Theory for underdoped high-T\textsubscript{c} superconductors: effects of phase fluctuations

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In underdoped cuprates, \( T_{\text{c}} \) is thought to be determined by Cooper pair phase fluctuations because of the small superfluid density \( n_s \). Experimentally, \( T_{\text{c}} \) is found to scale with \( n_s \). The fluctuation-exchange approximation (FLEX) in its standard form fails to predict this behavior of \( T_{\text{c}} \) since it does not include phase fluctuations. We therefore extend the FLEX to include them selfconsistently. We present results for \( T_{\text{c}}[n_s,x] \), where \( x \) is the doping.

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One of the striking properties of underdoped cuprates is the so-called strong pseudogap above \( T_{\text{c}} \). It appears below a characteristic temperature \( T_{\text{c}}^* \) in the underdoped regime and \( T_{\text{c}}^* \) approaches the superconducting transition temperature \( T_{\text{c}} \) near optimal doping, where \( T_{\text{c}} \) is maximal. The pseudogap evolves smoothly into the superconducting gap and has the same \( d \)-wave symmetry. A further characteristic property of underdoped cuprates is the low superfluid density \( n_s \). Furthermore, \( T_{\text{c}} \propto n_s(T=0)/m^* \) is observed experimentally\[1\] and there are indications of finite phase stiffness being proportional to \( n_s \) on short length and time scales in the pseudogap regime above \( T_{\text{c}} \). One interpretation is that at \( T_{\text{c}}^* \) Cooper pair formation occurs and that at \( T_{\text{c}} \) these Cooper pairs become phase coherent. In accordance with this physical picture we extend FLEX to include phase fluctuations.

Theory

As a microscopic model for high-\( T_{\text{c}} \) superconductors we use the single-band Hubbard model in 2D, with the nearest-neighbor hopping element \( t \) and
the local Coulomb repulsion $U$. The fluctuation exchange approximation (FLEX) is used to treat the superconducting state in the standard Nambu-Eliashberg formalism with the spin fluctuations of the FLEX as the pairing interaction.\textsuperscript{5,6,7} From the self-consistent solution of the Dyson equation one can determine $T^*_c$ as the highest temperature for which the off-diagonal self energy is non-vanishing. Usually this is the criterion for the critical temperature $T_c$, but this is only true if one can neglect the role of phase fluctuations. However, when the superfluid density is small, phase fluctuations will destroy phase coherence, while the charge carriers still form local Cooper pairs, which is signaled by a non zero amplitude of the superconducting order parameter.

To extend the FLEX to include phase fluctuations self-consistently, one has to know their self-energy contribution. In order to derive it we start with a phenomenological model of tight-binding electrons and an effective nearest-neighbor pairing interaction for electrons with opposite spins, leading to a superconducting $d$-wave order parameter in the mean-field approximation. We begin by writing down the action $S$ for the tight-binding electrons where the interaction term is decoupled by a Hubbard-Stratonovich transformation, introducing a decoupling field $\Delta_{ij}$, which turns out to be the superconducting order parameter:

\[
S[\Phi^*, \Phi; \Delta^*, \Delta] = \int_0^\beta d\tau \left\{ \sum_{i\sigma} \Phi^*_{i\sigma} (\partial_\tau - \mu) \Phi_{i\sigma} + t \sum_{<ij>\sigma} \Phi^*_{i\sigma} \Phi_{j\sigma} + \sum_{<ij>} \left[ \Delta_{ij} \Phi^*_{i\uparrow} \Phi^*_{j\downarrow} + \Delta^*_{ij} \Phi_{j\downarrow} \Phi_{i\uparrow} + \frac{|\Delta_{ij}|^2}{V} \right] \right\},
\]

where $\Phi_{i\sigma}$ represents the electron field at lattice site $i$ with spin $\sigma$. $V$ is the pairing interaction and $t$ is the hopping matrix element between nearest-neighbor sites. The doping is controlled by the chemical potential $\mu$. We now assume the local superconducting order parameter $\Delta_{ij}(\tau)$ to have a time and translational invariant amplitude $\Delta^0_{ij}$ with $d$-wave symmetry but a fluctuating phase suppressing superconducting order in the pseudogap regime below $T^*_c$. We perform the following transformation to decouple the phase and amplitude degrees of freedom of the order parameter:\textsuperscript{8}

\[
\psi_{i\sigma} = \Phi_{i\sigma} e^{-\frac{i}{2} \phi_i(\tau)}, \quad \Delta_{ij} = \Delta^0_{ij} e^{-\frac{i}{2} [\phi_i(\tau) + \phi_j(\tau)]},
\]

This leads to an expression for the action where the phase is directly coupled to the fermions by the elementary vertices shown in figure 1. After integrating out the fermionic degree of freedom, a loop expansion up to second order in the phase fields $\phi_i(\tau)$ leads to the effective action for the phases, taking the form of a time-dependent XY model on a cubic lattice. From the effective
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(a)  \(\bullet\) and  \(\blacksquare\) of our theory are shown. The solid line represent an in or outgoing electron and the wiggly the phase field. In (b) we show the diagrams contributing in lowest order to the effective action  \(S_{\text{eff.}}[\varphi]\) for the phases, here the solid line is the Nambu Green function.

\[
P_{\varphi\varphi}(q, i\nu_n) = \frac{8}{-\kappa(q, i\nu_n)(i\nu_n)^2 + \frac{n_s(q,i\nu_n)}{m^*}2(2 - \cos q_x - \cos q_y)}.
\]

where  \(\kappa(q, i\nu_n)\) is the density-density correlation function and the dynamical phase stiffness is given by  \(n_s(q, i\nu_n)/m^* = T + \Pi^{ij}(q, \omega)/e^2\). Here  \(T\) is the expectation value of the inverse band-mass operator and  \(\Pi^{ij}\) is the current-current correlation function calculated in the mean-field approximation. The superfluid density is the density of phase coherent Cooper pairs only, which are responsible for the Meissner effect. If no phase fluctuations are present it will take the value of the local Cooper-pair density  \(n_{cp}\). Since in the London theory  \(n_s\) is related to the London penetration depth by  \(\lambda_L = \sqrt{m^*c^2/(4\pi e^2n_s)}\) we can determine  \(T_c\) as the temperature where the Meissner effect and therefore the superfluid density  \(n_s(q=0, i\nu_n=0)\) referring to phase coherent Cooper pairs vanishes. This can be seen as the loss of rigidity against long-range phase fluctuations and is consistent with the transition from quasi long-range to short-range order in 2D. For  \(T > T_c\) the dynamical phase stiffness will be non-zero for certain  \(q > q_0\) and  \(\nu > \nu_0\) and will result in superconducting order on finite length and time scales and will finally vanish for all momenta and frequencies at  \(T_c^*\), where  \(n_{cp}\) goes to zero. From the generating functional for the fermions we determine the self-energy corrections due to phase fluctuations in lowest order. Combining this self-energy contribution with the contribution of standard FLEX and taking the renormalized propagator of the phase fluctuations, which means that one has to calculate  \(n_s(q, i\nu_n)\) and  \(\kappa(q, i\nu_n)\) with renormalized Green functions, gives a set of self-consistency equation for the renormalized Green functions. In this way we get an extension of the usual FLEX equations with
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Fig. 2. Dyson equation for the extended FLEX approximation. The straight double lines are renormalized Nambu Green function, whereas the single lines are bare ones. The zig-zag line in the second graph is the effective interaction of the FLEX, and the wiggly lines denote the propagator $\Pi^{\varphi\varphi}$ of the phase fluctuations.

the Dyson equation shown in figure 2.

Results

In figure 3 we show results for the critical temperature $T^*_c$ at which Cooper pairs are formed and for $T_c$ where the phase of the Cooper pairs become coherent. $T^*_c$ is determined within standard FLEX as the highest temperature for which the off-diagonal self energy is non-zero. $T_c$ is calculated using the Kosterlitz-Thouless criterion $\pi/2 \hbar^2 d n_s(T_c)/4m^* = k_B T_c$ for the temperature where phase coherence vanishes. Here $n_s(T)/m^*$ is calculated within FLEX approximation and $d$ is half of the $c$-axis lattice constant. Note the Kosterlitz-Thouless criterion neglects the coupling between amplitude and phase fluctuations, which is expected to be important for the overdoped regime. Also we show FLEX results for $n_s/m^*$ extrapolated to $T = 0$, indicating $T_c \propto n_s(T = 0)/m^*$ in the underdoped regime. We find $T_c = 1.691 h^2 d n_s/4m^* k_B$ [11] In accordance with experimental findings we expect that our results for $n_s(T = 0)/m^*$ and $T_c$ should decrease more rapidly for doping $x \rightarrow 0$ due to the vicinity of the antiferromagnetic transition which is not properly described in the FLEX. It is interesting to note, that $T_c \rightarrow T^*_c$ in the overdoped regime as expected for increasing Cooper pair density, although using the Kosterlitz-Thouless criterion neglects coupling of amplitude and phase fluctuations. We obtain $T_c \approx T^*_c$, since $n_s/m^*$ increases rapidly below $T^*_c$ as compared to the underdoped regime. The result for $n_s(T = 0)/m^*$ in the overdoped regime suggests that $T_c \propto n_s(T = 0)/m^*$ is no longer valid there. The scaled curve $T_c \propto n_s(T = 0)/m^*$ crosses $T^*_c$ at optimal doping. Our result for $T_c$ and $T^*_c$ already yield the observed behavior. We expect that a selfconsistent inclusion of phase fluctuations in FLEX will give better agreement with experiment, in particular a more rapid de-
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Fig. 3. Doping dependence of the temperatures $T_c^*$ where Cooper pairs are formed, of $T_c$ where Cooper pairs becomes phase coherent, and of the phase stiffness $n_s(T = 0)/m^*$. $T_c^*$ and $n_s(T)/m^*$ are calculated using FLEX and $T_c$ is calculated using the Kosterlitz-Thouless criterion for the vanishing of the phase coherence.

increase of $T_c$ for $x \to 0$. The extended FLEX theory shown in figure 3 should give for the underdoped superconductors $T_c \propto n_s$, $n_s(q=0, \nu=0) = 0$ at $T_c$ to obtain no Meissner effect above $T_c$, and the pseudogaps in the single-particle spectral density. Note, the coupling of the phase to its conjugate variable, the charge density, becomes important as the doping goes to zero. This may cause $T_c \to 0$ for $x \to 0$.

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REFERENCES

1. For a recent review see, e.g. T. Timusk and B. Statt , Rep. Prog. Phys. 62, 61 (1999).
2. Y. J. Uemura et al., Phys. Rev. Lett. 62, 2317 (1989).
3. J. Corson et al., Nature 398, 221 (1999).
4. V. J. Emery and S. A. Kivelson, Nature 374, 434 (1995).
5. N. E. Bickers and D. J. Scalapino, Ann. Phys. (N.Y.) 193, 206 (1989).
6. P. Monthoux and D. J. Scalapino, Phys. Rev. Lett. 72, 1874 (1994).
7. T. Dahm and L. Tewordt, Phys. Rev. Lett. 74, 793 (1995).
8. H.-J. Kwon and A. T. Dorsey, Phys. Rev. B 59, 6438 (1999).
9. T. M. Rice, Phys. Rev. 140, A1889 (1965).
10. J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1993).
11. 3D isotropic XY model gives instead of 1.691 the factor 2.202.