Influence of strong electron correlations on the electron-phonon coupling in high-T_c oxides

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Considering Hubbard models with infinite U, the leading terms of the electronic self-energy due to an on-site electron-phonon interaction are calculated within a $1/N$ expansion. In particular, the modifications of the Eliashberg function $\alpha^2 F(\omega)$ due to strong correlations are described and calculated for a simple square lattice as a function of doping. We find that the on-site electron-phonon coupling is in general slightly enhanced in forward scattering but dramatically suppressed for scattering with large momentum transfers by correlations. This implies at least in the single-band case that the electron-phonon coupling is greatly reduced in transport quantities and to a much smaller degree in $\alpha^2 F$ because of electronic correlations.

High-T_c oxides are characterized by strong electronic correlations and by, at least, a non-negligible electron-phonon interaction. In the past many investigations on the electron-phonon interaction in high-T_c oxides used the one-particle approximation for the holes and thus neglected strong correlation effects.[1–4] Considering electronic correlations Refs. 5 and 6 argue that the intersite "covalent" electron-phonon coupling is heavily suppressed by strong electronic correlations, especially, near the metal-insulator transition. In the following we study the influence of strong electronic correlations on the on-site "ionic" electron-phonon coupling in a systematic way keeping all terms of the leading order of a $1/N$ expansion. We will concentrate on the on-site electron-phonon interaction because it seems that this coupling is important in high-T_c oxides.[3] At the same time it allows a simpler treatment than a general electron-phonon interaction.

The Hamiltonian reads

$$
\begin{aligned}
H = & \sum_{\substack{i \\ p=0,\ldots,N}} E_{ip} X_i^{pp} + \sum_{\substack{ij \\ p=1,\ldots,N}} \frac{t_{ij}}{N} X_i^{p0} X_j^{0p} \\
& + \sum_{k\lambda} \omega(k\lambda)[a^\dagger(k\lambda)a(k\lambda)+\tfrac{1}{2}] \\
& + \sum_{\substack{ik\lambda \\ p=1,\ldots,N}} g_i(-k\lambda)[a^\dagger(k\lambda)+a(-k\lambda)] \\
& \times (X_i^{pp}-\langle X_i^{pp}\rangle) .
\end{aligned}
\tag{1}
$$

X_i^{pq} is a Hubbard X operator for the atomic site i where $p,q=0$ refer to the empty and $p,q=1,\ldots,N$ to a singly occupied state with spin directions p,q. The operators X obey the usual commutation and anticommutation rules

and we are interested in representations which fulfill the generalized constraint[7] $Q_i = \sum_{p=0}^{N} X_i^{pp} = N/2$. The corresponding Hilbert space is spanned by the eigenfunctions of X_i^{pp}. We specify it by the slave boson conditions $(X_i^{pp})^2 = X_i^{pp}$ for $p=1,\ldots,N$ plus the constraint. Though the constraint is treated quite differently than in slave boson calculations[8,9] it seems probable that our $1/N$ expansion is equivalent to the corresponding $1/N$ expansion of slave boson theory as long as only gauge invariant quantities are considered in the latter. The first two terms in Eq. (1) describe the electronic part of H; E_{ip} and t_{ij} are atomic energies and hopping amplitudes between neighbors. The third term in Eq. (1) is the free phonon part where $a^\dagger(k\lambda)$ creates a phonon with momentum k, branch index λ, and frequency $\omega(k\lambda)$. The fourth term in Eq. (1) represents the electron-phonon coupling with the coupling function g. It describes the simplest form of coupling where the phonons change just the local chemical potential at the lattice sites.[3] $\langle X_i^{pp} \rangle$ is the thermal average of X_i^{pp} and has to be introduced in the interaction to have $\langle a^\dagger(k\lambda)\rangle = 0$.

Following Ref. 10 we define nonequilibrium Green's functions with the fermionic Hubbard operators by

$$
G\begin{bmatrix} 0q_1 & p_20 \\ 1 & 2 \end{bmatrix} = -\langle TSX^{0q_1}(1)X^{p_20}(2)\rangle / \langle S\rangle ,
\tag{2}
$$

$$
S = T\exp\left[-\sum_{p_2q_2}\int d2 X^{p_2q_2}(2)K^{p_2q_2}(2) \right] .
\tag{3}
$$

1 stands for the site i_1 and the imaginary time τ_1, $1 \equiv (i_1,\tau_1)$. $\int d1$ means $\sum_{i_1}\int_0^\beta d\tau_1$. T is the time ordering operator, K an external source which couples to bosonic X operators corresponding to $p_2=q_2=0$ or $p_2>0,q_2>0$. G satisfies the Dyson equation

$$
\begin{aligned}
& \sum_{q_1q_2}\int d2 \left[\delta(2-1)\delta_{q_2q_1}\left(-\frac{\partial}{\partial \tau_2}+(E_{i_10}-E_{i_1q_1})-K^{00}(1)\delta_{q_1q_2}+K^{q_1q_2}(1) \right) \right. \\
& \left. -\Sigma\begin{bmatrix} 0q_1 & 0q_2 \\ , & \\ 1 & 2 \end{bmatrix} \right] G\begin{bmatrix} 0q_2 & p_1'0 \\ , & \\ 2 & 1' \end{bmatrix} = \delta(1-1')Q_{0q_1,p_1'0}(1) ,
\end{aligned}
\tag{4}
$$

which defines the self-energy Σ. Q is defined by

$$Q_{0q_1,p'_10}(1) = \langle [X^{0q_1}(1), X^{p'_10}(1)]_+ \rangle .\qquad (5)$$

It is convenient to introduce also the normalized Green's function

$$\widetilde{G}\begin{bmatrix} 0q_1 & 0q'_1 \\ & , \\ 1 & 1' \end{bmatrix} = \sum_{p'} G\begin{bmatrix} 0q_1 & p'0 \\ & , \\ 1 & 1' \end{bmatrix} Q^{-1}_{p'0,0q'_1}(1') .\qquad (6)$$

$\widetilde{G}$ satisfies Eq. (4) where the right-hand side has been replaced by $\delta(1-1')$. In the approach of Ref. 10 the source K is only used to obtain a formally closed equation for Σ. After that, K is put to zero and, in the absence of spontaneously broken symmetries, the original SU(N) symmetry of H is restored. As a result all quantities considered in the following such as G, Σ,..., become diagonal and independent of the indices p, q so we will drop them.

The leading terms $\sim O(1)$ of Σ read

$$\Sigma(11') = -\delta(1-1')N \int d2\, t(1-2)\widetilde{G}(2^+1)$$

$$+ t(1-1')\langle X^{00}(1)\rangle + \Sigma_{ep}(11') ,\qquad (7)$$

$$\Sigma_{ep}(11') = \int d2d3d4d5\, V(2-3)\widetilde{\Gamma}(14;2)\widetilde{G}(45)\widetilde{\Gamma}(51';3)$$
$$(8)$$

with $t(1-2) = t_{i_1 i_2}\delta(\tau_1-\tau_2)/N$. The first two terms in Eq. (7) are independent of phonons and represent a renormalization for the atomic levels and a renormalized hopping between different atoms.[7] These terms can be shown to be equivalent to the corresponding $O(1)$ terms of slave boson theory though there is no Bose condensation in the present approach. The last term in Eq. (7) is due to phonons and given explicitly by Eq. (8). V is the phonon-mediated interaction

$$V(1-2) = \sum_{k\lambda} g_{i_1}(-k\lambda)D^{ph}(k\lambda, \tau_1-\tau_2)g_{i_2}(k\lambda) ,\qquad (9)$$

where D^{ph} denotes the phonon Green's function. $\widetilde{\Gamma}$ is the electron vertex function defined by

$$\widetilde{\Gamma}(31';2) = \sum_{p=1}^{N} \frac{\delta\widetilde{G}^{-1}(31')}{\delta K^{pp}(2)} .\qquad (10)$$

Equations (4)–(10) can be most easily derived by the functional method of Ref. 10. The phonon variables have been eliminated, all spin summations carried out, and only terms of $O(1)$ have been kept. Assuming the electron-phonon interaction to be small, minor band renormalizations due to the electron-phonon interaction also have been omitted in Eq. (7).

The functional derivative in the definition of $\widetilde{\Gamma}$ is carried out by means of the modified Dyson equation (4) for $\widetilde{G}$ where the right-hand side contains the usual $\delta(1-1')$. Since Σ depends on K only via $\widetilde{G}$ and $\langle X^{pp}\rangle$ one obtains a formally closed equation for $\widetilde{\Gamma}$ with a kernel containing $\delta\Sigma/\delta\widetilde{G}$ and $\delta\Sigma/\delta\langle X^{pp}\rangle$. Keeping terms only of $O(1)$ it is sufficient to consider the first two terms in Eq. (7) in

calculating these functional derivatives. In this way one arrives at the following integral equation for $\widetilde{\Gamma}$:

$$\widetilde{\Gamma}(11';2) = \delta(1-1')\delta(1-2)$$

$$+ N\int d3d4d5[\delta(1-1')t(1-3)$$

$$+ t(1-1')\delta(1-3)]$$

$$\times \widetilde{G}(34)\widetilde{\Gamma}(45;2)\widetilde{G}(51^+) .\qquad (11)$$

The kernel in Eq. (11) consists of separable contributions which allows an analytic solution. If the Fermi energy is much larger than the phonon frequencies as will be assumed in the following, the frequency dependence of $\widetilde{\Gamma}$ can be neglected and Eq. (11) involves only spatial variables.

In the following we will consider a square lattice and only nearest-neighbor hopping. Writing $\widetilde{\Gamma}(11';3) = \gamma(1-1',1-3)\delta(\tau_1-\tau'_1)\delta(\tau_1-\tau_3)$ and performing Fourier transforms the following solution for γ is found:

$$\gamma(k,q) = \frac{1+b(q)-a(q)t(k)}{[1+b(q)]^2-a(q)c(q)} ,\qquad (12)$$

where

$$a(q) = \int \frac{d^2k}{(2\pi)^2} \frac{f[\xi(k)]-f[\xi(k+q)]}{\xi(k+q)-\xi(k)} ,\qquad (13)$$

$$b(q) = \int \frac{d^2k}{(2\pi)^2} t(k)\frac{f[\xi(k)]-f[\xi(k+q)]}{\xi(k+q)-\xi(k)} ,\qquad (14)$$

$$c(q) = \int \frac{d^2k}{(2\pi)^2} t(k)t(k+q)\frac{f[\xi(k)]-f[\xi(k+q)]}{\xi(k+q)-\xi(k)} .\qquad (15)$$

The k integrations in Eqs. (13)–(15) are to be extended over the first Brillouin zone. $\xi(k)$ is equal to $\epsilon(k)-\mu$ where $\epsilon(k)$ are the renormalized one-particle energies due to Σ of Eq. (7). For a small electron-phonon coupling, the phonon renormalization due to Σ_{ep} for $\epsilon(k)$ can be neglected so that $\epsilon(k)$ is independent of frequency. Furthermore, the first term in Eq. (7) can be absorbed into the chemical potential. As a result $\epsilon(k) = -2tq_0[\cos(k_x a)+\cos(k_y a)]$ where t is the nearest-neighbor hopping amplitude, a the square lattice constant, and $q_0 = \delta/2$ where δ is the doping defined at $T=0$ by $1-\delta = 2\int_{-\infty}^{\mu} N^*_\uparrow(\epsilon)d\epsilon$ and $N^*_\uparrow(\epsilon)$ is the density of renormalized one-particle states.

From Σ_{ep} the following expression for the Eliashberg function $\alpha^2F(\omega)$ is obtained if the density of renormalized states varies slowly over typical phonon energies[11]

$$\alpha^2F(\omega) = N^*_\uparrow(0)\sum_{\lambda} \ll |g(p,p-p'\lambda)|^2\delta(\omega-\omega(p-p',\lambda))$$

$$\times \gamma^2(p,p-p')\gg_{p}\gg_{p'} .\qquad (16)$$

$g(p,q\lambda)$ is related to $g_i(q\lambda)$ by a Fourier transform with respect to the site label i. $\langle\ \rangle_p$ denotes a Fermi surface average with respect to the momentum p. In the one-particle approximation (i.e., if $U=0$) $\alpha^2F(\omega)$ is also given by Eq. (16) except for two important changes: $N^*_\uparrow(0)$ is

replaced by the density of noninteracting particle states $N_\uparrow(0)$ whereas $N_\uparrow^*(0)$ in Eq. (16) denotes the density of renormalized states. Both densities are connected by $N_\uparrow^*(0)=N_\uparrow(0)/q_0$. The second change concerns γ: in the free particle approximation $\gamma=1$ whereas in our case with $U=\infty$, γ is the momentum-dependent function Eq. (12). This means that in the simplest possible approximation which takes electronic correlations into account, both self-energy and vertex corrections appear: The self-energy effect is frequency independent and can be interpreted as a changed prefactor describing a density of quasiparticle instead of free states. At the same time a momentum-dependent vertex has to be taken into account which, as we will see below, competes with the self-energy correction. In most previous calculations[12,13] using X operators only the self-energy effect has been considered.

Performing a similar calculation as above for the phonon-limited resistivity one finds that the resistivity is related to the function $\alpha_{tr}^2 F(\omega)$ as usual[11] and that $\alpha_{tr}^2 F(\omega)$ is given by Eq. (16) if the additional factor $[\mathbf{v}(\mathbf{p})-\mathbf{v}(\mathbf{p}')]^2/[2\langle\mathbf{v}(\mathbf{p})^2\rangle_p]$ is inserted before the Fermi surface averages are carried out. Correlations thus could change the ratio $\alpha_{tr}^2 F/\alpha^2 F$ if γ depends strongly on $\mathbf{p}-\mathbf{p}'$. Usually differences between $\alpha^2 F$ and $\alpha_{tr}^2 F$ have been attributed to the anisotropy of the electronic or phononic spectra or their couplings.[14]

The vertex function $\gamma(\mathbf{k},\mathbf{q})$ depends on $\mathbf{k}$ only via $t(\mathbf{k})$, i.e., only via the Fermi energy. The first argument is therefore constant for a given doping, denoted symbolically by k_F in the following. γ as a function of $\mathbf{q}$ is only restricted by the point group of the square lattice i.e., it depends in general on the direction of $\mathbf{q}$. Figure 1 shows γ as a function of $\mathbf{q}=(q,q)$ with q varying between 0 and the maximal momentum transfer occurring in $\alpha^2 F$. The three curves correspond to the dopings $\delta=0.04$ (dotted curve), $\delta=0.127$ (solid curve), and $\delta=0.539$ (dashed curve). The curves in Fig. 2 represent $\gamma(k_F,q)^2/q_0$ for the same dopings and the same direction of $\mathbf{q}$. Figure 2(a) gives a complete picture, Fig. 2(b) an enlargement of Fig. 2(a) for small values of the functions. They describe the total, momentum-dependent enhancement of $\alpha^2 F$ due to correlations relative to the uncorrelated case. Taking the limit $\mathbf{q}\to 0$ in Eqs. (12)–(15) one finds the following expression for the vertex

$$\gamma(k_F,0)=\frac{1}{1-2\bar{\mu}N_\uparrow^*(\mu)} \tag{17}$$

with the density of states

$$N_\uparrow^*(\epsilon)=\frac{1}{2\pi q_0}\Theta(2-|\bar{\epsilon}|)P_{-1/2}\left[\frac{\bar{\epsilon}^2}{2}-1\right]. \tag{18}$$

Θ and P are the theta and Legendre functions, respectively, and $\bar{\mu}$ and $\bar{\epsilon}$ are defined by $\bar{\mu}=\mu/q_0$, $\bar{\epsilon}=\epsilon/q_0$, respectively.

The dashed lines in Figs. 1 and 2 describing the case of a rather large doping depend only weakly on the momentum. If the doping is further increased the curves shrink more and more and become flatter until they collapse to one point in the limit $\delta\to 1$. In this limit $q_0\to\frac{1}{2}$, $\bar{\mu}\to -2$,
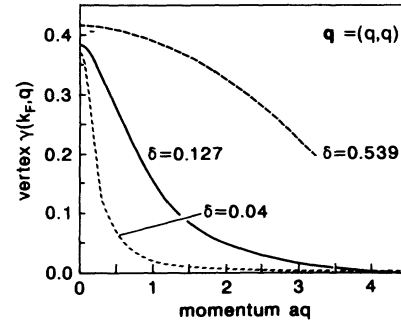

FIG. 1. Vertex function $\gamma(k_F,q)$ as a function of aq between 0 and the maximal momentum transfer for three dopings δ and $\mathbf{q}=[q,q]$.

$\gamma(k_F,0)\to 1/(1+4/\pi)\sim 0.440$, and $\gamma^2(k_F,0)/q_0 \to 2/(1+4/\pi)^2\sim 0.387$. Physically speaking, this limit describes a system of holes near the largest filling factor compatible with the constraint. Alternatively, this case can also be viewed as describing a few electrons in a renormalized band structure and interacting via renormalized vertices. The free electron value for the enhancement factor γ^2/q_0 is one, i.e., quite different from the above value due to the constraint. Figure 2 also shows that the momentum-averaged enhancement γ^2/q_0 de-
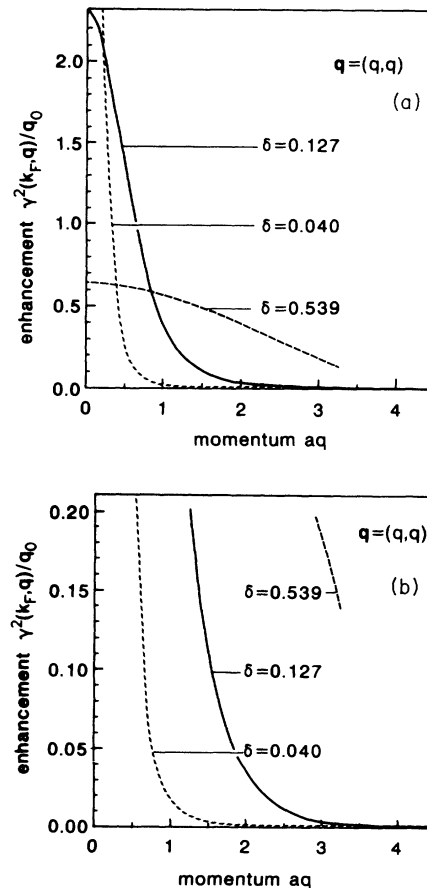

FIG. 2. Total enhancement $\gamma^2(k_F,q)/q_0$ as a function of aq for three different dopings δ and $\mathbf{q}=[q,q]$. (a) Overview; (b) Enlarged lower part.

creases by about 30% passing from $\delta=1$ to $\delta=0.539$.

The solid curve in Fig. 2 for the moderate doping $\delta=0.127$ exhibits two important features: (a) Its momentum-averaged value is around $\frac{1}{3}$ and thus has not changed much compared with its value for $\delta=0.539$. This means that correlation effects only moderately decrease the electron-phonon coupling in quantities which can be expressed by $\alpha^2 F$. Though the vertex functions suppress $\alpha^2 F$ by roughly one order of magnitude (see the solid line in Fig. 1) the band renormalization $2/\delta$ counterbalances this decrease to a large extent; (b) γ increases strongly at small momentum transfers as can be seen from the solid curve in Fig. 1. As a result, the enhancement curve becomes strongly peaked in the forward direction and decays rapidly at large momenta. The solid line in Fig. 2(a) illustrates this decay in more detail. For momentum transfers $k_F < q < 2k_F$ the effective electron-phonon interaction is only one per cent or less of the value of the uncorrelated case. According to Eq. (16) $\alpha^2 F$ is sensitive both to the strong increase of γ^2/q_0 at small momentum transfers and its huge suppression at large momenta. Both effects cancel each other to a large extent leading to an overall reduction of $\alpha^2 F$ of about a factor 3–4 due to correlations. Due to the extra factor $[v(\mathbf{p})-v(\mathbf{p}')]^2$ only the large momentum behavior of γ^2/q_0 enters $\alpha_{tr}^2 F$ which leads to a dramatic correlation-induced suppression of this function. For instance, for $\delta=0.127$ and for momentum-independent bare coupling functions and phonons $\alpha^2 F$ is suppressed by about a factor 100 compared to the uncorrelated case. Similar reductions should occur in transport quantities also for other scattering mechanisms such as impurity scattering. The strong momentum dependence of γ^2/q_0 is already present if the susceptibilities Eqs. (12)–(15) are evaluated in the continuum approximation where γ depends only on $|\mathbf{q}|$ and the anisotropy does not enter. The strong enhancement of $\alpha^2 F$ compared to $\alpha_{tr}^2 F$ and the difference between these two functions is therefore not as-

sociated with anisotropy but due to correlation effects.

For the very small doping $\delta=0.04$ the strong $\mathbf{q}$ dependence of γ and γ^2/q_0 is even more pronounced. The large band renormalization factor of 50 is nearly perfectly cancelled by vertex corrections yielding a momentum-averaged enhancement of similar magnitude as in the case $\delta=0.127$. In contrast to that, $\alpha_{tr}^2 F$ is quenched to very small values by correlation effects due to the extremely intense forward scattering and the extremely small scattering for larger momentum transfers [see the dotted line in Fig. 2(b)]. This means that electronic transport quantities are no longer determined by the scattering from phonons. Similar results as in Figs. 1 and 2 have been obtained for the direction $\mathbf{q}=[q,q/2]$. For $\mathbf{q}=[q,0]$ the curves in Figs. 1 and 2 are symmetric with respect to $aq=\pi$. As a result the enhancement of forward scattering is less pronounced in this case.

In conclusion, we have studied systematically the influence of strong electronic correlations on a simple but relevant model for the electron-phonon interaction in high-T_c oxides. We have shown that the leading terms in a $1/N$ expansion involve band renormalization and vertex corrections and that both compete with each other. We find for a one-band Hubbard model on a square lattice and an infinite U a strongly q-dependent vertex function for small and intermediate dopings with large values for small momentum transfers and small values for large momentum transfers. As a result, the transport function $\alpha_{tr}^2 F$ is heavily and the Eliashberg function $\alpha^2 F$ slightly suppressed by correlations. Our findings are consistent with the observability of an isotopic effect in nonoptimized high-T_c oxides and the view that the electron-phonon interaction is not dominant for electronic transport coefficients.

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