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Effective mass of quasiparticles in a t-J model with electron-phonon interactions

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The change of the spectral properties of the single-particle Green's function due to a coupling to optical phonons is investigated for strongly correlated electrons. The phonon-induced mass renormalization of the carriers that propagate in the t-J model on scale J is much larger than in the corresponding uncorrelated model, except in the limit of $J \to 0$ where the weight of the quasiparticle pole tends to zero. The enhancement is a consequence of the slow coherent motion of the spin polarons, which makes electron-phonon interactions more effective. Two scaling laws are determined which relate the mass renormalization to phonon frequency and coupling constant.

The role of electron-phonon (e-ph) interactions in the strongly correlated high-T_c superconductors (HTSC's) is still far from clear. On one side there is evidence of substantial e-ph interactions in a marked change of phonon frequency renormalization when passing through T_c,[1] that has been successfully described within the framework of strong coupling Migdal-Eliashberg theory.[2] On the other side it has been argued that these interactions are not particularly relevant to explain the high-T_c (Ref. 3) nor the isotope shifts.[4] The problem is complicated by the coherent motion of dressed carriers on a reduced energy scale J *and* with a reduced spectral weight, $a_k < 1$, which emerges from the strong correlations. As a consequence the Fermi energy is small, i.e., almost on the order of the phonon cutoff, which signals a possible breakdown of the standard strong coupling theory. In fact it has been suggested that the inclusion of Migdal-type vertex corrections may be sufficient to explain the large T_c.[5]

Our aim here is to study the changes of the quasiparticle properties of a single hole, i.e., relevant for the low doping regime, when a coupling to optical phonons is included in a generic model for the HTSC's, the t-J model. A central result is the observation that the relative mass renormalization due to phonons may be enhanced by an order of magnitude by the strong correlations, — a consequence of the reduction of the energy scale of coherent motion of quasiparticles.

The basic Hamiltonian to be studied

$$H = -t \sum_{<ij>s} \tilde{c}_{is}^{\dagger}\tilde{c}_{js} + J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{i\delta s} M_\delta \tilde{c}_{is}^{\dagger}\tilde{c}_{is}(b_{i+\delta}^{\dagger} + b_{i+\delta}) + \Omega \sum_i b_i^{\dagger} b_i, \quad (1)$$

consists of the usual t-J Hamiltonian, the first two terms, and coupling of charge carriers to Einstein phonons with energy Ω. The fermion operators $\tilde{c}_{is}^{\dagger} = c_{is}^{\dagger}(1 - n_{i\bar{s}})$ act in the space without double occupancy, M_δ is the e-ph coupling matrix element. The t-J part of the Hamiltonian may be rewritten in terms of slave fermions and Schwinger bosons, characterizing charge and spin degrees of freedom, respectively. It is advantageous to introduce at the outset the proper collective excitations describing the spin dynamics by applying linear spin-wave theory. After Fourier transformation and dropping an irrelevant constant we obtain[6–8]

$$\tilde{H} = \frac{1}{\sqrt{N}} \sum_{\mathbf{kq}} \left[h_{\mathbf{k-q}}^{\dagger} h_{\mathbf{k}} (\tilde{M}_{\mathbf{kq}} \alpha_{\mathbf{q}}^{\dagger} + M_{\mathbf{q}} \beta_{\mathbf{q}}^{\dagger}) + \text{H.c.} \right] + \sum_{\mathbf{q}} (\omega_{\mathbf{q}}\, \alpha_{\mathbf{q}}^{\dagger} \alpha_{\mathbf{q}} + \Omega\, \beta_{\mathbf{q}}^{\dagger} \beta_{\mathbf{q}}). \quad (2)$$

Here $h_{\mathbf{k}}^{\dagger}$, $\alpha_{\mathbf{q}}^{\dagger}$, and $\beta_{\mathbf{q}}^{\dagger}$ are creation operators for spinless fermions, antiferromagnetic magnons, and phonons, respectively. The fermion-magnon coupling is given by

$$\tilde{M}_{\mathbf{kq}} = 2\sqrt{2}\, t \left[\gamma_{\mathbf{k-q}} (\nu_{\mathbf{q}}^{-1} + 1)^{1/2} - \gamma_{\mathbf{k}} \operatorname{sgn} \gamma_{\mathbf{q}} (\nu_{\mathbf{q}}^{-1} - 1)^{1/2} \right],$$

where $\gamma_{\mathbf{q}} = (\cos q_x + \cos q_y)/2$, and $\nu_{\mathbf{q}} = (1 - \gamma_{\mathbf{q}}^2)^{1/2}$. The magnon dispersion equals $\omega_{\mathbf{q}} = 2J\nu_{\mathbf{q}}$, N is the number of lattice sites and the lattice constant is $a \equiv 1$. The fermion-phonon coupling $M_{\mathbf{q}}$ depends on the initial choice of the corresponding M_δ, and we consider local and longer-range couplings.

The corresponding Hubbard-Holstein model has been investigated recently by quantum Monte Carlo methods[9] with particular emphasis on superconducting properties. Yet until now only the nonretarded $\Omega \gg t$ case could be studied by these methods. Polaron[10] and bipolaron[11] formation was also studied in this model.

In the limit $t \to 0$ the bandwidth in the t-J model scales as t^2/J, hence the hole becomes localized and the exact solution of (2) can be obtained using the Lang and Firsov transformation.[12] The ground-state energy of the system is lowered by the (phonon-) polaron binding energy $\epsilon_b = |N^{-1} \sum_{\mathbf{q}} M_{\mathbf{q}}^2/\Omega|$. The exact single-particle Green's function consists of a sequence of poles spaced by Ω and with weights given by the Poisson distribution. The strength of the lowest pole equals $a_0 = \exp(-\epsilon_b/\Omega)$ and one expects a strongly reduced effective hopping $t \exp(-\epsilon_b/\Omega)$.[13]

In the following we will be interested in the opposite regime $J < t$ relevant for the copper oxides, which implies strong fermion-magnon coupling. The e-ph coupling will be considered weak. To clarify the further results we first briefly resume some large phonon-polaron properties for the case of usual fermions, i.e., dropping the single occupancy constraint in Eq. (1) and $J = 0$, where the hole can freely hop and the corresponding energy band is $\epsilon^0_{\mathbf{k}} = -2t\gamma_{\mathbf{k}}$. In the case of large bandwidth, $8t \gg \epsilon_b$, the hole has sufficiently large kinetic energy to escape the lattice distortion potential and the effect of phonons is mainly a renormalizaton of the effective mass $m = (\partial^2\epsilon_{\mathbf{k}}/\partial\mathbf{k}^2)^{-1}$, where $\epsilon_{\mathbf{k}}$ is a corresponding quasiparticle (QP) dispersion. For a single hole the second derivative has to be evaluated in the band minimum at $\mathbf{k} = (0,0)$, i.e., for nearest-neighbor hopping. The ratio between the effective and the bare mass $m_0 = (2t)^{-1}$ is a suitable measure for the e-ph coupling strength and is denoted with $m/m_0 \equiv 1 + \lambda$. This definition should be distinguished however from the λ in the theory of superconductivity which measures the renormalization of the mass at k_F and of the density of states.

For weak coupling the effective mass of an "unrestricted" fermion can be calculated using the lowest-order perturbation correction to the fermion self-energy,

$$\epsilon_{\mathbf{k}} - \epsilon^0_{\mathbf{k}} = \frac{1}{4\pi^2}\int d^2q \frac{M^2_{\mathbf{q}}}{\epsilon^0_{\mathbf{k}} - \epsilon^0_{\mathbf{k}-\mathbf{q}} - \Omega}. \tag{3}$$

From the second derivative around $k = 0$ we obtain an approximate result for m

$$\frac{1}{m} - \frac{1}{m_0} \simeq -\int_0^\infty dq \frac{4m_0\, M_q^2 q^3}{\pi(q^2+p^2)^3} = \frac{\lambda_0}{m_0}[1 + O(p^2)]. \tag{4}$$

Here $p^2 = 2m_0\Omega \ll 1$ was asumed (i.e., Ω small compared to bandwidth) and $\lambda_0 \equiv M_p^2 m_0/(2\pi\Omega)$. The integrand in Eq. (4) is a sharply peaked function around $q \sim p$, thus the coupling matrix element is evaluated at $q \sim p$ and ∞ was taken for the upper integration limit. From the expression $1 + \lambda = 1/(1 - \lambda_0)$ it is obvious that as long as the binding energy ϵ_b is small in comparison with the kinetic energy of a hole, the effective mass enhancement is small, $\lambda \sim \lambda_0 \ll 1$, and the problem falls into the category of large phonon polarons.

The strong correlations in the t-J model ($J > 0$) change the physics significantly. A quasiparticle peak with dispersion on scale J emerges together with a broad incoherent background which has considerable spectral weight. To study the influence of e-ph coupling onto the QP properties we treat $\tilde{H}$ within the self-consistent Born approximation (SCBA) for magnon and phonon interactions on the same footing

$$\Sigma_{\mathbf{k}}(\omega) = \frac{1}{N}\sum_{\mathbf{q}}\left[\tilde{M}^2_{\mathbf{kq}}G_{\mathbf{k}-\mathbf{q}}(\omega-\omega_{\mathbf{q}}) + M^2_{\mathbf{q}}G_{\mathbf{k}-\mathbf{q}}(\omega-\Omega)\right], \tag{5}$$

$$G_{\mathbf{k}}(\omega) = [\omega - \Sigma_{\mathbf{k}}(\omega)]^{-1}.$$

Such an approximation amounts to the summation of noncrossing diagrams to all orders. In the case of the pure t-J model the validity of this approach is well established. Agreement with exact calculation results for small clusters,[14] is not only qualitative but also quantitative for all relevant ranges of J/t.[7] The success of this approximation has roots in the vanishing of low-order magnon interaction vertex corrections as pointed out by several authors for systems where the hole is coupled to an antiferromagnetic spin background.[8,7,15] Similar arguments show that the lowest-order mixed exchange diagram formed by one magnon and one phonon line also vanishes because of the symmetry of the hole-magnon coupling. Yet the lowest order Migdal-type vertex formed by two phonons does not vanish. Thus we expect the SCBA to be limited to weak e-ph coupling but arbitrary J/t. In fact our study of the localized limit ($t = 0$) has shown a good agreement between the SCBA and the exact results for coupling strength $\epsilon_b/\Omega \lesssim 2$. In this coupling range the discrepancy in the calculation of the binding energy is almost completely repaired by the inclusion of the lowest-order vertex corrections. However, in our further study of the QP properties at finite t the relevant parameter is $\epsilon_b/t < 1$ rather than $\epsilon_b/\Omega < 1$.

We first choose a local Holstein e-ph interaction, thus $M_{\mathbf{q}} \equiv M$. The numerical method used for the full self-consistent solution of Eqs. (5) is essentially similar to Refs. 7 and 8. Our main interest was devoted to the effective QP mass. The corresponding coherent energy band, $\tilde{\epsilon}_{\mathbf{k}}$, was extracted from the numerical result as $\tilde{\epsilon}_{\mathbf{k}} = \Sigma_{\mathbf{k}}(\tilde{\epsilon}_{\mathbf{k}})$. A high $\mathbf{k}$-space resolution corresponding to a unit cell with 64×64 lattice sites was required to obtain convergent results. To calculate $\Sigma_{\mathbf{k}}(\omega)$ we used $\omega + i\eta$ in Eqs. (5) with a broadening parameter $\eta/t = 0.01$.

In order to exhibit the general influence of phonons we present in Fig. 1 for $J/t = 0.4$ the low energy part of the spectral function $A_{\mathbf{k}}(\omega) = -\frac{1}{\pi}\text{Im}G_{\mathbf{k}}(\omega)$ for wave vectors $\mathbf{k}$ along the principal directions $(\pi,0)\rightarrow(\frac{\pi}{2},\frac{\pi}{2})\rightarrow(0,0)$ in the Brillouin zone (BZ) for different values of phonon coupling. For comparison we show the pure t-J result,[7,8] Fig. 1(a). The average strength of the QP

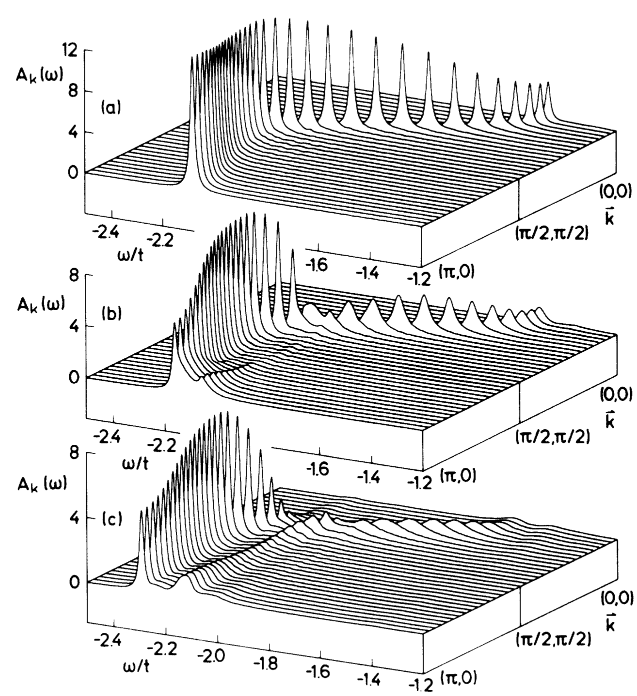

FIG. 1. Spectral function $A_{\mathbf{k}}(\omega)$ for $\mathbf{k}$ along $(\pi,0) \rightarrow (\frac{\pi}{2},\frac{\pi}{2}) \rightarrow (0,0)$ in the Brillouin zone for $J/t = 0.4$, $\Omega/t = 0.1$ and different e-ph coupling strengths (a) $M = 0$, (b) $M/t = 0.2$, and (c) $M/t = 0.4$.

peak is $\langle a_{\mathbf{k}}\rangle_{\rm BZ} \sim 0.3$. The peak is well separated from the incoherent part of the spectrum, which appears at higher energies. The effective QP band has its minimum at $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$, the effective mass tensor is highly anisotropic with a smaller eigenvalue $m_{\parallel}$ in the direction $(\frac{\pi}{2}, \frac{\pi}{2}) \to (0,0)$ and a larger $m_{\perp}$ in the perpendicular direction $(\frac{\pi}{2}, \frac{\pi}{2}) \to (\pi, 0)$. The spectral weight is largest along the line $(\pi, 0) \to (\frac{\pi}{2}, \frac{\pi}{2})$, and it is decreasing in the direction $(\frac{\pi}{2}, \frac{\pi}{2}) \to (0,0)$.

Already a weak e-ph interaction introduces some qualitative changes, Fig. 1(b). The QP peak remains undamped at the bottom of the band but its strength is reduced, especially near $(\pi, 0)$ while at energies of the order of Ω above the pole a new structure in the density of states appears. It corresponds to the multiphonon excitations found in the localized fermion limit. At higher phonon coupling strength, Fig. 1(c), these new features become more pronounced. Away from the bottom of the band the QP pole is strongly suppressed and broadened due to phonon-induced decay processes. The overall bandwidth is not significantly changed. But the effective mass of a single hole measured at the bottom of the band is strongly enhanced. Results presented in Fig. 1 resemble qualitatively the general situation for the whole investigated range of the parameters. We have also performed calculation with different forms of $M_{\mathbf{q}}$ (e.g., deformation potential-like[16]), but the results do not differ significantly provided the same ratio $\epsilon_b/t \lesssim 1$ is used. In the following we thus present only results for Holstein interaction.

Within the pure t-J model the mass $m_{\parallel}$ is much larger than the bare mass m_0. We focus now on the additional enhancement of the QP mass as function of the e-ph coupling strength. In particular we investigate the QP mass m^* along $(\frac{\pi}{2}, \frac{\pi}{2}) \to (0,0)$. The corresponding mass enhancement parameter λ^* is defined as before, $m^*/m_{\parallel} = 1 + \lambda^*$. As important energy scales we expect the polaron binding energy ϵ_b and the QP bandwidth. We thus calculate λ^* for different values of the relevant parameter ϵ_b/t, and vary the e-ph coupling M/t and phonon frequency Ω/t independently. The ratio λ^*/λ_0 is shown in Fig. 2(a) for different coupling strengths. The normalized results are essentially independent of M and are well described by $\lambda^* \propto J/t$. According to Eq. (4) a scaling $\lambda^* \propto M^2/(\Omega t)$ is expected in the perturbative limit for $m^*\Omega \ll 1$. In Fig. 2(b) we present the Ω/t dependence of the scaled quantity $JM^2/(\lambda^* t^3)$, which establishes the scaling rule $\lambda^{*-1} \propto \Omega/t$. We find that the scaling $\lambda^* \simeq c_\Omega\, \epsilon_b J/t^2$, $c_\Omega = 0.75/(1 + 1.5\,\Omega/t)$ provides a valid description of our data also outside the perturbative regime.

Comparing the above results for λ^* with λ_0 obtained for the free fermion case we see that when strong correlations come into play λ^* becomes up to an order of magnitude larger than the bare λ_0 in a large J/t range, except when $J/t \to 0$. This result, at first glance surprising, may be understood qualitatively within lowest-order perturbation theory with respect to phonon exchange, using a simple dominant pole approximation for the fermion Green's function

$$G_{\mathbf{k}}(\omega) = \frac{a_{\mathbf{k}}}{\omega - \tilde{\epsilon}_{\mathbf{k}}} + G_{\mathbf{k}}^{\rm inc}(\omega), \tag{6}$$

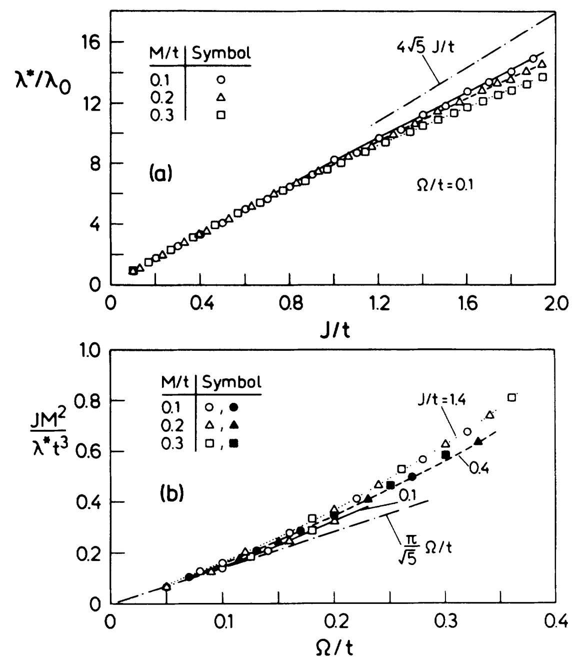

FIG. 2. (a) Phonon-induced mass renormalization λ^*/λ_0 vs J/t for three different M/t values and $\Omega/t = 0.1$. Here λ_0 is the renormalization for noninteracting fermions. (b) Ω/t dependence of $JM^2/(\lambda^* t^3)$ for different sets of parameters M/t and J/t. The dash-dotted lines indicate the perturbational results (large J/t) .

where the pole strength $a_{\mathbf{k}}$ and the QP band energy $\tilde{\epsilon}_{\mathbf{k}}$ are taken from a pure t-J model calculation.

For weak e-ph coupling one can generalize the perturbative expression, Eq. (4), to the case of a QP band appropriate for the t-J model with anisotropic mass tensor. Performing a similar calculation as in the perturbative case, Eq. (3), we obtain an expression for the effective mass which differs slightly from that for the case without coupling to spins, Eq. (4),

$$\frac{m^*}{m_{\parallel}} = 1 + \lambda^* = \left(1 - \frac{2}{\pi}\frac{M^2}{\Omega}\bar{a}\sqrt{m_{\parallel}m_{\perp}}\right)^{-1}. \tag{7}$$

Here one difference is in the numerical factor due to the four hole pockets forming the band minima at $\mathbf{k} = (\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ instead of a single one at $(0,0)$. Another difference is the appearance of an average pole strength $\bar{a} < 1$ in contrast to the uncorrelated fermion case where $\bar{a} \equiv 1$. In fact $\bar{a}$ is approximately given by $a_{|\mathbf{k}-\mathbf{p}|}$ with $|\mathbf{p}|$ of the order of $(m_{\parallel}m_{\perp})^{1/4}(2\Omega)^{1/2}$ and $\mathbf{k}$ is at the QP band minimum. Due to the anisotropy of the mass tensor the bare fermion mass m_0 is replaced by $(m_{\parallel}m_{\perp})^{1/2}$. The incoherent part of Green's function $G_{\mathbf{k}}^{\rm inc}(\omega)$ at high energies yields a small correction to Eq. (7) of $O[(\Omega/8t)^2]$ and is neglected.

The numerical results for λ^* can now be easily explained for large J/t values. The effective bandwidth in this limit is strongly reduced due to correlations. Nevertheless the hole motion can still be considered as coherent, and $a_{\mathbf{k}} \sim 1$ within Born approximation (the strict result for the limit $J \to \infty$ is $a_{\mathbf{k}} \to 0.82$ according to

Ref. 17). We meet a situation similar to the free fermion case. The only difference is a strongly reduced kinetic energy of the hole which is no longer necessarily large in comparison with the polaron binding energy. Thus the influence of phonons is enhanced. In this regime the transition from the large to small polaron physics is expected at correspondingly smaller e-ph coupling strength.[10] The QP bandwith within t-J model can be approximated by $m_{\parallel}^{-1} \sim 2t^2/J$ and $\bar{a} \sim 1$, so $\lambda^*/\lambda_0 = 4\,J/t\,(m_\perp/m_\parallel)^{1/2}$. This perturbative result is shown in Figs. 2(a) and 2(b) for $m_\perp/m_\parallel \sim 5$ as obtained from the t-J model calculation for $J/t \gtrsim 2$. This estimate for λ^* is strictly valid only for larger values of J/t. The reason why it reproduces the actual numerical solution so well for the whole range of J/t is nontrivial.

To explain the results for $J < t$ one has to consider the details of the QP properties. According to Eq. (7) it is clear that λ^* is determined by a subtle interplay of the masses ($\sim J^{-1}$), more precisely $m_{\parallel}^{-1} \sim 1.5\,t\,(J/t)^{0.79}$, and the reduced spectral weights ($\sim J^{\alpha}$).[7] As the J dependence of $a_{\mathbf{k}}$ is strongly $\mathbf{k}$ dependent, a precise determination of $\bar{a}$ is not easy. We find that the product of the QP pole strength and the effective mass in Eq. (7) tends either to zero or to a small constant value for $\mathbf{k} = (0,0)$ and $\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$, respectively, and $\bar{a}$ is between these two limiting cases. The phonon-induced renormalization is small in the limit $J \ll t$ because the spectral weight of the QP is small.

To give an estimate pertinent to the copper oxides we choose a polaron binding energy $\epsilon_b \sim 0.84$ eV (Ref. 18) as determined by Zhong and Schüttler[10] for Tl(2:2:1:2) with $t \sim 0.35$ eV and $\Omega \sim 50$ meV. This yields $\lambda_0 = \epsilon_b/4\pi t \sim 0.2$. Hence for $J/t = 0.4$ we expect a substantial mass enhancement $\lambda^* \sim 0.6$ and pronounced satellite structure in $G_{\mathbf{k}}(\omega)$.

We summarize by stressing that the mass renormalization due to e-ph coupling may be understood by visualizing the rapid hole motion (on scale t) hindered by a linear confining string potential due to the antiferromagnetic spin-background. As long as J/t is large, the hole excursions from the center of the spin polaron are restricted to a few lattice sites and the bandwidth is on scale t^2/J. The slow coherent motion of the polaron enhances the effect of the lattice distortion, resulting in a substantial QP mass enhancement. On the other hand, for $J \to 0$ the string potential becomes weak and the hole performs large excursions on scale t. The spectral weight in the coherent (QP) part of the spectrum tends to zero. The influence of phonons on such a QP becomes even smaller than λ_0 for J/t values below $J/t \sim 0.1$. Two scaling relations are shown to describe the mass renormalization over a wide range of the parameters J, M_q, and Ω. Further studies for finite-doping concentration are required to judge possible consequences for quasiparticle interactions and for the Migdal-Eliashberg theory of superconductivity.

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