in these quantities results from the more complicated interplay between collective degrees of freedom (order parameter fluctuations) and electronic degrees of freedom in the FEA than in either the BCS mean-field theory (which describes the change in single-electron energies but ignores order-parameter fluctuations) or descriptions based on Ginzburg-Landau functionals (which treat fluctuations of the order parameter, but ignore their effects on electronic quasiparticles). Although we do not mean to suggest that the details of the results for $D_s(T)$ or $C(T)$ from the FEA are correct, we do think that the FEA provides a valuable example of how calculated properties of a superconductor can be modified by mutual feedback between order-parameter fluctuations and quasiparticle properties when the feedback is included self-consistently.

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