Low-energy renormalization of the electron dispersion of high-\(T_c\) superconductors

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High-resolution ARPES studies in cuprates have detected low-energy changes in the dispersion and absorption of quasi-particles at low temperatures, in particular, in the superconducting state. Based on a new \(1/N\) expansion of the t-J-Holstein model, which includes collective antiferromagnetic fluctuations already in leading order, we argue that the observed low-energy structures are mainly caused by phonons and not by spin fluctuations, at least, in the optimal and overdoped regime.

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ARPES studies in cuprates have recently detected changes in the electronic spectral function near the Fermi energy at low temperatures and, in particular, in the superconducting state [1, 2]. The dispersion of quasi-particles changes its slope by about a factor 2 over an energy region of about 50 meV and this change occurs in a rather isotropic way around the Fermi surface. These results indicate that the particles near the Fermi surface interact with excitations characterized by an energy scale of about 50 meV with a dimensionless coupling constant of about 1. Possible candidates for these excitations are phonons or spin fluctuations. In particular, the collective spin excitation associated with the resonance peak of neutron scattering has been assumed to cause this new low-energy scale [3].

Band structure calculations yield an overall dimensionless coupling constant λ of electrons near the Fermi surface and phonons between 0.5 and 1.5 [4, 5, 6]. On the other hand, transport relaxation times indicate a very weak coupling λ_e ≪ 0.3 between electrons and phonons [5, 6] in the optimally doped case. One explanation for this is that electronic correlations make the effective electron-phonon coupling strongly momentum and frequency dependent suppressing large-momentum scattering [4, 5]. Below we will study whether a similar large reduction of the effective electron-phonon coupling by correlations occurs in the electronic self-energy and the renormalization function Z which determines the change in the quasi-particle dispersion. Another relevant point is the anisotropy of this renormalization. Assuming a bare, momentum-independent electron-phonon coupling the same correlation-induced momentum dependence in the effective coupling which suppresses transport scattering rates will make Z in general anisotropic. The calculation has to show whether this induced anisotropy is small enough to account for the rather isotropic behavior of the slope change observed in experiment.

Spin fluctuations within the usual 1/N expansion yield only small contributions to the electronic self-energy and to scattering rates at low energies [7]. Though the coupling between spin fluctuations and electrons is set by the large hopping integral t, the spin fluctuation spectrum at large N is rather structureless and extends in energy over several t’s. Most spin flips thus are high-energy excitations yielding only small renormalizations at low energies. Below we will present results from a different 1/N expansion which favors antiferromagnetic fluctuations and accounts for the resonance peak in the spin susceptibility already in leading order. This approach is convenient to make a fair comparison of phonon- and spin fluctuations-induced contributions to the electronic self-energy.

In the following we consider a slightly modified version of the Hamiltonian Eq. (1) of Ref. [1] describing the t-J model coupled to dispersionless phonons. First, we assume that the underlying internal symmetry is the symplectic group Sp(N/2) and not SU(N). Consequently, we split the internal index p in Eq. (1) of Ref. [1] into an index σ describing the two spin components and a flavor index μ running from 1 to N/2. Secondly, we modify the second term in Eq. (1) in the following way:

$$\sum_{p, p'} \frac{J_{ij}}{4N} X_i^{p\sigma} X_j^{p'\sigma} \to \sum_{i,j,\sigma',\sigma=1/2} \frac{J_{ij}}{4N} X_i^{\sigma\sigma'} X_j^{\sigma'\sigma'}.$$

In the modified term the sum over the flavor index is carried out independently in each X operator, whereas the sum over spins retains the old form. The two terms in Eq. (1) are identical in the physical case N=2. At large N they differ, however, and the label arrangement in the left and right terms in Eq. (1) favor RVB and antiferromagnetic correlations, respectively. Thirdly, we multiply the Hamiltonian with an overall factor 2 so that it coincides with the usual Hamiltonian for N = 2 and t and J have the usual meaning.

The 11 element of the electronic Green’s function matrix in a BCS superconductor has the following form,

$$G(i\omega_n, \mathbf{k}) = \frac{1}{i\omega_n - \epsilon(\mathbf{k}) - \Sigma(i\omega_n, \mathbf{k}) - \Delta^2(\mathbf{k})/(i\omega_n + \epsilon(\mathbf{k}) - \Sigma(i\omega_n, \mathbf{k}))}.$$

$$\omega_n = (2n+1)\pi T$$ is a fermionic Matsubara frequency and T the temperature. \(\Delta(\mathbf{k}) = \Delta(cos(k_x) - cos(k_y))\) describes a frequency-independent superconducting order parameter with d-wave symmetry which is a rather good approximation for the anomalous self-energy at large N [2]. The one-particle energy \(\epsilon(\mathbf{k})\) is in the leading O(1) of the 1/N expansion given by \(-2t(cos(k_x) + cos(k_y)) - 4\Delta^2 cos(k_x) cos(k_y)\). \(t = t_0 \delta/2\) and \(t' = t_0' \delta/2\) are renormalized hopping elements with \(t_0, t_0'\) being bare hopping matrix elements between nearest and second-nearest neighbors on the square lattice, respectively. \(\delta\) is the doping away from half-filling. In our modified 1/N expansion \(\epsilon(\mathbf{k})\) does not have any contribution from J as long as there is no long-range antiferromagnetic order. \(\Sigma\) is the diagonal self-energy due to the many-body interactions in H. In the leading O(1/N) \(\Sigma\) is additive in a purely electronic part \(\Sigma_{el}\) and a phononic part, \(\Sigma_{ph}\), renormalized by electronic correlations. We have analyzed all the contributions to \(\Sigma_{el}\) and found that the RPA-like term

$$\Sigma_{RPA}(k) = -\frac{T}{NN_c} \sum_{k_1} J(k_1) g_{\sigma}(k_1) G^{(0)}(k + k_1),$$

(3)
with the spin vertex \( \gamma_s(k_1) = 1/(1 - J|k_1|\alpha(k_1)/2) \), is the only term which may give rise to interesting structures at low energies. In Eq. (3) we combined the Matsubara frequency \( i\omega_{n_1} \) and the two-dimensional wave vector \( k_1 \) into a three-dimensional vector \( k_1 \). \( N_c \) is the number of cells and \( a(k_1) \) is defined below. The imaginary part of the remaining terms of \( O(1/N) \) exhibits a featureless \( \omega \) law at low energies and acquires structures only on the energy scales \( J \) or \( t \). This contribution is similar to the total \( O(1/N) \) contribution to the imaginary part of \( \Sigma \) in the usual \( 1/N \) expansion depicted in Fig. 5 of Ref. [10].

The phonon contribution \( \Sigma_{ph} \) is given in \( O(1/N) \) by

\[
\Sigma_{ph}(k) = \frac{2T}{NN_c} \sum_{k_1} G^{(0)}(k + k_1) \frac{16\lambda\omega_0^2}{(\omega_n - \omega_{n_1})^2 + \omega_0^2} \gamma_c(k_1 + k, -k_1)\gamma_c(k, k_1),
\]

where \( \omega_0 \) and \( \lambda \) denote the phonon frequency and the dimensionless electron-phonon coupling constant, respectively, and \( G^{(0)} \) is given by Eq. (2) with \( \Sigma = 0 \). The phonon vertex \( \gamma_c \) reads

\[
\gamma_c(k, k_1) = \frac{-1 - b(k_1) + 2a(k_1)t(k)}{1 + b(k_1)(1 + c(k_1)) - a(k_1)d(k_1) + a(k_1)J(|k_1|)/2}.
\]

\( t(k) \) is equal to \(-\epsilon(k)/\delta/2\). The four susceptibilities \( a, b, c, d \) are the generalizations of the normal state susceptibilities given in Eqs. (10)-(13) in Ref. [13] to the superconducting state. Omitting the term proportional to \( J \) in the denominator the expression for \( \gamma_c \) in Eq. (3) is identical with the \( J \rightarrow 0 \) limit of the expression obtained in the \( 1/N \) expansion used in Ref. [13].

Fig. 1 shows the imaginary part of the electronic self-energy in the superconducting state at \( T = 0 \) as a function of the frequency \( \omega \) for two momenta \( Q \) on the Fermi surface, namely, \( Q = (1.33, 1.33) = L \) along the diagonal (left panel) and \( Q = (3.14, 0.26) = X \) (right panel). The energy unit is an effective nearest neighbor hopping constant \( t \) of 150 meV. \( t'/t \) is equal to -0.25 and the value for \( J \), \( J = 1.11 \), is chosen such it reproduces the resonance peak in the spin susceptibility at the experimental value of about 40 meV. The doping \( \delta \) away from half-filling is \( \delta = 0.20 \). The definition of the coupling constant \( \lambda \), Eq. (7) of Ref. [1], is based on the bare coupling and an average density of states of \( 1/8t \). The dashed and solid lines have been calculated neglecting and including vertex corrections, respectively. The dash-dotted lines represent the spin fluctuation contribution, Eq.(2).

![Fig. 1. Imaginary part of the electronic self-energy \( \Sigma(Q, \omega) \) at the points L (left panel) and X (right panel). Solid, dashed, and dot-dashed lines correspond to the phonon contributions with and without vertex corrections, and the spin fluctuation contribution, respectively. Energies are given in units of \( t = 150 \) meV.](image)

The solid and dashed lines in Fig. 1 show a gap near the Fermi energy bounded by two sharp peaks with an energy distance of about \( 2(\Delta + \omega_0) \). The lines fall to zero below \( \omega \sim -2.5 \) and above \( \omega \sim 6 \) reflecting the finite electronic band-width. Comparing the left and right panel one recognizes that \( \Sigma_{ph} \) is rather isotropic in spite of the fact that the vertex corrections depend strongly on momentum and that the superconducting gap is anisotropic. The vertex
corrections $\gamma_c$, which represent one effect of electronic correlations, suppress large momentum transfers in the sum over $k_1$ in Eq. (4) but enhance small momentum transfers. Comparison of the dashed and solid lines shows that altogether the suppression prevails making the solid curves smaller by roughly a factor 2 compared to the dashed ones.

In order to discuss $\Sigma_{RPA}$ let us first consider the momentum integrated susceptibility $\chi''(\omega)$ at large $N$, shown in the left panel of Fig. 2. In accordance with previous work $\chi''(Q, \omega)$ develops a bound state in a very localized region around $Q = (\pi, \pi)$ with nearly no spectral weight left at higher energies at this momentum. Fig. 2 shows that also $\chi''(\omega)$ exhibits a sharp structure in the region around 40 meV. It consists of a stronger component at lower energy which comes from transitions near $(\pi, \pi)$ and corresponds to the resonance peak, i.e., an approximate pole in the denominator of $\gamma_s$. The upper weaker peak is mainly due to momenta near the X point and is caused by spin flip excitations across the superconducting gap. Experimentally, a two peak structure has been seen in inelastic neutron scattering in the momentum integrated spin susceptibility in $YBa_2Cu_3O_6.5$ and $YBa_2Cu_3O_6.7$ (Figs. 5 and 6 of Ref. [14]) but not in $\chi''(Q, \omega)$ for $Q = (\pi, \pi)$ in $YBa_2Cu_3O_6.7$ (Fig. 7 of Ref. [14]). The higher peak is sensitive to temperature, in contrast to the lower peak, and vanishes somewhere above the superconducting transition temperature $T_c$. Guided by the result of our calculation we identify the upper peak in the experimental $\chi''(\omega)$ with the pseudogap with energies of about 60 and 55 meV in $YBa_2Cu_3O_6.5$ and $YBa_2Cu_3O_6.7$, respectively. Accepting this interpretation the pseudogap increases slightly with decreasing doping which is in line with the well-investigated behavior of the pseudogap in the Bi-cuprates. Fig. 2 also illustrates that $\chi''(\omega)$ extends over a large energy region set by the band-width and that most of the spectral weight resides at high energies. Using the exact sum rule one finds that the resonance peak exhausts only about 1.5 per cents of the total spectral weight which agrees well with experiment [15,16].

![Graph](image-url)

**FIG. 2.** Left panel: Momentum-integrated susceptibility $\chi''(\omega + i\eta)$ using the same parameters as in Fig. 1; right panel: renormalization function $Z(Q, \omega)$ for interaction with phonons (“Ph”) at the point $Q = L$ for $T = 0$ (solid line), $T = 180K$ (dashed line), and with spin excitations (“RPA”) at $Q = L$ and $T = 0$ (dot-dashed line) and at $Q = X$ and $T = 0$ (dotted line).

The dash-dotted lines in Fig. 1 represent the imaginary part of $\Sigma_{RPA}$. In contrast to $\Sigma_{ph}$ $\Sigma_{RPA}$ is strongly anisotropic along the Fermi surface. The low-frequency spin fluctuations which are concentrated around momentum transfers of about $(\pi, \pi)$, can probe the superconducting gap if $Q$ is near the X but not the L point. Therefore sharp gap features appear only in the right but not in the left panel. One also notes that the dot-dashed lines are substantially smaller in absolute value at low energies and decay slower towards higher energies compared to the case of phonon scattering. The reason for this behavior can be inferred from $\chi''(\omega)$, as shown in the left panel of Fig. 2. Most of the spectral weight in $\chi''(\omega)$ is found at high energies which leads to the slow decay of the dash-dotted curves towards high energies. The rather small spectral weight associated with low energies and the resonance peak yields, together with $J$ as the coupling constant between electrons and spin fluctuations, only small values in the self-energy near the Fermi energy. The neutron resonance peak leads in the calculation of Ref. [3] to much larger effects in $\Sigma$ and $Z$. There the employed coupling constant and the frequency-integrated resonance peak are taken as 0.65 eV and...
13 per cents of the total sum rule, respectively. The corresponding values are in our case $J = 0.166 \text{eV}$ and 1.5 per cents, respectively. Our rather small spectral weight of the resonance peak agrees well with the experiment [15,16]. The present $1/N$ expansion also identifies in a unique way $J$ as the coupling constant between electrons and spin excitations.

The right panel in Fig. 2 shows the renormalization function $Z(Q, \omega) = 1 - \text{Re}(\Sigma(Q, \omega) - \Sigma(Q, 0))/\omega$, where $\text{Re}$ denotes the real part. The solid line is calculated from the phonon induced self-energy at the point L and at $T = 0$. A very similar curve is obtained for the point X. The solid line deviates substantially from 1 only in a narrow energy range around the Fermi energy set by the phonon energy and the superconducting gap assuming a value of 1.76 at $\omega = 0$. Defining a renormalized coupling function $\lambda(Q)$ by $Z(Q, 0) = 1 + \lambda(Q)$ one finds a rather isotropic $\lambda(Q)$ of 0.76. There are two competing effects due to electronic correlations in renormalizing the original bare coupling constant $\lambda$: Vertex corrections suppress $\Sigma_{ph}$ by roughly a factor 2, but density of state effects increase the effective $\lambda$ again so that $\lambda$ and $\lambda$ do not differ much. Calculating the related quantity $\lambda_{tr}$, which determines the coupling strength in transport phenomena, one has for the bare values $\lambda_{tr} = \lambda$ because the electron-phonon interaction was assumed to be momentum-independent. The renormalized quantity $\lambda_{tr}$ is, however, equal to 0.24, i.e., it is about three times smaller than $\lambda$. In this case the strong suppression of large-momentum scattering by vertex corrections dominates. Such a big difference between $\lambda$ and $\lambda_{tr}$ is needed to have agreement with experiment: The observed slope change in the quasi-particle dispersion by about a factor 2 corresponds to $\lambda \sim 1$, whereas the transport data suggest a three or four times smaller $\lambda_{tr}$ in the optimally doped case.

The dashed curve in the right panel of Fig. 2 describes the phonon-induced $Z$ at the L point at $T=180K$. It illustrates that its value at $\omega = 0$ is sensitive to temperature and thus would decrease the slope change substantially with increasing temperature. The dotted and dash-dotted curves in Fig. 2 represent the spin fluctuation induced renormalization factor. It is very anisotropic and in general much smaller than the phonon-induced contribution to $Z$. As shown in Ref. [10] the transport quantity $\lambda_{tr}$ tends generally to be larger than $\lambda$ in the case of spin fluctuations. The dotted and dash-dotted curves thus yield an effective $\lambda_{tr}$ of about 0.2 which is compatible with transport but indicates, on the other hand, that the spin fluctuation contribution to $Z$ is not the dominant one.

The left panel in Fig. 3 shows the evolution of the spectral function at low temperatures in the superconducting state as a function of frequency for six momenta approaching the Fermi wave vector in the direction L. The interaction with phonons as well as the parameters of Fig. 1 were used in calculating the self-energy. The dashed lines represent the spectral function without the self-energy. Going away from the Fermi surface in momentum space the quasi-particle peak disperses much weaker than the free peak away from the Fermi energy and loses rapidly spectral weight. The weak hump seen near the Fermi surface disperses roughly with the free particle dispersion at somewhat lower energy and becomes broad further away from the Fermi surface. Plotting the same as a function of momentum for a fixed energy one essentially obtains Lorentzians dispersing like free particles. All these properties are well reflected in the experimental data [1–4] showing that the self-energy is rather isotropic along the Fermi surface but strongly frequency-dependent.
FIG. 3. Left panel: Spectral function for phonon scattering for 6 momenta approaching the Fermi vector along the $(\pi, \pi)$-direction, dashed curves are obtained neglecting self-energy effects; right panel: imaginary part of $\Pi(Q, \omega)$ for three temperatures, using parameter values as in Fig. 1.

From this one concludes again that the spin fluctuation contribution to $Z$ cannot dominate in agreement with the right panel in Fig. 2.

The right panel in Fig. 3 shows the imaginary part of the total self-energy $\Pi$ associated with $G$, i.e., $\Pi(i\omega_n, \mathbf{k}) = -G^{-1}(i\omega_n, \mathbf{k}) + i\omega_n - \varepsilon(\mathbf{k})$. The curves in this Figure can directly be compared with the corresponding curves extracted from ARPES data, Fig. 2a of Ref. [17]. In the calculation we used for all temperatures the same $T=0$ gap $\Delta$ which approximately is found in the analysis of the data [17]. There is good agreement on a qualitative level. Quantitatively, there are, however, several discrepancies: in order to reproduce the absolute value of the hump (our energy unit $t$ corresponds to 150 meV) $\lambda$ should be increased by about a factor 2 which would tend to yield too large slope changes in the quasiparticle dispersion at the point $L$. At low temperatures the gap between the hump and zero energy is in our case much more pronounced than in the experiment. One reason for this discrepancy is our use of just one phonon frequency instead of the true, rather broad phonon density of states. It is also possible that the spin fluctuation contribution cannot be totally neglected at the point $X$ and enhance the dump-dip feature.

The situation is less clear in the underdoped region. Experimentally, the momentum-integrated susceptibilities, if integrated between 0 and 65 meV, are typically one order of magnitude or more larger than in the optimally doped case. For instance, $YBa_2Cu_3O_{6.7}$ exhausds in this region about 17 (10) per cent of the sum rule at $T=12K$ (200K) [14] whereas the resonance peak does only 1 per cent [15,16]. Using the experimental susceptibility in Eq. (3) instead of the calculated large $N$ susceptibility we find in the above case for $Q = L Z(\mathbf{Q}, 0) = 1.47(1.27)$ and for $Q = X Z(\mathbf{Q}, 0) = 3.30(2.31)$ at $T=12K$ (200K). Because $\lambda_{tr} \geq \lambda$ in the case of spin fluctuations the resulting values for $\lambda_{tr}$ seem to be too large to be compatible with the resistivity curves [15]. Also the large anisotropy in the slope change of the quasi-particle dispersion, implied by these values, seems not to be supported by the available experiments.

Using a $1/N$ expansion which takes into account the magnetic resonance peak already in leading order we have calculated the contributions of $O(1/N)$ to the electronic self-energy for a t-J-Holstein model. We find that the recently observed low-energy renormalization of quasi-particles in the superconducting state of cuprates can well accounted for taking a phonon energy of 35 meV and a dimensionless coupling constant of about $0.75-1$. In calculating the spin fluctuation part to the self-energy our approach does not contain any adjustable parameter. Due to the rather small value of $J$, which acts as the coupling constant, and due to the structureless $\chi''$ at large $N$ we find that this contribution is rather small and strongly anisotropic along the Fermi surface. This means that it does not play the dominant role in the observed low-frequency renormalization of quasi-particles, at least, in the optimal and overdoped regime.

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