Evidence of a Pseudogap above the Critical Temperature in the Attractive Hubbard Model

J.J. Rodríguez-Núñez[1,3*], S. Schafroth[2], R. Micnas[1†],
T. Schneider[1], H. Beck[3] and M.H. Pedersen[1,2]
[1] *IBM Research Division, Zurich Research Laboratory, CH-8803 Rüschlikon, Switzerland,*
[2] *Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland,*
[3] *Institut de Physique, Université de Neuchâtel, Rue A.L. Breguet 1, CH-2000 Neuchâtel, Switzerland*

We explore the effect of fluctuations for $T \geq T_c$ in the two-dimensional negative Hubbard model within the framework of the self-consistent T-matrix formalism, which goes beyond the BCS approximation and includes pair fluctuations. We enter the regime in which correlations are important, namely $U/t = -4.0$, where t denotes the hopping matrix element between nearest neighbors and U is the strength of the on-site interaction. Our results show the following: (i) Compared to the free case, the distribution function, $n(\mathbf{k})$, reveals considerable renormalization. Thus we conclude that the Fermi surface is blurred for correlated electron systems. (ii) There is a pseudogap in the density of states, $N(\omega)$, around the chemical potential, μ. (iii) The real part of the T-matrix, at zero frequency and zero momentum, vs. T/t exhibits a divergence at a particular temperature. This shows that more approximate T-matrix calculations, i.e. extended to $T = 0$, are meaningless.

High-T_c superconducting materials are extreme type-II superconductors with short correlation length and pronounced uniaxial anisotropy. As a consequence, thermal fluctuations are essential and known to mediate critical point universality [1]. These fluctuations invalidate mean-field theories around T_c, but away from T_c, the pronounced uniaxial anisotropy of cuprates leads to a crossover from three dimensions (3D) to quasi two-dimensional (2D) behavior, where fluctuations are again essential. In this Rapid Communication, we explore the pair fluctuation effects above T_c in the 2D attractive Hubbard model [2] within the framework of the fully self-consistent T-matrix formalism [3] and in the regime where weak coupling treatments do not apply. Previous fully self-consistent T-matrix calculations have been performed numerically [4,5] for a weaker coupling than in the one we investigate and analytically [6] for both, but only for the special case of parabolic bands. The pairing of electrons, which does not necessarily imply the occurrence of superconductivity, is usually described by the anomalous Green's function, $F(\mathbf{x}\tau,\mathbf{x}'\tau')$. In terms of the operator

$$Q(\mathbf{x}\tau) \;\equiv\; c_\downarrow(\mathbf{x}\tau)c_\uparrow(\mathbf{x}\tau) \quad , \tag{1}$$

the expectation value

$$\Delta \;\equiv\; -U < Q(\mathbf{x}\tau) > \tag{2}$$

defines the pairing order parameter below T_c.

Beyond BCS one has to include pair fluctuations above T_c. For this purpose, we introduce the pair Green's function, G_2, defined

$$G_2(\mathbf{x}\tau,\mathbf{x}'\tau') \;\equiv < T_\tau Q(\mathbf{x}\tau)Q^\dagger(\mathbf{x}'\tau') > \quad . \tag{3}$$

In the weak coupling limit (and above T_c), the pair G_2 factorizes

$$G_2(\mathbf{x}\tau,\mathbf{x}'\tau') \;=\; G(\mathbf{x}\tau,\mathbf{x}'\tau')G(\mathbf{x}\tau,\mathbf{x}'\tau') \quad , \tag{4}$$

where T_τ means time ordering. For a finite U, however, there are additional contributions owing to the correlations between particles. In fact, the evaluation of Eq. (3) (in Fourier space) yields

$$G_2(\mathbf{q},i\epsilon_m) \;=\; \frac{\chi(\mathbf{q},i\epsilon_m)T(\mathbf{q},i\epsilon_m)}{U} \quad , \tag{5}$$

where T is the T-matrix and χ is given by the right-hand side of Eq. (4), which in k-space can be written as

$$\chi(\mathbf{q},i\epsilon_m) \;\equiv\; \frac{1}{\beta N}\sum_{\mathbf{k},\omega_n} G(\mathbf{k},i\omega_m)G(\mathbf{q}-\mathbf{k},i\epsilon_m-i\omega_n) \quad , \tag{6}$$

where $\epsilon_m(\omega_n)$ are the bosonic (fermionic) Matsubara frequencies. The T-matrix is expressed as

$$T(\mathbf{q},i\epsilon_m) \;\equiv\; \frac{U}{1+U\chi(\mathbf{q},i\epsilon_m)} \quad . \tag{7}$$

The difference with respect to the free case is that the T-matrix at zero frequency and zero momentum diverges at a particular temperature. This temperature can be taken as an estimate for the critical temperature, T_c, indicating the instability of the normal state against gauge symmetry breaking (Thouless criterion). The other equations which close the T-matrix approach can be found in Ref. [4,5].

In this report we present numerical results for $U/t = -4.0$, including (i) the distribution function, $n(\mathbf{k})$, (ii) the density of states, $N(\omega)$, (iii) the phase shift, $\delta\phi(\mathbf{q},\omega)$, and (iv) the real part of the T-matrix zero frequency and at zero momentum. Correlations are important for this value of U/t, because $|U|$ is half the bandwidth, W ($W = 8t$ in 2D).

In Fig. 1 we show the distribution function, $n(\mathbf{k})$, along the diagonal of the Brillouin zone, i.e., $\mathbf{k} \equiv (Q,Q)$ and compare it to the free distribution function, i.e., for $U/t = 0$. The temperature is $T/t \equiv 0.17$. We have calculated the parameter α [7], which measures the relative number of excited quasiparticles. With 32×32 points in the Brillouin zone and 1024 Matsubara frequencies, we obtain $\alpha \equiv 20\%$. This implies that 10% of electrons are now excited from below to above the Fermi wave vector of the noninteracting system, which in turn would imply that the Fermi surface is probably not a well-defined quantity for this value of the interaction, because the distribution function has a less abrupt change as a function of momentum than for the free case.

Another quantity of interest is the density of states (DOS), $N(\omega)$. In Fig. 2 we show the DOS for $n/2 \equiv 0.10$ for different temperatures. We observe that for a temperature of $T/t \equiv 0.22$ there is no pseudogap. Then, for temperatures between 0.20 and 0.17 the opening of the pseudogap is observed. That the pseudogap does not fully develop when the temperature decreases is probably due to the choice of the damping factor, $\delta \equiv 0.25$. (To go from imaginary (Matsubara) frequencies to real frequencies, we have to make the analytical continuation value of δ is taken to avoid having any additional structure that could appear away from the chemical potential due to finite size effects. We should mention that the temperature of pair formation, T_p, can be estimated in different ways. First, it can be defined by a mean-field BCS approximation. Second, the disappearance of the pseudogap in the DOS can be evaluated numerically [8]. This way of calculating T_p is probably not very precise. We note that the presence of fluctuations above T_c can produce the opening of a pseudogap in DOS within the framework of the Ginzburg-Landau approach in the self-consistent Hartree approximation (if a cutoff parameter is extended down to the lattice scale) by allowing randomness in $\Delta(\mathbf{r})$ down to the atomic scale [9]. From a microscopic point of view, Moreo et al. [10], using quantum Monte Carlo simulations for $U/t = -4.0$ and $n = 0.87$, found a pseudogap above T_c and a fully developed gap at T_c. Our formalism is more suitable for lower densities.

The existence of fluctuating pairs above the critical temperature is also signaled by the appearance of Θ-like functions in the phase shift vs. frequency for large momentum [11,12]. The phase shift is defined as

$$\delta\phi(\mathbf{q},\omega) \equiv \tan^{-1}\left(\frac{\mathrm{Im}[T(\mathbf{q},\omega)]}{\mathrm{Re}[T(\mathbf{q},\omega)]}\right) \quad , \tag{8}$$

where Re(Im)(...) denotes the real (imaginary) part of what follows. Figure 3 shows that for large momenta, Θ-like behavior saturates at large frequencies. These features resemble bound or resonant states.

In a fully self-consistent T-matrix formalism, we have the critical temperature, which can be estimated in terms of the real part of the T-matrix at zero frequency and at zero momentum [3]. At T_c, this quantity diverges and signals the formation of stable pairs, i.e., a symmetry breaking and $\Delta \neq 0$. Below this temperature, however, the formalism must be generalized. Some authors [12] have extended the T-matrix approach down to zero temperatures without taking a finite Δ. They found that the chemical potential, for any density and for any coupling strength, approaches the potential given by bound pairs (see, for example, Fig. 3 of [12]). Figure 4 shows the real part of the T-matrix vs. temperature for $U/t \equiv -4.0$ and $n/2 \equiv 0.05$, revealing a divergence around $T/t = 0.16$. The critical temperature is a quantity that must be calculated by a fully self-consistent T-matrix approach, i.e., a perturbative calculation will yield a different value for T_c [13]. To check our estimates for T_c, we consider the chemical potential as a function of temperature for the same density and same number of k-points and Matsubara frequencies. The numerical data shown in Fig. 5, even when we artificially extended our calculations below T_c, is qualitatively very close to that of [12]. Again, we should say that we cannot use the T-matrix formalism below the critical temperature unless we modify the formalism to include off-diagonal, one-particle Green's functions.

In conclusion, we have evaluated several quantities in the fully self-consistent T-matrix formalism and in the regime where correlations are important for the attractive Hubbard model. In contrast to the BCS weak coupling approximation, the presence of fluctuating pairs above T_c has important effects on the density of states, the phase shift and the distribution function. This distribution function indicates that the Fermi surface is more blurred in correlated systems than in weakly interacting ones. In other words, the fully self-consistent T-matrix approach can be used more properly to describe the high-T_c superconductors, because they are characterized by strong fluctuations. In addition, we have used the full T-matrix formalism to evaluate the critical temperature, the results of which show that calculations that use the nonconserving T-matrix approach down to zero temperature are not correct unless the approach is modified to include anomalous Green's functions. The presence of pairs also has a dramatic effect on electronic quantities, such as the spectral function for the single-particle Green's function. These results will be published elsewhere. Finally, we should remark that in the T-matrix formalism the Thouless criterion is formally equivalent to the appearance of a pairing order parameter, i.e., $\Delta \neq 0$.

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* Permanent address: Grupo de Física de Sólidos, Departamento de Física, FEC-LUZ, Apartado 526, Maracaibo, Venezuela.

† Permanent address: Institute of Physics, Adam Mickiewicz University, Solid State Theory Division, Matejki 48/49, 60-769 Poznán, Poland

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FIG. 1. Distribution function, $n(\mathbf{k})$, for $U/t = -4.0$, $T/t = 0.17$, $n/2 = 0.16$. We have chosen a damping factor, δ, of 0.25 in Green's function to go over to real frequencies. The number of lattice sites is $N_x \times N_y = 32 \times 32$ and that of Matsubara frequencies is $NMats = 1024$; n denotes the number of electrons per site. We show only 11 points of the Brillouin zone and the units are $\pi \times Q/16$.

FIG. 2. Density of states, $N(\omega)$, for different temperatures and the same interaction as in Fig. 1. The density per spin is $n/2 = 0.10$ and the damping factor is $\delta = 0.25$. The values of $N_x \times N_y$ and $NMats$ are the same as in Fig. 1. The energy is measured with respect to the chemical potential.

FIG. 3. The phase shift for different values of momenta along the diagonal of the Brillouin zone. The parameters are the same as in Fig. 2.

FIG. 4. Real part of the T-matrix at zero frequency and zero momentum vs. temperature. The interaction is the same as in Fig. 1. The density per spin is 0.05 and the damping factor is 0.1. The number of lattice sites is $N_x \times N_y = 22 \times 22$ and that of Matsubara frequencies is $NMats = 1024$.

FIG. 5. T/t vs. μ/t for the same parameters as in Fig. 4. The form presented here is similar to the one in [12].