Condensation energy in the spin-fermion model for cuprates

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We use the Scalapino-White relation between the condensation energy and the difference between the dynamical structure factor in the normal and the superconducting states to compute the condensation energy in the spin-fermion model. We show that at strong coupling, the extra low-frequency spectral weight associated with the resonance peak in the dynamical structure factor in a superconductor is compensated only at energies ~ J which are much larger than the superconducting gap Δ. We argue that in this situation, the condensation energy is large and well accounts for the data for cuprates.

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The understanding of the mechanism of superconductivity is an important step towards the general understanding of the physics of cuprates. It has been known from the studies of BCS superconductors, that the information about the pairing boson can be extracted from measurements of the upper critical field. Specifically, the increase of the kinetic energy in a superconductor is over-compensated by the decrease of the potential energy associated with the feedback effect from superconductivity on the bosonic mode which is responsible for pairing. The energy difference is called a condensation energy Ec and is directly related to the measurable thermodynamic critical field by Ec = V0 \( H_c^2/(8\pi) \) where V0 is the volume of the unit cell.

Recently, Scalapino and White applied this reasoning to high \( T_c \) superconductors. They argued that if the pairing is mediated by spin fluctuations, then the difference in the dynamical structure factor \( S(q, \Omega) \) between the normal and the superconducting states, integrated over frequency and momentum with the weighting factor \( \cos q_x + \cos q_y \) should be positive and of the same order as \( E_c \). This yields a relation

\[
\frac{H_c^2}{8\pi} = \frac{3N}{2} \alpha J \int \frac{d^2q}{4\pi^2} \int_0^\infty \frac{d\Omega}{\pi} \left( S_n(q, \Omega) - S_{sc}(q, \Omega) \right) (\cos q_x + \cos q_y),
\]

where \( \alpha < 1 \) is a numerical factor which accounts for the fact that the condensation energy is smaller than the decrease in the potential energy, and \( N (= 2 \text{ for } YBCO \text{ and } Bi2212) \) is the number of layers in the unit cell.

Neutron scattering experiments in YBCO and Bi2212 demonstrated that in a superconducting state, \( S_{sc}(q, \Omega) \) possesses a resonance peak at momenta near \( Q = (\pi, \pi) \) and at frequencies below \( 2\Delta \) where \( \Delta \ll J \) is the maximum of the \( d \)-wave gap. The integrated intensity of the resonance peak yields the r.h.s. of the above relation consistent with the data on \( H_c \). However, it is not clear a priori to which extent the contribution from the resonance peak measures the actual condensation energy in a system. The relevant issue here is whether the spectral weight of the resonance peak is compensated by the depletion of the spectral weight in \( S_{sc}(q, \Omega) \) at energies comparable to \( \Delta \), or the compensation comes from energies comparable to \( J \), i.e., from \( |q - Q| \sim \Delta/J \ll 1 \), or the compensation comes from energies comparable to \( J \), i.e., from \( |q - Q| \sim \Delta/J \ll 1 \).

In the first case, the geometrical \( \cos q_x + \cos q_y \) factor is nearly constant for relevant \( q \) and can be omitted. Since \( \int d^2q d\Omega S(q, \Omega) = S(S+1)/3 \) where \( S \) is the average value of the on-site spin (this is the sum rule for spin structure factor), the r.h.s. of the above relation just measures the difference in \( S \) between normal and superconducting states. In general, this difference is finite due to a possibility for double occupancy for which case \( d \)-wave superconductivity favors a spin singlet, \( S = 0 \). However, in cuprates double occupancy is energetically unfavorable (Hubbard \( U \) is large), and the condensation energy should be small.

In the second case, however, typical \( q \) are far from \( Q \), and the momentum dependence of the geometrical factor cannot be neglected. In this situation, one can expect that the condensation energy is not reduced by the sum rule constraint and, generally, is of the same order as the unscreened contribution from the resonance peak.

There are two qualitatively different explanations of the resonance peak. One was presented by us, and is based on strong coupling calculations within the spin-fermion model. These calculations extend earlier weak-coupling results by others. We argued that the resonance peak is in the particle-hole channel and is related to the fact that in a superconductor, the damping of a spin fluctuation due to a decay into a particle-hole pair is strong only at frequencies above \( 2\Delta \), while below \( 2\Delta \) it is strongly reduced because of a lack of phase space for a decay. By a Kramers-Kronig relation, this reduction produces a real part of the spin polarization bubble. At low energies, this real part scales as \( \omega^2 \), i.e spin collective modes in a superconductor behave as propagating magnons. This behavior obviously gives rise to a peak in \( S_{sc}(q, \Omega) \) at \( \Omega = \Omega_{res} \propto \xi^{-1} \), where \( \xi \) is the magnetic correlation length.

Another explanation was presented by Demler and Zhang in the context of \( SO(5) \) theory of superconductivity. They conjectured that the peak seen in neu-
tron scattering is an antibound state in the spin-triplet, particle-particle channel at total momentum \( Q \) (\( \pi \) resonance). Below \( T_c \), particle-particle and particle-hole channels are mixed, and the antibound state appears as a pole in the spin susceptibility.

Demler and Zhang recently argued that the measurement of the condensation energy is a way to distinguish between the two theories. They conjectured on general grounds that if the \( \pi \) resonance is the correct explanation, then it is likely that the compensation of the peak spectral weight comes from high energies. Their argumentation is that in the spin-fluctuation theory of the peak, the compensation of the spectral weight is confined to a vicinity of \( 2\Delta \), and hence the condensation energy is small.

In the present paper we show that this is not the case. We compute \( S(q,\Omega) \) in the spin-fermion model and show that the compensation of the spectral weight associated with the resonance peak in fact comes from high energies. Their argumentation is that at strong coupling, the low-energy antibound state in the particle-particle channel does not exist because fermionic incoherence washes out the upper boundary of fermionic dispersion.

The point of departure for our consideration is the spin-fermion model for cuprates. It describes low-energy fermions interacting with their collective spin degrees of freedom. Of interest here is the form of the full dynamical spin susceptibility. It has been derived in earlier studies, and we just quote the results. Both in the normal and the superconducting state, the full spin susceptibility can be written as \( \chi^{-1}(q,\Omega) = \chi_0^{-1}(q) - \Pi_q(\Omega) \), where \( \chi_0 \) is the bare susceptibility which is made of fermions with energies comparable to bandwidth, and \( \Pi_q(\Omega) \) is the universal (i.e. cutoff independent) contribution from low-energy fermions.

The form of \( \chi_0 \) is the input for low-energy calculations. As before, we assume that \( \chi_0 \) is peaked at \( Q \) or near \( Q \), and has a simple Ornstein-Zernike form i.e. \( \chi_0(q) = \chi_0 \delta^2 / (1 + (q - Q)^2\xi^2) \).

The universal contribution to the dynamical susceptibility involves low-energy fermions and therefore has to be computed fully self-consistently within the spin-fermion model. Near \( q = Q \), one can neglect \( q \) dependence in \( \Pi \) (it yields only a small correction to already exciting dispersion in \( \chi_0(q) \)) and restrict with \( \Pi_Q(\Omega) = \Pi_\Omega \). The full susceptibility then has the form

\[
\chi(q,\Omega) = \frac{\chi_0 \delta^2}{1 + (q - Q)^2\xi^2 - \Pi_\Omega}.
\]

We absorbed \( \chi_0 \xi^2 \) factor into the redefinition of \( \Pi_\Omega \).

In the normal state, \( \Pi_\Omega \) is purely imaginary and for any coupling strength is almost linear in \( \Omega \): \( \Pi_\Omega = i\Omega / \omega_{sf} \) where \( \omega_{sf} \propto \xi^{-2} \). The deviations from the linear behavior result from the corrections to the particle-hole vertex which at \( \xi = \infty \) are logarithmical in \( \omega \). However, the prefactors are small, and the deviations from linearity become relevant only in the extremely tiny region near \( \xi = \infty \) which we will not study here.

Consider now the superconducting state. Here the form of \( \Pi_\Omega \) is more complex because spin polarization is cut below \( 2\Delta \). By Kramers-Kronig relation, this cut in \( Im\Pi_\Omega \) creates Re\( \Pi_\Omega \) which, as we said before, gives rise to a resonance peak in \( \chi''(Q,\Omega) \) below \( 2\Delta \).

In general, the spin polarization operator in a superconductor is a sum of bubbles made of normal and anomalous Green’s functions. Both fermions in the bubble has to be near the Fermi surface to satisfy the constraint on energy conservation. For \( q \approx Q \), this restricts the momentum integration to the vicinity of hot spots. Their ar-

Here \( R = \tilde{g} / (v_F\xi^{-1}) \) is a dimensionless parameter which governs the strength of the spin-fermion coupling (we use the same notations as in - \( \tilde{g} \) is the effective spin-fermion coupling, \( v_F \) is the Fermi velocity at a hot spot). There are numerous reasons to believe that at and below optimal doping \( R \approx 1 \). To shorten notations, we included a bare \( \omega \) term in \( G^{-1}(k,\omega) \) into the self-energy.

We discuss the solution of (3,4) below but first consider what we actually need to compute. Our goal is to check how the extra spectral weight in local \( S_{sc}(\Omega) \) is redistributed compared to the normal state. For this purpose, it is sufficient to compute the integral in (4) without the geometrical \( cos q_x + cos q_y \) factor and just check at which scales the sum rule is recovered.

Without \( cos q_x + cos q_y \), the momentum integration in the r.h.s. in (4) can be performed exactly, and at \( T \rightarrow 0 \), we obtain using \( S(q,\Omega) = 2\chi''(q,\Omega) / (1 - e^{-\hbar \Omega / T}) \)

\[
I = \int \frac{d^2q d\Omega}{4\pi^3} \left( S_{sc}(q,\Omega) - S_n(q,\Omega) \right) = \frac{\chi_0}{4\pi^2} \int_0^\infty d\Omega F(\Omega),
\]
where

\[ F(\Omega) = \arctan \frac{\omega_{sf}}{\Omega} - \arctan \frac{1 - Re\Pi_\Omega}{Im\Pi_\Omega}. \]

We see that the rate of convergence of the r.h.s. of (3) depends on the forms of both \(Re\Pi_\Omega\) and \(Im\Pi_\Omega\) above the superconducting gap.

We now obtain these forms from Eq. (1). Qualitatively, the solution of this set has been obtained earlier [2,3,4,5]. Here we present quantitative results for \(\Pi_\Omega\).

At \(R \gg 1\), the normal state self-energy has a Fermi-liquid form \(\Sigma(\omega) \propto Z^{-1}(\omega + i\omega / (4\omega_{sf}))\) with \(Z \propto R^{-1} \sim (\omega_{sf}/\bar{g})^{1/2}\) at energies smaller than, and at larger frequencies crosses over into a non-Fermi liquid, quantum-critical regime \(\Sigma(\omega) \propto \exp(i\pi/4) / \sqrt{\bar{g}/|\omega|}\). A simple experimentation shows that the solution of (3) depends on the ratio between \(\omega_{sf}\) and the measured superconducting gap which is \(\bar{\Delta} = \Delta Z\) if \(\omega_{sf} \gg \Delta\), and \(\Delta \sim \Delta^2/\bar{g}\) if \(\omega_{sf} \ll \Delta \ll \Delta\). In the first case, at typical frequencies \(\sim \Delta\) the system behaves in the normal state as a Fermi-liquid, while in the second case, which is more relevant to optimally doped and underdoped cuprates [4,5], fermions with \(\omega \sim \bar{\Delta} \gg \omega_{sf}\) display in the normal state the quantum-critical, \(\sqrt{\omega}\) behavior.

![FIG. 1. Schematic representation of \(F(\Omega)\) from Eq. (3) for (a) weak coupling case \(\omega_{sf} \gg \bar{\Delta}\) and (b) strong coupling case \(\omega_{sf} \ll \bar{\Delta} \ll \Delta\). Here \(\bar{\Delta}\) and \(\Delta\) are measured superconducting gaps at weak and strong coupling, respectively, \(\Omega_{res}\) is the frequency of the neutron resonance peak in a superconductor, and \(\omega_{sf}\) is a typical spin relaxation frequency in the normal state. Observe that in both cases, the frequency integral of \(F(\Omega)\) is confined to frequencies, which are much larger than the measured superconducting gap.](image)

We now consider the two cases separately. At \(\omega_{sf} \gg \bar{\Delta}\), the quasiparticle residue just renormalizes the superconducting gap \((\Delta \to \bar{\Delta})\), and the system behavior is the same as at weak coupling. In this situation [3,4] \(Im\Pi_\Omega = 0\) for \(\Omega < 2\bar{\Delta}\), while \(1 - Re\Pi_\Omega\) changes sign at \(\Omega_{res} = 2\bar{\Delta}(1 - O(e^{-\omega_{sf}/\bar{\Delta}}))\). Above \(2\bar{\Delta}\), the analytical form for \(\Pi_\Omega\) can be obtained in the limit of \(\Omega \gg 2\bar{\Delta}\). We found \(Re\Pi_\Omega(\Omega) \propto \pi \bar{\Delta}^2/(\Omega \omega_{sf})\) and \(Im\Pi_\Omega(\Omega) = (\Omega/\omega_{sf}) + (2\bar{\Delta}^2/\Omega \omega_{sf}) \log(\Omega/\bar{\Delta})\). Substituting these results into (3) we find after a simple algebra that below \(2\bar{\Delta}\), \(F(\Omega)\) is negative except for a tiny range between \(\Omega_{res}\) and \(2\bar{\Delta}\), while above \(2\bar{\Delta}\), \(F(\Omega)\) is positive and scales as \(F(\Omega) \propto (1/\Omega) \log \Omega/\bar{\Delta}\) for \(\Omega < \omega_{sf}\) and as \(F(\Omega) \propto (1/\Omega)^3\) for \(\Omega > \omega_{sf}\). This behavior is schematically shown in Fig. (a). Splitting the integral in (3) in two parts, \(I = I_1 + I_2\), where the first is the integral over frequencies up to twice the measured gap and the second is the integral over larger frequencies, and performing integration we obtain with the logarithmical accuracy

\[ I_1 \approx \frac{\chi_0}{4\pi^2} \left( \frac{\pi(2\bar{\Delta} - \Omega_{res})}{2\bar{\Delta}^2} - \frac{2\bar{\Delta}^2}{\omega_{sf}} \right) \approx -\frac{\chi_0}{2\pi^2} \frac{\bar{\Delta}^2}{\omega_{sf}} \]

\[ I_2 \approx \frac{\chi_0}{2\pi^2} \frac{\bar{\Delta}^2}{\omega_{sf}} \int_{\sim \Delta}^{\omega_{sf}} \frac{d\Omega}{\Omega} \log \frac{\Omega}{\bar{\Delta}} \approx \frac{\chi_0}{4\pi^2} \frac{\bar{\Delta}^2}{\omega_{sf}} \log^2 \frac{\omega_{sf}}{\bar{\Delta}} \]

We see that the contribution from low frequencies is negative - the vanishing of \(Im\Pi_\Omega\) overshadows the contribution from the resonance peak which for \(\omega_{sf} \gg \bar{\Delta}\) has an exponentially small residue. However, the contribution from frequencies above \(2\bar{\Delta}\) is positive and parametrically larger than negative \(I_1\), such that \(I = I_1 + I_2 > 0\).

It is essential that although typical frequencies in \(I_2\) are \(\Omega \sim \omega_{sf} \gg \bar{\Delta}\), still \(I_2\) converges at \(\omega \sim \omega_{sf}\) and therefore does not depend on system behavior far away from \(Q\). Indeed, at \(\omega \sim \omega_{sf}\), typical \(q - Q\) are of the order of inverse correlation length (see [4]). The geometrical \(cos q_s + cos q_f\) factor is then nearly a constant (= -2) for all relevant \(q\) and hence a nonzero value of the condensation energy just reflects the fact that in the absence of no double occupancy constraint, the average on-site spin in the \(d\)-wave superconducting state is smaller than in the normal state. Notice that the magnitude of \(I\) is much smaller than \(\chi_0 \bar{\Delta}\) which would be the contribution from the resonance peak if its residue was \(O(1)\).

Consider now the opposite case of \(\omega_{sf} \ll \bar{\Delta} \ll \Delta\) where, we remind, \(\Delta \sim \Delta^2/\bar{g} \sim \Delta^2/\omega_{sf}\) is the measured gap in this limit. Below \(2\bar{\Delta}\) we still have \(Im\Pi_\Omega = 0\), but the resonance frequency (the one at which \(Re\Pi_\Omega = 1\)) is now much smaller than the gap: \(\Omega_{res} \sim (\Delta \omega_{sf})^{1/2} \ll \bar{\Delta}\). At \(\Omega \gg \Delta\) but still \(\Omega \ll \bar{g}\), we find from [3,4] that \(Im\Pi_\Omega\) approaches the normal state form \(\Pi_\Omega/\omega_{sf}\), but \(Re\Pi_\Omega\) saturates at \(Re\Pi_\Omega = (\pi \bar{\Delta}/(2\omega_{sf}))(1 + \pi^{-1} \log 2)\) and preserves this value as long as the fermionic propagator has a non-Fermi liquid, \(\sqrt{\omega}\) form. At very large frequencies \(Re\Pi_\Omega\) indeed decreases, but the decrease begins only at \(\Omega \sim \Omega_{max}\), where either the fermionic propagator recovers Fermi-liquid behavior, i.e., bare \(\omega\) term exceeds \(\sqrt{\omega}\) contribution from the self-energy, or typical \(q - Q\) in \(S(q,\Omega)\) become \(O(1)\), i.e., lattice effects become relevant. For \(\bar{g} \ll v_F k_F\), the recovery of the Fermi-liquid behavior comes first, and \(\Omega_{max} \sim \bar{g}\). For \(\bar{g} \gg v_F k_F\) (which in Hubbard-model language implies \(U \gg t\)), lattice effects become relevant first, and \(\Omega_{max} \sim (v_F k_F)^2/\bar{g} \sim J\).

Substituting the results for \(\Pi_\Omega\) into (3) we find that \(F(\Omega)\) is now positive at frequencies below \(2\bar{\Delta}\), except
for very low $\Omega < \Omega_{res} \ll 2\Delta$. However, $F(\Omega)$ is also positive above $2\Delta$ and, moreover, due to a saturation in $Re\Pi_0$, it behaves as $F(\Omega) \propto 1/\Omega$ up to $\Omega_{max}$ which again causes a logarithmical behavior of the frequency integral. This behavior of $F(\Omega)$ is schematically shown in Fig. (6). Evaluating the integral in (6), with the logarithmical accuracy we obtained

$$I_1 = \frac{\chi_0}{4\pi} (\Delta - \Omega_{res}) \approx \frac{\chi_0}{4\pi} \tilde{\Delta}$$

$$I_2 = \frac{\chi_0}{8\pi} \tilde{\Delta} \beta \int_{\Delta}^{\Omega_{max}} \frac{d\Omega}{\Omega} = \frac{\chi_0}{8\pi} \tilde{\Delta} \beta \log \frac{\Omega_{max}}{\Delta}$$

(8)

where $\beta = 1 + \pi^{-1}\log 4$. We see that $I_1$ is positive, i.e., the appearance of the resonance peak below $T_c$ gives rise to an extra integrated spectral weight below $2\Delta$ and hence yields a positive contribution to the condensation energy. As we discussed before, this extra spectral weight should be compensated by a depletion of the spectral weight at somewhat higher frequencies. We see however that due to non-Fermi liquid behavior of the fermionic propagator above $2\Delta$, this compensation comes from frequencies larger than $\Omega_{max}$. Moreover, the integrated contribution from energies between $2\Delta$ and $\Omega_{max}$ is logarithmically larger than the contribution from the resonance peak. Further, for $g \gg v_F k_F$ (the case when the no double occupancy constraint is almost exact), $\Omega_{max} \sim \omega_{sf} \xi^2$ and hence typical momenta in $\chi(q, \Omega)$ are $(q - Q) \xi^2 \sim \Omega_{max}/\omega_{sf} \sim \xi^2$, or $q - Q = O(1)$. In this situation, the geometrical $\cos q_x + \cos q_y$ factor in (1) cannot be approximated by a constant and effectively reduces the contribution from high energies. In other words, even if $\int d^2 q d\Omega S(q, \Omega)$ does not change between normal and superconducting states, there is still a finite, positive condensation energy which is even larger than the net contribution from the resonance peak. This is the central result of the paper.

The magnitude of the contribution to $E_c$ from the resonance peak in optimally doped $YBCO$ has been estimated in [1] without invoking any theory but rather using the experimental results for $\int \chi''(q, \Omega)$ [2]. They found $E_c \sim 0.03\alpha J$ where, we recall, $\alpha < 1$ accounts for the reduction of $E_c$ due to the increase in the kinetic energy. Using $J \sim 1500$, one obtains $E_c \sim 45\alpha K$ which, as Demler and Zhang argued [3] agrees with $E_c \sim 3 - 12K$ extracted from penetration depth and specific heat measurements. Our results show that the actual magnitude of $E_c$ is even higher due to an extra positive contribution from frequencies above $2\Delta$. Furthermore, we found that this extra contribution to the condensation energy is larger than the one from the peak. From this perspective, the above estimate for $E_c$ yields a lower boundary for the condensation energy.

To summarize, in this paper we considered the condensation energy within the spin-fermion model for cuprates. At strong coupling, this model predicts that in a superconducting state, $\chi''(Q, \Omega)$ possesses a sharp resonance peak below twice the maximum of the measured $d$-wave gap. We demonstrated that the appearance of this peak does not cause the depletion of the spectral weight in local $\chi''$ up to frequencies of order $J$. We computed the condensation energy $E_c$ using Scalapino-White relation between $E_c$ and $\chi''$ and found that the dominant, positive contribution to $E_c$ comes from a wide range of frequencies between $2\Delta$ and $J$. Our results disagree with the assertion in [4] that a large condensation energy cannot be obtained in the spin-fermion model and therefore would require a resonance in the triplet particle-particle channel ($\pi$-resonance).

We on the contrary didn’t find any indication of a sharp resonance in the $\pi$ channel at strong coupling. This resonance can only emerge as an antibound state and requires a sharp upper boundary of the fermionic spectrum. We, however, found that strong fermionic self-energy transforms the spectral weight from the quasiparticle peak to higher frequencies and washes out a sharp upper boundary of fermionic excitations. We caution however, that our analysis is valid for a Fermi surface with hot spots. Without hot spots, the fermionic decay is forbidden, and at least in some range of couplings, the fermionic spectrum preserves a sharp upper boundary in which case the system possesses an antibound state in the $\pi$ channel.

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