Abstract: We present calculations of the single-particle excitation spectrum for a 2D strong-coupling superconductor in a conserving approximation. Spectral weight at low frequency is substantially reduced as the superconducting transition is approached from the normal state. The suppression of low-energy excitations is a consequence of Cooper-pair fluctuations that are described self-consistently in the fluctuation exchange approximation. The static and uniform electromagnetic response provides a measure of the super fluid density and a fully self-consistent indication of the superconducting transition temperature.

The pseudogap observed in the normal state of the high-temperature superconductors has focused interest on fluctuations directly associated with superconductivity (Emery and Kivelson 1995, Randeria, et al. 1992, Doniach and Imui 1990). The occurrence of superconductivity in two-dimensional copper-oxide layers encourages speculation that Cooper-pair fluctuations affect the low-energy excitation spectrum irrespective of the pairing mechanism.
or of the symmetry of the order parameter. It has been proposed that fluctuations of the phase of the order parameter suppress the physical transition temperature, i.e. the temperature at which macroscopic signatures of phase coherence first appear, below the temperature at which a gap forms in the single-particle excitation spectrum (Emery and Kivelson 1995, Trivedi and Randeria 1995). Here we investigate the excitation spectrum in a self-consistent calculation that includes fluctuations of both the amplitude and phase of the order parameter.

The short coherence lengths characteristic of the high-temperature superconductors suggest that an appropriate description lies somewhere between the BCS picture and Bose condensation of bound fermion pairs (Randeria et al. 1989). The experimental observation of what is apparently a well defined Fermi surface in the high-temperature superconductors and the presence of a sharp drop in $n(k)$ for $|U| \sim W/2$ in quantum Monte Carlo calculations on the Hubbard model with an attractive two-body interaction (Trivedi and Randeria 1995), indicate that a pairing interaction of intermediate coupling strength on the scale of a typical electronic bandwidth may be of physical interest. Recent angle-resolved photoemission experiments on BSCCO have been interpreted as being consistent with a large Fermi surface and therefore a high electronic density (Ding et al. 1997). The nature of the crossover from the overlapping Cooper pairs of BCS theory to a Bose condensation of preformed pairs has been explored by several authors in the context of continuum and lattice models (Leggett 1980, Nozières and Schmitt-Rink 1985, Eagles 1969, Randeria et al. 1992, Luo and Bickers 1993, Micnas et al. 1990, and Sá de Melo et al. 1993). Taken together, these works highlight the importance of collective behavior in the particle-particle channel, which is expected to play a significant role, particularly for large interaction strength, in determining the transition temperature, the nature of the phase transition, and, of central interest here, the electronic excitation spectrum.

In a previous work (Deisz et al. 1998a), hereafter called DHS, we explored superconductivity in the fluctuation exchange approximation (FEA) (Bickers et al. 1989), a conserving approximation (Baym 1962) beyond mean field theory. The superfluid density, its temperature derivative, and the specific heat all show dramatic effects of fluctuations, and scale slowly with increasing lattice size. This slow scaling so far precludes an unambiguous determination of the type of phase transition, and could even be consistent with a Kosterlitz-Thouless transition, but in any case it is of interest to know how Cooper-pair fluctuations affect the electronic excitation spectrum in a theory in which fluctuations are powerful enough to correctly renormalize the transition temperature from mean-field theory. To address this question, we calculate single-particle spectral functions in the FEA and show the temperature evolution of the excitation spectrum side-by-side with the superfluid density calculated on lattices of $128 \times 128$ momentum points. We consider a density $n = 0.75$ roughly consistent with that obtained in electronic structure calculations. This provides a connection with the discussion of the nature of the transition presented in DHS which also shows that transition temperatures obtained on small lattices at this density are in good agreement with quantum Monte Carlo calculations. While it is expected that phase fluctuations are most important for the suppression of long-range order, the FEA contains fluctuations of both the amplitude

1By contrast, for a sufficiently strong pairing interaction, all electrons are expected to participate in the formation of ‘dielectronic molecules’ and no Fermi surface is expected.
and phase of the order parameter.

The central results of this paper are contained in Fig. 1 which shows the electronic spectral weight accessible to a photoemission experiment at four temperatures. Spectral weight is indicated by color in an energy \((y)\)-axis momentum \((x)\)-axis plane. The momenta shown are along the \((1, 0)\) direction from \(\Gamma\) to \(X\) in the square Brillouin zone. Red indicates the largest spectral weight; spectral weight decreases from red descending in the order of the colors of the spectrum to the smallest indicated by indigo. Only for the lowest temperature (Panel 1) is there a non-zero superfluid density; it is very small compared to that for zero temperature. The spectrum for the highest temperature, shown in Panel 4, is consistent with a band of short-lifetime excitations broadened by correlations and by thermal fluctuations. As the temperature is lowered, narrow yellow and red regions appear in the electronic excitation spectrum for some momenta above and below the Fermi surface. The ‘sharpening’ of these single-particle excitations\(^2\) signals the evolution and emergence of quasiparticle excitations\(^3\) with energies above and below the chemical potential \(\mu\). For momenta nearer to the Fermi surface, excitations do not ‘sharpen’ and the light green color indicates that spectral weight at low-energy decreases as the temperature is lowered. As we explicitly show below for a point very near the Fermi surface in the \((1, 0)\) direction, spectral weight at zero energy is suppressed significantly as the transition is approached; relative to the ‘sharp excitations’ the maxima of the spectral functions associated with low-energy excitations are reduced by approximately 50%. Our results suggest a simple model discussed below.

We begin with a model of coupled Cooper-pair fluctuations and electrons that consists of the Hubbard Hamiltonian with an attractive interaction \(U < 0\) threaded by a flux \(\phi_B\),

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

together with the FEA. Here \(-t\) is the nearest-neighbor hopping matrix element, \(U(<0)\) is an on-site attractive interaction and \(\phi_o = hc/e\).

To self-consistently identify a superconducting phase transition in this model, we calculated the internal energy \(E\), and free energy \(F\), as a function of an applied flux using the self-consistently determined self-energy and fully renormalized propagator. A finite superfluid density \(D_s\) leads to a non-zero curvature in \(E(\phi_B)\) and \(F(\phi_B)\) at \(\phi_B = 0\) (Yang 1962, Fisher et al. 1973, Scalapino et al. 1992),

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

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

\(^2\)To be more precise, by ‘sharpening’ we mean that the peak in the spectral functions for these momenta becomes narrower and spectral weight at the maximum increases.

\(^3\)While these excitations are relatively ‘sharp,’ the temperature dependence of their lifetime is not consistent with expectations for a Fermi liquid. This may not be surprising given the high temperature and the relatively large energy of these excitations. In any event, this is not the central point of this paper, and will not be pursued further here.
Figure 1: Single-particle spectral weight represented by color with darkest blue (indigo) corresponding to zero and red to $\sim 1.4$. Spectral weight increases in the order of the colors of the rainbow. Panel 1 is for $T = 0.12$; temperature increases by 0.02 going from panel to panel from left to right. The $x$-axis in each panel indicates momentum from $\Gamma$- to $X$-points along the $(1,0)$ direction and the $y$-axis indicates energy from $-5.5$ to 2.0. The white line indicates the position of the chemical potential. Spectral weight at low energy above the transition is suppressed with decreasing temperature (from 4 to 1) as indicated by the light green region sandwiched between the evolving red peaks. Each panel corresponds to an arrow in Fig. 2. Here, as in all figures, $U = -4$ and the density is 0.75.

This procedure is equivalent to obtaining $D_s(T)$ from the long-wavelength and zero-frequency limit of the fully self-consistent electromagnetic response function. DHS examined signatures of the phase transition in $D_s(T)$ and $dD_s(T)/dT$ for lattice sizes from $4 \times 4$ up to $64 \times 64$ and for temperatures as low as 87 K (taking the bandwidth to be 1 eV).

To study the effect of Cooper-pair fluctuations on the single-particle excitation spectrum, we examine the fully renormalized propagator and self-energy obtained from numerical solutions of the equations for the FEA with $\phi_B = 0$. A detailed description of the FEA together with a summary of our computational methods can be found elsewhere (Serene and Hess 1991, Deisz, et al. 1994, Deisz, et al. 1998a, Deisz, et al. 1998b). Central to our discussion of the single-particle excitation spectrum is Dyson’s equation, which relates the fully renormalized propagator $G$ to the self-energy $\Sigma$ and to the dispersion relation $\epsilon_k$ of the noninteracting system,

$$G^{-1}(k, i\varepsilon_n) = \{i\varepsilon_n - \xi_k - \Sigma(k, \varepsilon_n)\},$$  \hspace{1cm} (4)

where $\xi_k = \epsilon_k - \mu$, $\mu$ is the chemical potential and $\varepsilon_n = (2n+1)\pi T$ are Matsubara frequencies.
The FEA self-energy includes, in addition to the Hartree term, the second-order term and the exchange of spin-fluctuations, density-fluctuations and Cooper-pair fluctuations,

\[
\Sigma(r, \tau) = U^2 [\chi_{ph}(r, \tau) + T_{pp}(r, \tau) + T_{sf}(r, \tau)] G(r, \tau) + U^2 T_{pp}(r, \tau) G(-r, -\tau).
\]  

Here \(T_{pp}\) and \(T_{sf}\) are density and spin-fluctuation \(T\)-matrices, and \(T_{pp}\) is the Cooper-pair fluctuation \(T\)-matrix. For \(U < 0\) and sufficiently low temperature, \(T_{pp}\) provides the largest contribution to the self-energy; it is given by

\[
T_{pp}(q, \omega_n) = \frac{U \chi_{pp}(q, \omega_n)^2}{1 + U \chi_{pp}(q, \omega_n)}.
\]

where \(\chi_{pp}(r, \tau) = G(r, \tau) G(r, \tau)\). We have included all contributions to the FEA self-energy since this leads to a self-energy that is more accurate at high frequency (Deisz, et al. 1997).

In Fig. 2, we show the superfluid density calculated for \(U = -4\) and a density \(n = 0.75\) on a \(64 \times 64\) and on a \(128 \times 128\) lattice.\(^\text{[4]}\) The sharp upturn in \(D_s(T)\) signals the transition to superconductivity; the finite size of the lattice is evident in the changes in \(D_s(T)\) even for these large lattice sizes (Deisz et al. 1998a). As shown in the inset, the chemical potential becomes increasingly negative with increasing temperature as expected for a self-consistent conserving approximation that includes particle-particle ‘ladder diagrams’ (Serene 1989), as observed in quantum Monte Carlo calculations (Randeria et al. 1992), and in contrast to calculations in the ‘ladder approximation’ that are not self-consistent (Schmitt-Rink et al. 1989).

The single-particle spectral function \(A(k, \varepsilon)\), provides a measure of the number of states accessible to an injected electron or hole. Roughly speaking, the product of \(A(k, \varepsilon)\) and a Fermi function may be observed in angle-resolved photoemission experiments. The spectral function is related to the retarded propagator

\[
A(k, \varepsilon) = -\frac{1}{\pi} \text{Im} G^R(k, \varepsilon) = -\frac{1}{\pi} \frac{\text{Im} \Sigma^R(k, \varepsilon)}{(\varepsilon - \xi_k - \text{Re} \Sigma^R(k, \varepsilon))^2 + (\text{Im} \Sigma^R(k, \varepsilon))^2}.
\]

We calculate \(A(k, \varepsilon)\) from the retarded self-energy \(\Sigma^R(k, \varepsilon)\) which we obtain by analytic continuation from the imaginary frequency axis using Padé approximants (Vidberg and Serene, 1977). In contrast to quantum Monte Carlo data, our self-energies have no numerical noise of statistical origin, but do contain roundoff errors dependent on the criterion for convergence; we converged our self-energies so that the modulus of the largest change in \(\Sigma\) for any \(k\) point or Matsubara frequency from one iteration to the next is less than \(1.0 \times 10^{-7}\) for \(64 \times 64\) lattices and less than \(1.0 \times 10^{-8}\) for \(128 \times 128\) lattices. The density was held fixed at \(n = 0.75\) to the same accuracy.

In Fig. 3a, we compare single-particle spectral functions \(A(k, \varepsilon)\) for several temperatures at one point inside but very near the Fermi surface \(k_0 = (23, 0)\pi/32\). The highest temperature shown \((T = 0.20)\) for these calculations on a \(128 \times 128\) lattice is well above any sign of superconductivity as shown in Fig. 2. At \(T = 0.20\), \(A(k_0, \varepsilon)\) has a single rather broad peak\(^\text{[5]}\). As the temperature is lowered in increments of 0.02, the peak in \(A(k_0, \varepsilon)\) shifts to

\(^{4}\)We measure all energies and temperatures in units of the hopping matrix element \(t\).

\(^{5}\) The large width of the peak and the temperature dependence of the width is not consistent with a quasiparticle of a Landau Fermi liquid. We do not pursue this point here.
Figure 2: Superfluid density as a function of temperature for a 128 × 128 lattice (●) and 64 × 64 lattice (○). The arrows indicate the temperatures at which the excitation spectra are shown in panels 1 through 4 in Fig. 1. The inset shows the self-consistent chemical potential as a function of temperature. The (temperature independent) Hartree contribution to the self-energy is included in the chemical potential.

lower energies; at the lowest temperature shown \( T = 0.12 \), spectral weight is suppressed at \( \varepsilon = 0 \) and it appears that the formation of a second peak for \( \varepsilon > 0 \) is incipient; calculations on 64 × 64 lattices at lower temperatures clearly show a second peak for \( \varepsilon > 0 \) (Hess et al 1996). Fig. 3b shows the real part of the denominator of the retarded Green’s function, \( \text{Re} \left[ G^R(\mathbf{k}_0, \varepsilon) \right]^{-1} = \varepsilon - \xi_{\mathbf{k}_0} - \text{Re} \Sigma^R(\mathbf{k}_0, \varepsilon) \). The zero crossing of this expression, which corresponds to the energy of a quasiparticle excitation, occurs nearly at the peak in \( A(\mathbf{k}_0, \varepsilon) \). With decreasing temperature the zero crossing shifts to lower energy. Structure in \( \text{Re} \left[ G^R(\mathbf{k}_0, \varepsilon) \right]^{-1} \) at low energy also evolves with decreasing temperature. For the 128 × 128 lattice, a perceptible superfluid density is only evident for the lowest temperature (see Fig. 2). To better understand the evolution of the peak for \( \varepsilon > 0 \) in \( A(\mathbf{k}_0, \varepsilon) \) with decreasing temperature, we also consider \( \text{Im} \Sigma^R(\mathbf{k}_0, \varepsilon) \). As seen in Fig. 3c, structure evolves in \( \text{Im} \Sigma^R(\mathbf{k}_0, \varepsilon) \) with decreasing temperature that is more complex than that which evolves in \( \text{Re} \left[ G^R(\mathbf{k}_0, \varepsilon) \right]^{-1} \). An examination of Fig. 3a shows that these changes do not lead to significant changes in the shape of the spectral function for the higher temperatures where the only apparent change in \( \text{Re} \left[ G^R(\mathbf{k}_0, \varepsilon) \right]^{-1} \) is the shift of the zero crossing to lower energy. A more careful examination shows that while changes in the energy dependence of \( \text{Im} \Sigma \) are reflected in \( A(\mathbf{k}_0, \varepsilon) \), \( |\text{Im} \Sigma| \) is still rather large and changes of \( \text{Re} \left[ G^R(\mathbf{k}_0, \varepsilon) \right]^{-1} - \text{Re} \Sigma(\mathbf{k}_0, \varepsilon) \) dominate. Included in these are changes in the chemical potential required to hold the den-
Fig. 3d shows the spectral weight at $\varepsilon = 0$ as the temperature is decreased; a reduction of some 20% is evident as $T_c$ is approached and in the absence of any signature of superconductivity.

![Figure 3](image)

**Figure 3:** Contributions to the spectral function for $k_0 = (23, 0)\pi/32$, a point near the Fermi surface shown for $T = 0.20$ (dash-dot), 0.18 (long-dash), 0.16 (dash), 0.14 (dotted), and 0.12 (solid): (a) single-particle spectral weight, (b) Real part of the denominator of the fully renormalized retarded Green’s function $\varepsilon - \xi_k - \text{Re} \Sigma^R(k, \varepsilon)$, and (c) Imaginary part of the self-energy. Also shown in (d) is the spectral weight at zero energy as a function of temperature. Comparison with the superfluid density and it’s derivative in Fig. 2 suggests that the slight kink around $T = 0.135$ is another signature of the phase transition to superconductivity.

The total DOS is a sum of $A(k, \varepsilon)$ over all momenta in the zone; our results suggest that the DOS will show a similar suppression of spectral weight. The suppression will differ quantitatively from that shown in Fig. 3d, which tracks the peak of what might be regarded as the ‘coherent part’ of the (non-Fermi liquid) quasiparticle excitation. Changes from incoherent parts of spectral functions for other $k$ are included in the DOS. Depending in detail on how $\text{Im} \Sigma(k, \varepsilon = 0)$ changes with temperature for $k$ near $k_F$, these may lead to additional reduced contributions to the DOS as coherent quasiparticle excitations or possible gap structure in the low-energy excitation spectrum attempt to evolve. The evolution of these ‘dimples’ in the spectral function for $k$ near $k_F$ as $\varepsilon \rightarrow 0$ would be analogous to those observed as a coherent state evolves in the Anderson lattice model (McQueen *et al.* 1993).

These changes in single-particle excitation spectra are accompanied by the self-consistent formation of a sharp peak in $T_{pp}(q, \omega_m)$ at $q = 0$ and $\omega_m = 0$ which evolves as an instability is
approached (see Fig. 3 of DHS). For larger lattices, $T_{pp}$ is more sharply peaked with a larger $T_{pp}(0,0)$. Supposing that this peak leads to the dominant contribution to the self-energy, we find,

$$\Sigma(k, i\varepsilon_n) = \frac{T}{N} \sum_{m,q} G(-k + q, -\varepsilon_n + \omega_m) T_{pp}(q, \omega_m)$$

where $\tilde{t}_{pp} = T/N \sum_{|q|<\xi} T_{pp}(q, 0)$, $\xi$ is an appropriate correlation length, and $N$ is the number of sites. Inserting this result into Dyson’s equation leads to a connection between $G$ at $(k, \varepsilon_n)$ and the time reversal conjugate point $(-k, -\varepsilon_n)$ as expected for a pairing interaction. Taking $k$ to be on the Fermi surface and using Dyson equations for $G$ for two $(k, \varepsilon_n)$ points related by time reversal conjugation, we find for the single-particle spectral function,

$$A(k_F, \varepsilon) = \frac{1}{2\pi \tilde{t}_{pp}} \sqrt{4\tilde{t}_{pp}^2 - \varepsilon^2}; \quad |\varepsilon| < 2\sqrt{\tilde{t}_{pp}}.$$

This is a parabolic shaped spectral function centered on $\varepsilon = 0$ with a maximum value $\propto 1/\sqrt{\tilde{t}_{pp}}$ and with all spectral weight contained in the interval $|\varepsilon| < 2\sqrt{\tilde{t}_{pp}}$. As $\tilde{t}_{pp}$ increases, the maximum is reduced and the size of the interval increases so that the sum of all spectral weight at any given $k$-point is unity. This is not the entire contribution to the self-energy, but this contribution is rapidly changing, leading to a suppression of spectral weight for any $k$-point at the Fermi surface. We note in passing that spectral weight is pushed away from the Fermi surface, and for $k$-points off of the Fermi surface, a second peak appears in the spectral function consistent with particle-hole coherent Bogoliubov-like excitations. While this model is too simplistic to correctly capture the essential features of the full calculation, it does illustrate how a superconducting transition in two dimensions that separates two disordered phases might occur in the FEA without giving rise to a finite gap but still leading to a suppression of low-energy spectral weight in the normal state.

We return now to the excitation spectra shown in Fig. 1 for $k$ along the $(1,0)$ direction in the zone, which shows that the quasiparticle excitations are still evolving as the superconducting transition is approached, intermingled in a self-consistent way with the evolution of superconducting fluctuations. As the temperature is lowered, the suppression of spectral weight at zero energy is evident in the failure of a sharp peak to emerge in the narrow green region sandwiched between much sharper (red) quasiparticle and quasihole peaks slightly above and below zero energy. The largest value of the spectral functions occurs at the lowest temperature shown and is $\sim 1.4$. We have noted that the spectral weight at the point closest to the Fermi surface decreases strongly below $T \sim 0.18$ and falls by some 20% just above $T_c$. So, relative to the sharp quasiparticle excitations above and below the Fermi surface, spectral weight at the peak of the quasiparticle excitation near the Fermi surface is suppressed by roughly 50%. At the lowest temperature, a finite superfluid density exists (see Fig. 2), finite but small spectral weight exists at zero energy, and hints of additional structure emerging from the region around zero-energy are evident. These “satellite” peaks suggest the coherent coupling of particle and hole excitations expected for a superconducting state, Bogoliubov excitations.

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\(^{6}\) A similar model was considered by Patton (1971).
While we have explicitly shown that spectral weight at low-energy is suppressed for this sizeable density, the quantitative result is less than observed in experiments for BSCCO which show a large reduction in spectral weight. The quantitative dependence of the spectral weight just above \( T_c \) on the interaction strength and density is so far unknown. The dependence on the symmetry of the order parameter is also a subject of current research (Engelbrecht 1997). It is also largely unknown how Cooper-pair fluctuations interact with other possible mechanisms for the formation of the pseudogap that are not a consequence of superconductivity. Further work seeking to elucidate these issues is underway.

We have presented fully self-consistent calculations of the temperature dependent superfluid density together with the single-particle excitation spectrum for a strong coupling superconductor with an attractive interaction of half the bare bandwidth in two dimensions on large 128 \( \times \) 128 lattices. We have taken the electronic density to be roughly that expected from electronic structure calculations. Our calculations show the evolution of quasiparticle excitations self-consistently intermingled with superconducting fluctuations, and explicitly demonstrate a significant suppression of spectral weight at low energy as the superconducting transition is approached from above. For temperatures just below the transition temperature, a gap is not evident. A simplistic self-consistent model was presented to illustrate how the FEA might produce a phase transition between disordered states in two dimensions without producing a finite gap in the single particle excitation spectrum.

Acknowledgements

DWH acknowledges the support of the Office of Naval Research, and J.J.D. acknowledges the support in part of NSF Grant ASC-9504067. This work was also supported by a grant of computer time from the DoD HPC Shared Resource Centers: Naval Research Laboratory Connection Machine facility CM-5; Army High Performance Computing Research Center under the auspices of Army Research Office contract number DAAL03-89-C-0038 with the University of Minnesota. DWH would like to thank J. Erwetowski for a history of superb administrative support.

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