Renormalization of the electron-phonon coupling in the one-band Hubbard model

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We investigate the effect of electronic correlations on the coupling of electrons to Holstein phonons in the one-band Hubbard model. We calculate the static electron-phonon vertex within linear response of Kotliar-Ruckenstein slave-bosons in the paramagnetic saddle-point approximation. Within this approach the on-site Coulomb interaction $U$ strongly suppresses the coupling to Holstein phonons at low temperatures. Moreover the vertex function does not show particularly strong forward scattering. Going to larger temperatures $kT \sim t$ we find that after an initial decrease with $U$, the electron-phonon coupling starts to increase with $U$, confirming a recent result of Cerruti, Cappelluti, and Pietronero. We show that this behavior is related to an unusual reentrant behavior from a phase separated to a paramagnetic state upon decreasing the temperature.

The relevance of phonons for high-temperature superconductivity has been debated since the discovery of the high-$T_c$ cuprates. Recently, strong renormalization effects of the electrons near the Fermi surface, observed in angle-resolved photoemission in several cuprates, have been at least partially ascribed to phonons $\delta$. Furthermore, quantum Monte Carlo simulations of the Hubbard-Holstein model suggest that the electron-phonon coupling shows forward scattering and no substantial suppression at large $U$ and small dopings $\delta$, similar as in the $1/N$ expansion for the t-J model $\delta$. On the other hand, it has been pointed out $\delta$ that at small dopings the Kotliar-Ruckenstein (K-R) slave-boson approach $\delta$ might yield results quite different from the $1/N$ expansion. Below we study the influence of strong electronic correlations on the electron-phonon coupling using the K-R approach. The quantity of interest is the static vertex function $\Gamma$ which acts as a momentum-dependent, multiplicative renormalization factor for the bare electron-phonon coupling.

We consider the one-band Hubbard model on a square lattice with nearest and next-nearest neighbor hopping, $t$ and $t'$, respectively,

$$ H = -t \sum_{\langle i,j \rangle, \sigma} c_{j \sigma}^\dagger c_{i \sigma} + t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} c_{j \sigma}^\dagger c_{i \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow}. \quad (1) $$

For the non-interacting system the dispersion relation is

$$ \varepsilon_k = -2t(\cos(k_x) + \cos(k_y)) - 4t' \cos(k_x) \cos(k_y), \quad (2) $$

and because the saddle-point density of states has a logarithmic van Hove singularity at $4t'$. For this model we want to study the influence of electronic correlations on the coupling of electrons to an external field $V_i$. The bare coupling has the form $H' = \sum_{i, \sigma} n_{i \sigma} V_i$. Writing $V_i = g u_i$, $H'$ describes also the interaction of electrons and atomic displacements $u_i$ with coupling constant $g$. The linear change in the one-particle Green’s function $G(p)$ due to $V_q$ is,

$$ \frac{\delta G(p)}{\delta V_q} = G(p) \Gamma(p, q) G(p + q), \quad (2) $$

with the charge or electron-phonon vertex $\Gamma(p, q) = \frac{-\delta G^{-1}(p)}{\delta V_q}$. The components of the three-dimensional vectors $p$ and $q$ consist of a frequency and a two-dimensional momentum. For the calculation of the vertex we use the slave-boson technique of Kotliar and Ruckenstein $\delta$. The basic idea of our approach $\delta$ is to calculate linear responses by linearizing the saddle-point equations for the perturbed system about the homogeneous saddle-point solution. We consider only paramagnetic solutions. Then there are three slave-bosons, $c$, $p$, and $d$, describing empty, singly, and doubly occupied sites, and two Lagrange parameters $\lambda^{(1)}$ and $\lambda^{(2)}$ enforcing consistency between slave-fermions and slave-bosons. The linear response to a charge-like perturbation of a given wave-vector can be determined by solving the $5 \times 5$ system of linear equations given in $\delta$. Considering only static fields $V_q$ we find

$$ \Gamma(p, q) = \frac{\delta \lambda^{(2)} B}{\delta V_q} + \delta z (\varepsilon_p + \varepsilon_{p+q}) \frac{\delta z}{\delta V_q}. \quad (3) $$

The first term in Eq. (3) is due to the explicit dependence of $G^{-1}$ on $V$, the remaining terms are obtained by taking the derivative of the self-energy with respect to $V$. $\Gamma$ does not depend on frequencies because we assumed zero frequency in $q$ and because the saddle-point self-energy is frequency-independent. $z$ is given by the Kotliar-Ruckenstein choice

$$ z = \frac{(e + d)^2}{\sqrt{1 - p^2} - d^2 \sqrt{1 - e^2 - p^2}}. \quad (4) $$

In the limit $U \to \infty$ our approach reduces to method (II) of Ref. $\delta$, and we have checked that for large $U$ we recover the results given in their Fig. 1.

While it was shown that the slave-boson linear-response method gives very good results for the charge susceptibility (see, e.g., Fig. 1 of Ref. $\delta$ for a comparison with exact diagonalization), it is not clear a priori how well it will work for the charge vertex $\Gamma(p, q)$. As a check we have calculated the static vertex for a small system using exact diagonalization. The result for the scattering of an electron from a state just below, to a state just above the Fermi surface is shown in Fig. $\delta$ Considering the fact that in exact diagonalization the number of
particles is fixed, while the slave-boson calculations are performed in the grand canonical ensemble, the agreement between both methods is remarkably good. This indicates that the slave-boson approach should work well at zero temperature.

To find out how well the slave-bosons work at finite temperatures we compare to the quantum Monte Carlo (QMC) calculations of Ref. [2]. Fig. 4 of that work shows the effective electron-phonon coupling $g(p, q)$, as defined in their Eq. (7), for the Hubbard model on an 8×8 lattice with filling $n = 0.88$, calculated at the lowest fermionic Matsubara frequency, for an inverse temperature of $\beta = 2$. For comparison, we show in Fig. 2 the results of our slave-boson linear response calculations for the same model at $\omega = 0$ and a slightly different filling $n = 0.875$. Also here we find a remarkable agreement. In particular, we find that after an initial decrease the coupling for forward scattering (small $q$) starts to increase for $U \gtrsim 8$. This seems to indicate that the slave-boson method also works well at finite temperatures. Moreover, Eq. (3) naturally explains why the QMC results for different electron momenta $p$, shown in Fig. 4 of Ref. [2], are so similar.

After comparing the results of the slave-boson linear response calculations to more accurate methods, which are, however, limited to small systems (exact diagonalization) or finite temperatures (quantum Monte Carlo), we now turn to very large systems at very low temperatures. First we calculate the electron-phonon vertex for electrons on the Fermi surface, where in Eq. (4) $\varepsilon_p$ and $\varepsilon_{p+q}$ are both replaced by the Fermi energy of the non-interacting system. Fig. 3 shows the vertex for momentum transfer $q$ along high symmetry lines in the Brillouin zone for the Hubbard model at essentially zero temperature. The effect of next-nearest neighbor hopping is illustrated by comparing calculations for $t' = 0$ and $t' = -0.35 t$. We find that in both cases the on-site Coulomb interaction strongly reduces the electron-phonon coupling. This is not completely unexpected as the charge response should be strongly suppressed by an on-site Coulomb interaction. It is, however, in striking difference to the behavior at higher temperature (Fig. 2). Also, while $\Gamma(q)$ shows a broad peak around $q = 0$, we do not find a particularly pronounced forward scattering. In fact, the electron-phonon vertex is often strongest close to $q = (\pi, 0)$. This is different from what was found within an 1/N expansion [3]. The 1/N expansion relies on the smallness of $1/\delta N$, i.e., it breaks down at small dopings $\delta$. This can be seen from the fact that the charge-charge correlation function remains in leading order finite for $\delta \to 0$ though the exact correlation function vanishes in this limit. The Kotliar-Ruckenstein method, on the other hand, reproduces this limit correctly in leading order which makes it plausible that in this case the charge vertex is smaller than in the 1/N expansion, especially at smaller dopings [4]. Which of the two methods is more reliable, in particular, near optimal doping, is not clear and can probably only be judged by comparison with exact numerical methods.

To assess the importance of the electron-phonon coupling for superconductivity we calculate the renormalization factor

$$\Lambda_\alpha = \frac{\int_{FS} dp \int_{FS} dp' \varepsilon_{p+q} \langle \alpha | g_\alpha(p) \Gamma(p, p' - p) g_\alpha(p') | \alpha \rangle}{z^2 \int_{FS} dp \int_{FS} dp' g_\alpha^2(p)}$$

for the pairing channels $g_\alpha(p) = 1$, $g_\alpha^*(p) = \cos(p_x) + \cos(p_y)$, $g_{p_x}(p) = \sin(p_x)$, $g_{a_{-x-y}}(p) = \cos(p_x) - \cos(p_y)$, and $g_{a_{+x}}(p) = \sin(p_x) \sin(p_y)$. $\Lambda_\alpha$ is equal to the ra-
tio $\lambda_n/\Lambda^{(0)}$, where $\lambda_n$ and $\Lambda^{(0)}$ denote the dimensionless electron-phonon coupling constants in the interacting and non-interacting cases, respectively. To judge the importance of forward scattering we also calculate the renormalization factor for transport,

$$\Lambda_{tr} = \frac{\int_{FS} dp \frac{d\Gamma(\mathbf{q})}{d\mathbf{p}} \int_{FS} dp' \frac{d\Gamma'(\mathbf{q})}{d\mathbf{p}'} | \mathbf{v}(\mathbf{p}) - \mathbf{v}(\mathbf{p}') |^2}{2 z^2 \int_{FS} dp \frac{d\Gamma(\mathbf{q})}{d\mathbf{p}} \int_{FS} dp' \frac{d\Gamma'(\mathbf{q})}{d\mathbf{p}'} | \mathbf{v}(\mathbf{p}) |^2}.$$

The results are shown in Fig. 4. We find that for $U \lesssim 10$ the $s$-wave couplings decrease almost exponentially with $U$. For the special case of the Hubbard model with nearest neighbor hopping only ($t' = 0$) we have $\Lambda^{s} = \Lambda_{tr}$, since $g_s^*$ is constant on the Fermi surface. Moreover $\Lambda_{tr} \approx \Lambda_{tr}$, reflecting that there is no pronounced forward scattering; only for larger $U$ does $\Lambda_{tr}$ become somewhat smaller than $\Lambda_{tr}$. But by then both coupling constants are already very small. The higher pairing channels are even weaker, starting from zero at $U = 0$, going through a maximum around $U = 2$ only to decay almost exponentially. We can thus conclude that within Kotliar-Ruckenstein slave-boson theory, restricting the system to be paramagnetic, the contribution of Holstein phonons to superconductivity should be very small.

We now come back to the surprising upturn of the electron-phonon vertex for $U \gtrsim 8$ shown in Fig. 2 and also found in the QMC calculations of Ref. 2. Calculating $\Gamma(\mathbf{q})$ at $kT \approx t$, we indeed find a drastically different behavior than for $T \to 0$: Instead of monotonically decreasing with $U$, the coupling starts to increase and develops a very strong forward scattering peak. An example is shown in Fig. 5. Looking at the charge response function $\chi(\mathbf{q})$ in the paramagnetic phase we find that this behavior is a precursor of a phase-separation instability — a divergence of $\chi(\mathbf{q} = 0)$. This has already been pointed out in Ref. 3. Calculating the phase diagram, we find a very peculiar reentrant behavior around the phase separated region as shown in Fig. 6. When cooling down the system phase separates, but at low enough temperature it reverts back to the paramagnetic phase. Since in our calculations we only allow for a paramagnetic phase, other phases might mask the phase separation. Also, since slave-bosons may have problems at high temperatures, it is not clear if the Hubbard model really shows such an reentrant behavior. Nevertheless, we find a qualitatively similar behavior in the limit $U \to \infty$ in the gauge invariant $1/N$ expansion (i.e., a theory without Bose condensation). Phase separation at finite $T$ has also been proposed in Refs. 3, 7, 10. Moreover the good agreement with the quantum Monte Carlo calculations of Ref. 3 suggests that our approach might indeed capture the relevant physics. It would therefore be interesting to test the phase diagram shown in Fig. 6 with QMC: A calculation for, e.g., $\beta = 1$ and $U = 4\ldots8$, i.e., at temperatures and values of $U$, where QMC has little problems, should show clear signs of phase separation. Of course, these calculations should be done at $\omega = 0$ as the extrapolation from finite Matsubara frequencies might be

FIG. 3: Electron-phonon vertex $\Gamma(\mathbf{q})$ for scattering electrons on the Fermi surface. Calculations are for the Hubbard model on a 1000 x 1000 lattice with $t' = 0$ (top) and $t' = -0.35 t$ (bottom) at an inverse temperature $\beta = 500/t$. Fillings and Hubbard $U$ are indicated in the plots. We find that in all cases the vertex function is strongly reduced with increasing $U$. For large $U$ the changes become small and eventually $\lim_{U \to \infty} \Gamma(\mathbf{q})$ is reached.
FIG. 4: Renormalization constants $\Lambda_\alpha$ for different pairing channels and $\Lambda_{tr}$ relevant for transport for the Hubbard model with $t' = 0$. Calculations were performed for lattices of increasing size at decreasing temperatures, performing the $p$ integrals over the whole Brillouin zone and weighting with minus the derivative of the Fermi-Dirac distribution $-f'(\varepsilon_p) = \beta f(\varepsilon_p)(1 - f(\varepsilon_p))$, which becomes a delta function for $T = 0$. Convergence of the $T \to 0$ extrapolation has been checked by comparing $\Lambda_s$ and $\Lambda_1$, which only for $T = 0$ are equal. Error-bars for the extrapolation are plotted, but are usually smaller than the size of the plotting symbols.

FIG. 5: Electron-phonon vertex $\Gamma(q)$ for scattering on the Fermi surface. Calculations are for the Hubbard model on a $100 \times 100$ lattice with $t' = 0$ and filling $n = 0.80$ at an inverse temperature $\beta = 1$. The plot should be compared to the uppermost panel on the right of Fig. 6.

FIG. 6: Phase separation: The lines enclose the region where the paramagnetic slave-boson saddle-point solution is unstable against phase separation. Calculations are for the Hubbard model on a $100 \times 100$ lattice with $t' = 0$. For $t'/t > 0$ the region of phase separation tends to increase, for $t'/t < 0$ it tends to decrease, in particular, for large doping.

difficult close to an instability.

In conclusion, we have studied the influence of strong electronic correlations on the electron-phonon interaction for the Hubbard-Holstein model using the Kotliar-Ruckenstein slave boson method. For high temperatures the boundaries of the phase-separated state were determined in the $T - U$ plane for different dopings and the increase of the static vertex $\Gamma$ near the boundaries was studied, confirming and extending recent results of Ref. 7. At low temperatures and moderate or small dopings we found that $\Gamma$ does not exhibit pronounced forward scattering behavior and that $\Gamma$ reduces dramatically the electron-phonon coupling. It seems that exact numerical calculations are necessary to judge the reliability of the $1/N$ and the Kotliar-Ruckenstein approaches.

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