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Influence of d-wave order parameter fluctuations on spin fluctuations in underdoped high-T_c cuprates

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Abstract. – We consider the effect of fluctuations of the superconducting $d_{x^2-y^2}$-wave gap above T_c for the 2D Hubbard model. The order parameter fluctuations (OPFL) lead to a decrease of T_c and to a suppression of the dynamical spin susceptibility below a crossover temperature T_* which can be much larger than T_c. The temperature T_* increases while T_c decreases with increasing strength of OPFL, or decreasing doping. The resulting neutron scattering intensity and NMR relaxation rates decrease below T_* for decreasing T. This agrees qualitatively with the observed spin gap behavior in the underdoped high-T_c cuprates.

There are many different attempts to explain the unusual properties of high-T_c cuprates in the normal state in the underdoped regime. The ^{63}Cu spin-lattice relaxation rate $1/T_1$ and the spin-echo decay rate $1/T_{2G}$ [1], the uniform susceptibility, and the in-plane resistivity, all exhibit a sequence of crossovers for decreasing temperature T. First one observes at T_{cr} a crossover from non-universal mean-field behavior with a dynamical exponent $z = 2$ to $z = 1$ pseudoscaling behavior, and then at T_* a crossover to spin pseudogap behavior [2], [3]. Recently, a counterpart to the NMR spin pseudogap behavior has been found, namely, a quasiparticle gap above T_c in angle-resolved photoemission (ARPES) experiments in Bi2212 [4], [5]. It has been proposed that the physical origin of this normal-state gap are preformed d-wave pairs without pair-pair coherence [6], [7]. In contradiction to this scenario, it has been proposed that the pseudogap behavior is associated with a preformed spin-density wave gap [3].

In this letter we show that another mechanism may be responsible for the suppression of the spin fluctuations and of T_c, namely, coupling to d-wave order parameter fluctuations which are treated by the classical Aslamazov-Larkin theory [8]. Particle-hole and particle-particle

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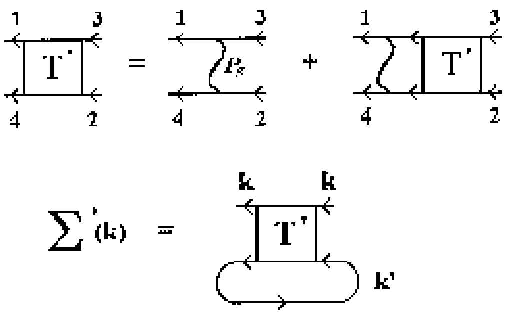

Fig. 1. – Bethe-Salpeter equation for particle-particle scattering matrix T' in the ladder approximation with full pairing interaction $P_{\mathrm{s}} = (3/2)U^2\chi$ (wavy line), and self-energy contribution Σ' arising from T' (the solid line is the dressed-particle propagator).

scattering together were first considered in the FLEX (fluctuation exchange) approximation for the two-dimensional (2D) Hubbard model [9]. The effect of particle-particle scattering is to reduce the T_{c} for $d_{x^2-y^2}$-wave pairing which is obtained from the FLEX approximation for spin fluctuations alone [10]-[12]. In analogy with [9], we generalize the FLEX approximation of [10]-[12] by taking into account, besides the self-energy contribution due to particle-hole scattering, the self-energy Σ' due to particle-particle scattering T'. Here we are led by weak-coupling theory where the propagator for scattering of two particles with momenta $\mathbf{k}_3 + \frac{\mathbf{q}}{2}$, $\frac{\mathbf{q}}{2} - \mathbf{k}_3$ and total energy ω into $\mathbf{k}_1 + \frac{\mathbf{q}}{2}$, $\frac{\mathbf{q}}{2} - \mathbf{k}_1$, ω is given by [8]

$$T'(\mathbf{k}_1, \mathbf{k}_3; \mathbf{q}, \omega) = -\frac{\psi(\mathbf{k}_1)\psi^*(\mathbf{k}_3)}{\bar{N}\left[\frac{|T-T_{\mathrm{c}}|}{T_{\mathrm{c}}} + \xi^2 q^2 - i\omega\tau\right]}. \tag{1}$$

The function ψ is the basis function of the "embryonic" superconducting state, here $\psi = \cos(k_x a) - \cos(k_y a)$ for $d_{x^2-y^2}$-wave pairing, $\bar{N} = (4\pi t)^{-1}$ is the average density of states, ξ the superconducting coherence length, and τ the relaxation time. In analogy with eq. (1), we have calculated $T'(k_1, k_3; q = k_1 + k_4)$ in the ladder approximation for the full pairing interaction, $P_{\mathrm{s}}(k_1 - k_3) = (3/2)U^2\chi(k_1 - k_3)$, where χ is the dynamical spin susceptibility[12] (see fig. 1). The homogeneous part of the integral equation for $T'(k_1, k_3; q = 0)$ is just the linearized gap equation whose eigensolutions $\phi(\mathbf{k}, \omega)$ and eigenvalues λ have been calculated previously[12]. From this it is clear that the term $(T - T_{\mathrm{c}})/T_{\mathrm{c}}$ in eq. (1) has to be replaced by $[1 - \lambda_d(T)]$, and $\psi(\mathbf{k})$ by $\phi_d(\mathbf{k}, \omega)$, where λ_d is the eigenvalue of the $d_{x^2-y^2}$-wave eigensolution $\phi_d(\mathbf{k}, \omega)$. For finite $\mathbf{q}$ and ω of the embryonic pair we obtain in the denominator of T', besides the term $(1 - \lambda_d)$, quantities corresponding to $\xi^2 q^2$ and $-i\omega\tau$ in eq. (1).

Going to the real-frequency formulation and separating $\Sigma'(\mathbf{k}, \omega)$ into odd- and even-ω parts, $\omega[1 - Z(\mathbf{k}, \omega)]$ and $\xi(\mathbf{k}, \omega)$, we obtain the following normal-state self-energy equations:

$$\begin{aligned}\omega[1 - Z(\mathbf{k}, \omega)] = \sum_{\mathbf{k}'} \int_0^\infty \mathrm{d}\Omega\, \left[\mid \phi_d(\mathbf{k}, \omega) \mid^2 K(\mathbf{k} - \mathbf{k}', \Omega) + P_{\mathrm{s}}(\mathbf{k} - \mathbf{k}', \Omega)\right] \times \\ \times \int_{-\infty}^{\infty} \mathrm{d}\omega' I(\omega, \Omega, \omega') A_0(\mathbf{k}', \omega'),\end{aligned} \tag{2}$$

$$K(\mathbf{q}, \Omega) = \frac{g}{4\pi\bar{N}} \frac{(g/4)\,\tau\Omega}{\left[(1 - \lambda_d) + (g/4)\,\xi_0^2 q^2\right]^2 + \left[(g/4)\,\tau\Omega\right]^2}. \tag{3}$$

The expressions for the superconducting coherence length ξ_0 at $T = 0$ and for the relaxation time τ are essentially the same as those which have been derived from Ginzburg-Landau-Gorkov (GLG) theory [8]. The coupling constant g is approximately equal to

$$g = (3/2)\,(U/t)^2\,\mathrm{Re}\,(\chi(\mathbf{Q},0)t)\,4\pi\,(\Delta q)^2\,\gamma\,, \tag{4}$$

where Δq and γ are the half-widths of the peak $\mathrm{Re}\,\chi(\mathbf{q},\nu)$ around $\mathbf{q} = \mathbf{Q}$ and $\nu = 0$, respectively. The equation for the energy shift $\xi(\mathbf{k},\omega)$ is obtained from eq. (2) by changing the sign in front of the term $|\phi|^2 K$, and by replacing the spectral function A_0 by $A_3(\mathbf{k}',\omega')$. The eigenvalue λ_d is obtained from the linearized equation for the order parameter $\phi_d(\mathbf{k},\omega)$ [12]. The spin-fluctuation interaction P_s, the spectral functions A_0 and A_3, and the kernel I are given in [12].

We consider here a tight-binding band $\epsilon(\mathbf{k})$ whose 2D Fermi line is similar to that of the YBaCuO and Bi2212 compounds. Then the spin-fluctuation interaction $P_\mathrm{s}(\mathbf{q},\omega)$ exhibits a broad peak centered at $\mathbf{q} = \mathbf{Q} = (\pi,\pi)$. In contrast to this, the order parameter fluctuation interaction $K(\mathbf{q},\Omega)$ (see eq. (3)) exhibits a peak centered at $\mathbf{q} = 0$ whose width is of the order ξ_0^{-1}. These two interactions are coupled via the irreducible spin susceptibility χ_0 which is determined by the quasiparticle spectral function $N(\mathbf{k},\omega) = A_0 + A_3$. The latter functions are renormalized by the self-energies $\omega(1-Z)$ and ξ. Equation (2) for $\omega(1-Z)$, and the corresponding one for $\xi(\mathbf{k},\omega)$, are calculated self-consistently together with the eigenvalue equation for λ_d and $\phi_d(\mathbf{k},\omega)$, and with the interactions P_s [12] and K (see eq. (3)). We want to emphasize that the eigenvalue λ_d and the eigenfunction $\phi_d(\mathbf{k},\omega)$ are calculated self-consistently, which takes into account the renormalization of the order parameter fluctuations by the spin fluctuations, and vice versa. It is interesting that $\phi_d(\mathbf{k},\omega)$ has about the same $\mathbf{k}$- and ω-dependence as the gap function below T_c [12]: there occurs a maximum of $\mathrm{Im}\,\phi_d(\mathbf{k},\omega)$ at about $\omega \simeq 0.4t$ and a corresponding dispersive behavior of $\mathrm{Re}\,\phi_d(\mathbf{k},\omega)$ with a zero at $\omega \simeq 0.7t$.

We present now our results for a $\mathbf{q}$-dependent Coulomb repulsion $J(\mathbf{q})$ (see [12]) with $J(\mathbf{Q}) \equiv U = 3.2t$ (t is the nearest-neighbor hopping energy) and a chemical potential $\mu = -1.1$ corresponding to a renormalized band filling $n = 0.92$. The superconducting coherence length ξ_0 and the relaxation time τ are given in [8] in terms of the tight-binding band $\epsilon(\mathbf{k})$. For d-wave pairing ξ_0 varies from about $5a$ to a as the band filling n varies from $n = 0.85$ to half-filling $n = 1$. A typical value for the relaxation time τ is obtained from the Ginzburg-Landau expression, *i.e.* $\tau\Omega = \pi\Omega/8T_\mathrm{c} \simeq 6(\Omega/t)$. The superconducting transition temperature T_c is given by that temperature where, for decreasing T, the eigenvalue $\lambda_d(T)$ passes through unity. Without order parameter fluctuations we find $T_{\mathrm{c}0} = 0.028t$. This T_c is reduced in proportion to decreasing ξ_0 and τ, *i.e.* $T_\mathrm{c} \simeq 0.015t$ for $\xi_0 = 4$, $\tau = 8$, and $T_\mathrm{c} \simeq 0.01t$ for $\xi_0 = 2$, $\tau = 4$ at fixed $g = 1$. The value of $g = 1$ for the coupling constant has been estimated from eq. (4) by using the results for $\mathrm{Re}\,\chi(\mathbf{q},\nu)$ (see fig. 2(b)). This effect of decreasing T_c for increasing strength of the order parameter fluctuations (OPFL), or decreasing ξ_0 and τ, might be the reason why T_c decreases in the underdoped regime for $n \to 1$.

In fig. 2(a) we show the spectral density of the spin susceptibility at $\mathbf{Q}$, $\mathrm{Im}\,\chi(\mathbf{Q},\omega)$, without (dashed line) and with OPFL for $g = 1$, $\xi_0 = 4$ and $\tau = 8$ (solid lines). One sees that the spin susceptibility is suppressed by the OPFL at the same temperature T. Considered as a function of T, one finds that $\mathrm{Im}\,\chi(\mathbf{Q},\omega)$ increases monotonically with decreasing T in the absence of OPFL, while in the presence of OPFL this function increases down to a temperature $T_* \simeq 0.035t$ where it passes through a maximum, and then decreases slowly as T decreases from T_* downwards to T_c. At the same time, the position of the maximum, ω_sf, decreases first with decreasing T down to T_* where it passes through a minimum, and then increases as T decreases further towards T_c. For the parameter set $g = 1$, $\xi_0 = 2$, $\tau = 4$, we obtain somewhat smaller values of the spin susceptibility and a crossover temperature $T_* \simeq 0.038t$. An analogous

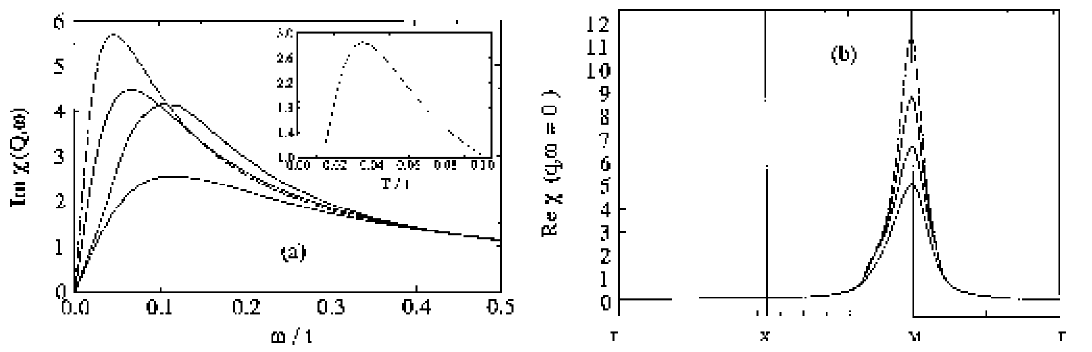

Fig. 2. – Dynamical spin susceptibility $\chi(\mathbf{q},\omega)$ in the absence of order parameter fluctuations (OPFL) at $T = 0.035t$ (dashed line), and in the presence of OPFL for superconducting coherence length $\xi_0 = 4$ and relaxation time $\tau = 8$ (solid lines). (a) $\mathrm{Im}\,\chi(\mathbf{Q},\omega)$ at $\mathbf{Q} = (\pi,\pi)$ *vs.* ω, with solid lines for $T = 0.1t$ (lowest curve), $T_* = 0.035t$ (uppermost curve), and $T = 0.015t$ (intermediate curve). The inset shows this quantity for fixed $\omega = 0.024t \simeq 6\,\mathrm{meV}$ as a function of T. (b) $\mathrm{Re}\,\chi(\mathbf{q},\omega = 0)$ *vs.* $\mathbf{q}$ along a path running from $\Gamma = (0,0)$, to $X = (\pi,0)$ to $M = (\pi,\pi)$ and back to Γ, with solid lines for the same T as in (a).

behavior is found for the $\mathbf{q}$-dependence of $\mathrm{Re}\,\chi(\mathbf{q},\omega = 0)$. In fig. 2(b) we have plotted this function *vs.* $\mathbf{q}$ along a path in the Brillouin zone running from $\Gamma = (0,0)$ to $X = (\pi,0)$ to $M = (\pi,\pi)$ and back to Γ. One sees that without OPFL (dashed line) the peak centered at $\mathbf{Q}$ is higher and narrower than that with OPFL (solid lines) at the same T. Moreover, in the former case the height of the peak increases monotonically with decreasing T, while with OPFL the height of the peak passes through a maximum at about $T_* \simeq 0.035t$. At the same time the half-width of the peak, $\Delta q \propto \xi_{\mathrm{AF}}^{-1}$, decreases monotonically with T in the absence of OPFL, while it passes through a minimum at T_* in the presence of OPFL.

These completely different behaviors of the spin susceptibility with and without OPFL are reflected in the temperature dependence of the spin-lattice relaxation rate $1/T_1$ and of the spin-echo decay rate $1/T_{2G}$. In fig. 3(a) we have plotted our results for $1/T_1T$ *vs.* T (with constant form factor) for our two parameter sets of ξ_0 and τ. One sees that $1/T_1T$ first increases with decreasing T, passes through a maximum at about $T_* \simeq 0.035t$ for $\xi_0 = 4$, $\tau = 8$ ($T_* \simeq 0.038t$ for $\xi_0 = 2$, $\tau = 4$), and then decreases as T tends to T_{c}. Thus, T_1T has about the same T-dependence as ω_{sf}. We identify the temperature T_* approximately with the crossover temperature to spin pseudogap behavior which has been observed in the underdoped cuprates [2], [3]. One recognizes from fig. 3(a) that T_* increases while T_{c} decreases as one goes from the parameter set $\xi_0 = 4$, $\tau = 8$, to $\xi_0 = 2$, $\tau = 4$. We obtain ratios of about $T_*/T_{\mathrm{c}} \simeq 2.5$ and 4, respectively, which agree qualitatively with the observed ratios for $YBa_2Cu_3O_{6.63}$ and $YBa_2Cu_4O_8$ [2]. In fig. 3 we have also included our result for coupling strength $g = 0.3$ and $\xi_0 = 4$, $\tau = 8$ in eq. (3). One sees that for decreasing OPFL T_* decreases while T_{c} increases ($T_* \simeq 0.03t$ and $T_{\mathrm{c}} \simeq 0.02t$). In contrast to this behavior, we obtain in the absence of OPFL a function $1/T_1T$ which increases continuously with decreasing T down to T_{c}, in agreement with data on YBaCuO in the overdoped regime [1], [2] (see fig. 3(a)).

The calculated spin-echo decay rate $1/T_{2G}$ (with constant form factor) increases continuously with decreasing T without OPFL, while it passes through a maximum at about T_* in the presence of OPFL. Thus, we can say that T_{2G} has roughly the same T-dependence as the half-width $\Delta q \propto \xi_{\mathrm{AF}}^{-1}$ of the commensurate peaks (see fig. 2(b)). This leads to an almost

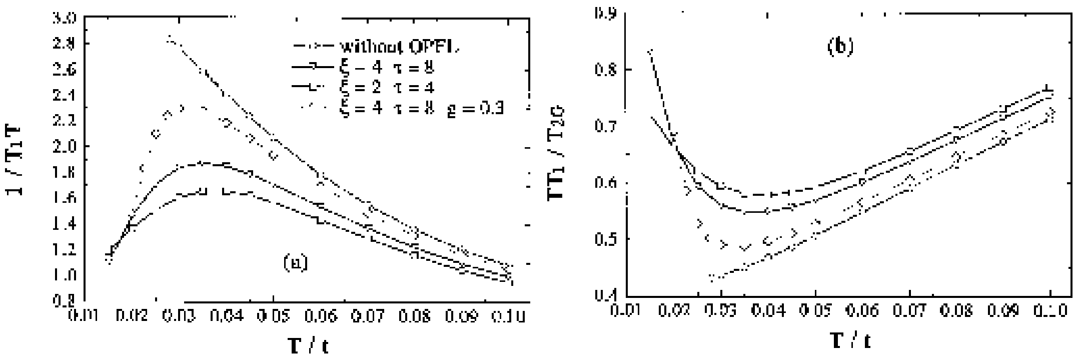

Fig. 3. – (a) The quantity $1/T_1T$ *vs.* T, where $1/T_1$ is the spin-lattice relaxation rate, without order parameter fluctuations (OPFL) (dashed line and circles) and with OPFL for coupling strength $g = 1$ and for superconducting coherence lengths and relaxation times $\xi_0 = 4$, $\tau = 8$ (solid line and triangles), and $\xi_0 = 2$, $\tau = 4$ (solid line and squares). The dotted line (with diamonds) refers to $g = 0.3$ and $\xi_0 = 4$, $\tau = 8$ in eq. (3). The maxima occur at the crossover temperature T_*. (b) Ratio T_1T/T_{2G} *vs.* T, where $1/T_{2G}$ is the spin-echo decay rate, for the same parameter sets as in fig. 3(a). The minima occur at about the same T_* as the maxima in (a).

temperature-independent ratio T_1T/T_{2G}^2 without OPFL corresponding to $z = 2$ overdamped spin excitations [2], [3]. In fig. 3(b) we have plotted the ratio T_1T/T_{2G} *vs.* T, in the absence of OPFL and for our two sets of ξ_0 and τ in the presence of OPFL. One sees that without OPFL this ratio decreases almost linearly with decreasing T while in the presence of OPFL the curve for this ratio first runs almost parallel to the former curve, then below a temperature $T_{\rm cr}$ this curve bends upwards until it reaches a minimum at about T_*, and below T_* this curve increases as T decreases further to $T_{\rm c}$. The behavior of T_1T/T_{2G} in the range from $T_{\rm cr}$ to T_*, and below T_*, is similar to the observed behavior of this ratio for the underdoped cuprates in the $z = 1$ pseudoscaling and spin pseudogap regimes [2], [3].

Our calculations show that the inclusion of order parameter fluctuations (OPFL) in the FLEX approximation for the 2D Hubbard model is capable of explaining some of the unusual properties of the high-$T_{\rm c}$ cuprates in the underdoped regime. First, one obtains a reduction of $T_{\rm c}$ for increasing strength of OPFL corresponding to increasing coupling strength g and/or decreasing superconducting coherence length ξ_0 and relaxation time τ. From our results for $\chi(\mathbf{q}, \omega)$ for different doping values $x = 1 - n$ away from half-filling, we find with the help of eq. (4) that g increases with decreasing x. Furthermore, ξ_0 and τ decrease with decreasing x [8]. Second, the spin susceptibility $\chi(\mathbf{q}, \omega)$ for $\mathbf{q}$ near $\mathbf{Q} = (\pi, \pi)$, and in turn the NMR relaxation rates $1/T_1$ and $1/T_{2G}$, exhibit for decreasing T a crossover at a temperature T_* to spin pseudogap behavior [2], [3] (see figs. 3(a) and (b)). This crossover temperature T_* increases for increasing strength of OPFL. We remark that T_* decreases while $T_{\rm c}$ increases for increasing U. Third, $\mathrm{Im}\,\chi(\mathbf{Q}, \omega)$ at fixed small ω passes through a maximum at T_* for decreasing T (see inset of fig. 2(a)). This agrees qualitatively with the neutron scattering data on underdoped $YBa_2Cu_3O_{6+x}$ [13].

We want to emphasize that our finite values of $T_{\rm c}$ in the presence of order parameter fluctuations in two dimensions are not in conflict with Hohenberg's theorem [14] which states that there is no long-range order possible in two dimensions at finite temperatures. The temperature at which $\lambda_d(T)$ reaches unity is the temperature at which the d-wave pair field susceptibility diverges and thus it will be an approximation of the Kosterlitz-Thouless transition temperature. This has been studied carefully by Luo and Bickers [15] for the attractive Hubbard model.

In summary, we studied the competition between spin fluctuations and order parameter fluctuations within an extension of the FLEX approximation. The latter become sufficiently strong near T_c because the superconducting coherence length is relatively small for the high-T_c cuprates. We find that d-wave order parameter fluctuations above T_c can explain very well the observed spin gap in the underdoped cuprates for wave vectors $\mathbf{q}$ near $\mathbf{Q} = (\pi, \pi)$. However, we cannot explain the spin pseudogap at $\mathbf{q} = 0$ and the quasiparticle gap. This raises the question whether the latter gaps might have a different physical origin which is not described by the present FLEX approximation.

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