Pair fluctuation effects above $T_c$

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We explore the occurrence of pairing effects above $T_c$ in the 2D attractive Hubbard model. The presence of pairs above $T_c$ goes beyond the BCS approximation, in which pair formation and condensation occur at the same temperature. Using the fully self-conserving $T$-matrix formalism, which is valid above $T_c$, we find that (1) the distribution function, $n(k)$, shows a 10% change of the weight from “below” to “above” $k_F$ with respect to the free case, and (2) the phase shift, $\delta\phi(\omega,k)$, shows $\Theta$-like behavior as a function of $\omega$ for large momentum $k$ along the diagonal of the Brillouin zone. Our calculations have been carried out for an interaction of $U/t = -4.0$ and a temperature of $T/t = 0.125$, where $t$ is the hopping matrix element between nearest neighbors. We conclude that for such an interaction value the Fermi surface is not a well-defined quantity.

The high-$T_c$ materials with their short coherence length and their large penetration depth are leading condensed-matter physicists to consider the effect of pair fluctuations above $T_c$, i.e., to investigate the exotic properties of the normal state. To include fluctuations above $T_c$, we must go beyond the BCS approach, which is mean-field approximation, and where, therefore, pair formation and superconductivity occur at the same temperature. The next level of approximation to BCS is the fully self-consistent $T$-matrix formalism, which includes the effect of fluctuations in a natural way by means of the self-energy of the system. The effect of fluctuations invalidates mean-field theory close to $T_c$; but away from $T_c$, the pronounced uniaxial anisotropy of cuprates leads to a crossover from three dimensions (3D) to quasi-2D behavior, where fluctuations are again essential.

We explore the pair fluctuation effects above $T_c$ in the 2D attractive Hubbard model within the fully self-consistent $T$-matrix formalism. Our basic assumption is that there are fluctuation pairs above the critical temperature and that at $T_c$ there is Bose-Einstein condensation of pairs. The signaling of an order parameter in the $T$-matrix approach is given by the divergence of the real part of the $T$-matrix evaluated at zero momentum and zero frequency (Thouless criterion).

We have evaluated the distribution function, $n(k)$, for an interaction of $U/t = -4.0$ along the diagonal of the Brillouin zone, and compare it with the distribution function for $U/t = 0.0$. The temperature chosen is $T/t = 0.125$, and the total density is $n = 0.32$. These two distribution functions are shown in Fig. 1. We have gone up to 11 points of the Brillouin zone, with the wave number in units of $\pi Q/16$. The parameter $\alpha$, as defined in Ref. [4], measures the relative number of excited quasiparticles. Here $\alpha$ is equal to 20%, which indicates a considerable renormalization of the distribution function with respect to the non-interacting case. Also, we observe that the distribution function, instead of being sharp, is rather smeared out. This leads us to conclude that the Fermi surface is not a well-defined quantity when correlations are relevant. This distribution function can be fitted with a fluctuating BCS gap, i.e., by an auxiliary fluctuating field, $\Delta$, in the partition function.

Next we calculated the phase shift, $\delta\phi(\omega)$, for large values of momenta along the diagonal of the Brillouin zone. The results are presented in Fig. 2 for a density of $n = 0.20$. We observe that for higher momenta the phase shift tends to saturate. The appearance of $\Theta$-like behavior for the
phase shift is an indication of resonant or bound states. Their contribution can be estimated in the ring approximation for the thermodynamic potential, which gives one density contribution that stems purely from band effects and one that is due to bound or resonant states. We have worked with $32 \times 32$ points in the Brillouin zone and 1024 Matsubara frequencies.

In conclusion, we have shown that, when correlations are important, the inclusion of pair fluctuations above $T_c$ in the fully self-consistent $T$-matrix formalism produces considerable renormalization of the distribution function. The fact that the distribution function is not as sharp as in the free case leads us to conclude that the Fermi surface is not a well-defined quantity for a system in which correlations are important. At the same time, we obtain the signatures of resonant or bound states by studying the phase shifts for large momenta and large energies. We should add that the $T$-matrix formalism, for the case of diagonal Green’s function, should be used for temperatures up to the critical temperature, $T_c$, which is given by the divergency of the real part of the $T$-matrix at zero frequency and zero momentum.

We gratefully acknowledge the support of the Swiss National Science Foundation. RM acknowledges partial support from the Committee for Scientific Research (KBN Poland, project No. 2 P3 02 057 04). JJRN thanks for partial support from the project N°. F-139 (CONICIT) and CONDES-LUZ. We would also like to thank María D. García for reading the manuscript.

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Figure 1. The momentum distribution function along the diagonal of the Brillouin zone.

Figure 2. The phase shift as function of frequency for large momenta, $Q$, along the diagonal of the Brillouin zone ($32 \times 32$). The $Q$-values are integers.

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