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Electron-phonon interaction in strongly correlated electron systems: relevance of antiferromagnetic correlations.

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Abstract. The interplay between electron-phonon interaction and strong electronic correlation is analyzed by means of Dynamical Mean Field Theory. Suppressing all antiferromagnetic correlations, the electron-phonon interaction is found to be strongly suppressed by Coulomb repulsion. In particular, close to the Mott transition at half-filling the electron-phonon interaction has very little effect on quasiparticles: In fact it is possible to describe the low-energy physics in terms of an effective Hubbard model with a slightly renormalized repulsive coupling. The situation changes completely if antiferromagnetic correlations are included: Electron-phonon interaction has a strong effect on the electronic self-energy even for large values of the Coulomb repulsion. Phonon-induced modifications of electronic properties like, e.g. photoemission spectra, are therefore expected to be more pronounced in underdoped cuprates where antiferromagnetic correlations are stronger than in overdoped.

1. Introduction
More than twenty years after their discovery [1], high-temperature superconducting cuprates still represent one of the biggest challenges of current solid-state research. There is a lively debate not only on the nature of the superconducting bosonic mediator, but also on whether or not a “superconducting glue” exists at all [2, 3]. In the attempt to identify the origin (spin, lattice, . . .) of the bosonic degrees of freedom electrons interact with, people have been looking for “signatures” of such modes in various quantities. However, it is often quite difficult to interpret such experiments because of the strongly correlated nature of cuprates: In spite of the recent spectacular progresses in the development of technical tools to study such systems, we still know fairly little about the interplay between Coulomb interaction and electron-boson interaction. Moreover, when interpreting experiments, it is often quite tricky to distinguish between clear hallmarks and phenomena which are related to superconductivity in a roundabout and misleading way. There are however some unambiguous experimental evidences that the electron-phonon interaction (EPI) plays an appreciable role for a number of properties: Certain phonons show a large softening and broadening under doping [4, 5], suggesting a strong interaction with doped holes. This is, for instance, seen for the so-called half-breathing copper-oxygen bond stretching phonon, apical oxygen phonons and the oxygen B_{1g} buckling phonon. Photoemission spectroscopy (PES) experiments show the formation of small polarons for the undoped cuprates [6], and a kink in the nodal k-direction also suggests strong EPI [7]. While
there is only a weak isotope effect on $T_c$ for optimally doped samples, a strong isotope effect has been seen away from optimum doping [8]. Recent STM work suggests that a phonon mode plays a role in superconductivity [9], although other interpretations are possible [10]. In particular, an isotope effect has been observed [9]. While the phonon contribution to superconductivity remains unclear, it seems clear that phonons can be important for other properties.

The EPI has been studied very extensively in the local density approximation (LDA) [11] of the density functional formalism [12], which is particularly appropriate for systems where correlation effects are not very strong. This approach has been shown to be very successful for conventional superconductors [13, 14, 15, 16]. For cuprates [17] a rather weak EPI was found, which alone would not be sufficient to explain the superconductivity [18]. However, the calculated width [19] of the half-breathing phonon is an order of magnitude smaller than the reported experimental value [20], raising questions about the accuracy of the LDA in this context [21]. An even larger width and softening has been observed for an apical oxygen phonon [4]. The coupling to this mode is mainly electrostatic and probably too efficiently screened in the LDA [22]. The interest has therefore recently focused on whether the interplay between the Coulomb interaction and the EPI can explain experimental signs of a strong EPI.

A powerful approach to study the interplay between Coulomb repulsion and electron-phonon interaction is Dynamical Mean Field Theory (DMFT). DMFT is non-perturbative and therefore it allows one to study the most interesting situations, namely those where the two interactions directly compete with one another. These regimes are indeed very hard to attack with standard theories, as both interaction strengths are comparable to the electronic bandwidth (or even larger). DMFT represents therefore a convenient tool in this regard and it has been applied several times to the Hubbard-Holstein model [23, 24, 25, 26, 27, 28, 29, 30]. Here we review some of the results, in particular the study of the Mott-Hubbard transition in the presence of electron-phonon interaction [25] and the analysis of the role of antiferromagnetic correlations in the undoped case [29].

2. Mott-Hubbard transition in the presence of electron-phonon interaction

Paramagnetic DMFT (P-DMFT) has been extensively used to study the half-filled Hubbard model, showing that, in the metallic region close to the Mott transition, the spectral function presents three features: the high-energy Hubbard bands at energy $\pm U/2$ and a narrow resonance at the Fermi level, whose width is proportional to the quasiparticle residue $Z = (1 - \partial \Sigma(\omega)/\partial \omega|_{\omega=0})^{-1}$, a quantity which decreases for increasing $U$ and vanishes at the Mott transition ($U = U_c$ is the electronic half-bandwidth). Since P-DMFT neglects all non-local correlations, starting from the situation described above we can expect EPI to give essentially two effects: The first is a reduction of $Z$ (which, due to the momentum independence of the self-energy, is equivalent to an enhancement of the effective mass $m^*/m = 1/Z$). This effect is responsible for the polaron crossover for weak repulsion. The second effect is a phonon-mediated retarded attraction between electrons with opposite spins, which opposes the Hubbard repulsion leading to an effective dynamical interaction $U_{eff}(\omega) = U - \frac{2g^2\omega_0}{\omega_0^2 - \omega^2}$. In the antidiabatic limit $\omega_0 \to \infty$ the attraction becomes static and equals the bipolaronic binding energy $2g^2/\omega_0$. While the first effect opposes to the electronic motion, the second effect instead favors the motion by screening the Hubbard repulsion and should lead to an enhancement of $Z$. The overall effect of the EPI coupling on the correlated metallic phase is therefore hard to predict on intuitive grounds.

In the P-DMFT solution of the half-filled Hubbard-Holstein model the quasiparticle weight $Z$ is very weakly dependent on the dimensionless electron-phonon coupling $\lambda = g^2/\omega_0 D$: On the metallic side of the Mott transition it is basically identical to that of the pure Hubbard model (i.e. $Z \propto 1 - U/U_{c2}$) and the electron-phonon coupling $\lambda$ adds only a very slow linear
increase with respect to it. The increase of $Z$ due to the phonon-mediated attraction, which results in a reduction of the total repulsion, is therefore actually visible, as we have speculated above [26, 25]. This is the result of P-DMFT as long as $\lambda < U/D$ [26, 25]. The increase of $Z$ can therefore be attributed to the reduction of the effective repulsion, which prevails over the polaronic renormalization of the hopping in this region. If instead $\lambda$ gets of the order of $U/D$, $Z$ starts to decrease and eventually goes to 0, due to bipolaron formation [31].

Empirically one can determine an effective static repulsion $U_{\text{eff}}(U, \lambda, \omega_0)$, as the value of $U$ for which a pure Hubbard model has the same $Z$ as the full Hubbard-Holstein model. Since in the antiadiabatic limit $U_{\text{eff}} = U - 2\lambda D$, one can try to parameterize the effective repulsion as $U_{\text{eff}} = U - 2\eta \lambda D$, where $\eta$ is a dimensionless free parameter that is determined by fitting directly $Z(U, \lambda)$ with this functional form. For relatively small $\omega_0/U$, we found that $\eta$ has a linear behavior in $\omega_0/U$, and bends over for larger phonon frequency closely following the functional form $\eta = 2\omega_0/U/(1 + 2\omega_0/U)$ and eventually reaching the asymptotic value $\eta = 1$. This functional form is in agreement with what derived from an expansion of the effective Kondo coupling [32].

![Figure 1](image_url)

**Figure 1.** The electron spectral function for the Hubbard-Holstein model (dashed line), compared with a pure Hubbard model with $U = U_{\text{eff}} = U - 2\eta \lambda D$ (solid line), for different values of $U$ and $\omega_0$ (the dot-dashed vertical line indicates $\omega_0$). In the three upper panels we take $\lambda = 0.5$, in the lowest $\lambda = 0.25$. Since we used exact diagonalization as DMFT impurity solver the Hubbard bands are made of a small number of discrete features. The Kondo peak at the Fermi level ($\omega = 0$) is instead hardly affected by the discretization.

The analysis of the quasiparticle weight suggests that the effect of EPI interaction on the strongly correlated metallic phase of the Hubbard model is a partial screening of the repulsion, and the degree of screening is controlled by $\omega_0/U$ when this quantity is not too large. This latter factor contains the information about the lattice dynamics in an effective way. Of course, at this level, this result could sound of little physical significance, since it basically arises by a simple
fit procedure. Nonetheless, $Z$ also measures the width and weight of the low-energy feature in the single-particle spectral function. Thus, it is tempting to compare the spectral function for the Hubbard-Holstein model with the correspondent quantity for the equivalent Hubbard model with reduced repulsion. As far as $U \gg \omega_0$, we find that the low-energy part of the spectrum is basically identical in the two models, while differences develop in the high-energy part, where phonon satellites at energies of the order $\omega_0$ appear in the system coupled to phonons. This can be seen in Fig.1, where the spectra for four different cases (see caption) are shown. Moreover, even if the effect of phonons is visible in the high-energy Hubbard bands, their position is more or less coincident in the Hubbard-Holstein model and in the effective Hubbard model. This is remarkable, since the rescaling of $U$ has been derived only be requiring the same value for the quasiparticle weight.

Our analysis of the half-filled Hubbard-Holstein close to the Mott transition shows that the phonon-induced modifications on the low energy physics of the Hubbard-Holstein model can be accounted for by a slight renormalization of the static Hubbard repulsion. In other words, according to P-DMFT, the effects of EPI on quasiparticles are strongly suppressed. This implies that to explain the conclusion of PES studies [6, 22] of polaronic behavior in undoped cuprates, an unrealistically large value of $\lambda$ would be necessary in P-DMFT. However, going beyond the level of approximation of P-DMFT, one expects polaronic features in the spectrum to appear for a much smaller $\lambda$, at least for the undoped system. One way of going beyond P-DMFT is to include antiferromagnetic correlations allowing for long-range antiferromagnetic order. This is nothing else than effectively introducing an Ising-like superexchange $J_\sigma$, and it can be done by employing an antiferromagnetic bath (AF-DMFT) [35, 36, 37]. In the following section we show how this is enough to get polaron formation in the undoped system for $\lambda$ smaller than 1, as the PES experiments and other numerical studies suggest [33].

3. Effects of antiferromagnetic correlations

In this section we present results for the half-filled Hubbard-Holstein model, obtained with AF-DMFT [29]. As we already discussed in the previous section, we want to understand how much of the strong suppression of the EPI found in the proximity of the Mott transition is due to the absence of antiferromagnetic correlations in P-DMFT. A positive effect of antiferromagnetic correlations on the EPI has been predicted in the framework of the $t$-$J$-Holstein model [38, 39, 33, 40, 41]. In particular it has been found that a single hole experiences a strong EPI due to the presence of the antiferromagnetic background which provides a sort of “pre-localizing” effect. One therefore expects that similar results have to be present in the Hubbard-Holstein model at half-filling. Indeed, we know that the half-filled Holstein-Hubbard model must be an insulator for large $U$. In the P-DMFT this can only happen via $Z \to 0$. It follows that this strongly suppresses the EPI, at least in the weak-coupling limit [34]. In the AF-DMFT, on the other hand, it is possible to have an insulating state with $Z > 0$. Moreover, notice that P-DMFT is equivalent to solving an Anderson impurity model (with a self-consistent host). We consider the electron Green’s function, describing, for instance, the removal of an electron in photoemission. We focus on the corresponding final states close to the Fermi energy, i.e., in the Kondo resonance. These states have essentially the same occupancy of the local level as the ground-state, since the electron removed in the photoemission process is replaced by an electron hopping in from the host [42]. Actually, in the limit of infinite orbital degeneracy and an infinite $U$, the occupancy of the local level is unchanged [43]. Seen from the phonons, coupling to the net charge of the local level, a photoemission process corresponding to the Kondo peak then leads to no change. As a result, Holstein phonons have only an indirect influence on these states due to a renormalization of the parameters [42, 24]. In the Holstein-Hubbard model, however, an electron filling the hole created in photoemission comes from another $3d$ level, which also couples to phonons, and in general this may be expected to influence the spectrum also close to
the Fermi energy.

We have applied the AF-DMFT method to the Holstein-Hubbard model on a Bethe lattice using exact diagonalization for solving the impurity problem [29]. The results for $Z$ are shown in Fig. 2. The results for $U = 0$ shows how $Z$ is reduced from $Z = 1$ for $\lambda = 0$ to $Z \approx 0$ for $\lambda = \lambda_c = 0.33$. We use this as the criterion for (small) polaron formation. For $\lambda = 0$, an increase of $U$ leads to a decrease of $Z$. However, $Z$ deceases more slowly with $\lambda$ for a finite $U$, and polaron formation happens at a somewhat larger value $\lambda_c$. Thus the Coulomb interaction moderately suppresses polaron formation, at least in AF-DMFT. This is also shown in Fig. 3.

It is important to notice that in the half-filled large $U$ case, there is no polaron formation in the ground-state unless $\lambda >> U/D$, since $U$ suppresses charge fluctuations. The Green’s function describes the final state after an electron has been removed (in, e.g., photoemission) and $Z \to 0$ describes how the corresponding hole localizes due to polaronic effects. This is different from the Holstein model, where polaron formation means the formation of polarons also in the ground-state.

Macridin et al. [44] performed a dynamical cluster calculation (DCA) for the Holstein-Hubbard model using a $2 \times 2$ cluster. Using a different definition of polaron formation, they found $\lambda_c \sim 0.5$, similar to the result in Fig. 2. They emphasized the synergistic cooperation between the EPI and AF correlations. As a result they found that the AF transition temperature at finite doping is enhanced by the EPI. Macridin et al. [44] and Fu et al. [45] pointed out that the EPI can contribute to a charge density modulation seen experimentally.

To see the effects of the antiferromagnetic correlations we compare with polaron formation in the ferromagnetic state (F in Fig. 3), where antiferromagnetic correlations are completely suppressed. We then find that $\lambda_c$ is very large. When the antiferromagnetic correlations are reintroduced, $\lambda_c$ is strongly reduced (see Fig. 3), meaning that the electron-phonon coupling

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{\footnotesize $Z$ as a function of $\lambda$ for different $U$ and for $\omega_0 = 0.0125W$, where $W$ is the band width. The figure shows how the Coulomb interaction moderately suppresses polaron formation ($Z \to 0$) (after Sangiovanni et al. [29]).}
\end{figure}
Figure 3. Critical value $\lambda_c$ for polaron formation ($Z \to 0$) in the half-filled Holstein model ($U = 0$) as well as in the large $U$ Holstein-Hubbard model in the antiferromagnetic (AF) or ferromagnetic (F) states. The figure illustrates that AF correlations help the EPI (smaller $\lambda$ needed for polaron formation) but that the net effect of $U$ is a moderate suppression of the EPI.

becomes more efficient, as expected.

Although the antiferromagnetic effects, caused by $U$, strongly reduce $\lambda_c$, the net effect of $U$ is still an increase of $\lambda_c$, due to other effects of $U$. We may then ask what this is due to. The Green’s function of the ferromagnetic half-filled state, describes the creation of a hole in an otherwise filled spin up band. In the absence of phonons, this hole could move completely freely, and if the system has electron-hole symmetry, this state is equivalent to a Holstein model with a single electron at the bottom of the band. We need therefore to know how polaron formation differs between the half-filled and the single electron case in the Holstein model. We first consider the $\lambda \ll 1$ limit and $\omega_0 \ll t$ for a nearest neighbor hopping $t$ with a single electron Holstein model. Using the weak-coupling expression of the self-energy of the single-electron case (see, e.g. Ref. [34]) one can define an effective electron-phonon coupling $\lambda = \lambda_0$ via the quasiparticle weight $Z$ or the effective mass

$$\left. \frac{d^2E_k/dk^2}{d^2\varepsilon_k/dk^2} \right|_{k=0} = \frac{1}{1 + \lambda_0},$$

where $E_k = \varepsilon_k/(1 + \lambda_0)$ ($\varepsilon_k$ being the bare dispersion) and

$$\lambda_0 = \frac{g^2}{4\pi t \omega_0}.$$  

Both methods give the same $\lambda_0$ for this model in the weak-coupling limit [47]. Instead of the Holstein model with a single electron, we can study the half-filled model assuming a constant density of states. Defining $\lambda$ via the expression for $Z(k)$ recovers the $\lambda$ defined as

$$\lambda = \frac{2g^2}{\omega_0} N(0)$$

and leads to $\lambda = \pi \lambda_0$, since $N(0) \simeq 1/(8t)$. The increase in $\lambda$ is partly due to the fact that the self-energy at the bottom of the band only has contributions from higher states while in the half-filled case there are contributions from both higher and lower states and partly due to the DOS at the bottom of the band being smaller than the average DOS [29]. The weak-coupling argument above shows how the effects of EPI are stronger for the half-filled case. Let us now consider strong coupling: Polaron formation has been studied extensively for the Holstein model [48, 49, 50, 51, 52, 53, 33, 54]. For noninteracting electrons, polaron formation is often associated with bipolaron formation [53, 54]. Since on-site bipolaron formation is strongly suppressed by the large on-site $U$ relevant for cuprates, we focus on polaron formation here. We use $Z \to 0$ as the criterion for polaron formation. For the nearest neighbor Holstein model
with a single electron and $\omega_0 = 0.0125W$ this was found to happen for $\lambda_c = 1.2$ [33], where $W$ is the band-width and $\lambda$ is here defined as $\lambda = g^2/\omega_0 D$, corresponding to the assumption $N(0) = 1/W$ in Eq. (3). For the half-filled case with a semi-elliptical DOS in AF-DMFT we find that $\lambda_c = 0.33$ (see Fig. 2), again using $\omega_0 = 0.0125W$ and putting $N(0) = 1/W$ in the definition of $\lambda$. Similar results were found by several other groups [51, 52, 53, 54]. As in the weak coupling limit, there is a large difference between the single electron and half-filled cases [29]. To better understand where this difference comes from, we consider polaron formation in the adiabatic limit by comparing free electron states with states of perfectly localized electrons [55, 29]. The energy for free electrons is $E_{\text{free}} = -4t$ per electron for the single electron case and $E_{\text{free}} = -16t/(3\pi) \approx -1.7t$ for the half-filled case. In the localized case, $E_{\text{loc}} = -g^2/\omega_{\text{ph}}$ per electron for both cases. For simplicity, we assume that polarons form when $|E_{\text{loc}}| > |E_{\text{free}}|$. This leads to a large $\lambda_c = 1$ for the single electron case and a much smaller $\lambda_c = 0.42$ for the half-filled case, in rather good agreement with more accurate calculations. The large difference between the two cases is due to the large difference in kinetic energy per electron. In the single electron case, the electron is at the bottom of the band and has the maximum (absolute) kinetic energy, while in the half-filled case the average kinetic energy is much smaller. The electron-phonon interaction energy can then win more easily and lead to polaron formation. This is illustrated in Fig. 3.

Comparing the half-full Holstein model and the single electron Holstein model one can therefore conclude that $\lambda_c$ is much larger in the single electron case, because the absolute value of the hopping energy per electron is much larger. Counterintuitively, $\lambda_c$ is therefore larger for the ferromagnetic Holstein model than for the half-filled Holstein model because the hopping energy of the hole to be localized in the ferromagnetic case is larger, although the total hopping energy is strongly suppressed. As shown in Fig. 3 the critical value for polaron formation found with AF-DMFT at half-filling (“U large Half (AF)” in the figure) is (slightly) larger than that of the half-filled case with $U = 0$ (“U=0 Half in the figure), but (much) smaller than the one found for the single-electron case (“U large Half (F)” in the figure). Therefore we can conclude that Coulomb repulsion has, as a net effect, that of moderately suppressing the EPI. To isolate the contribution of AF correlations, one has to compare the critical lambda obtained for a large $U$ in the antiferromagnetic and ferromagnetic cases. The result of this comparison is that AF correlations alone help polaron formation very much, enhancing the effects of the EPI on electronic properties.

The AF-DMFT calculation can also be applied to the doped system. In Ref. [29] it has been found that, as the filling is reduced (doping increases) the critical $\lambda_c$ for polaron formation increases. The reason is that AF correlations decrease with increasing doping, which reduces the effects of the EPI. This is consistent with the experimental observation [6] that polaron formation is gradually suppressed as the system is doped. In addition to the effect discussed here, the calculated strong coupling to apical oxygen phonons [22] becomes more efficiently screened as the system is doped, also reducing the tendency to polaron formation.

4. Conclusions
We presented results showing the interplay between Coulomb repulsion and electron-phonon interaction crucially depends on the inclusion of antiferromagnetic correlations. DMFT is very well suited to directly compare the paramagnetic with the antiferromagnetic case: In the former all antiferromagnetic correlations are neglected while in the former the $J$ term is included at a (dynamical) mean field level. The outcome of this comparison is that quasiparticle formation is strongly affected by the antiferromagnetic correlations: In the absence of AF correlations the effect of the EPI on quasiparticles is strongly suppressed. In contrast, this is not the case when including AF correlations: The self-energy renormalization is still substantially visible and AF-DMFT gives polaron formation for $\lambda$ less than 1, in line with experiments.
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