Effective electron-phonon coupling and polaronic transition in the presence of strong correlation

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We study the Hubbard-Holstein model using slave-boson mean-field and a variational Lang-Firsov transformation. We identify weak and strong e-ph coupling solutions, whose stability depends both on the bare e-ph coupling and on the correlation strength. At mean field level the evolution from weak to strong electron-phonon coupling occurs via a first-order polaronic transition if the adiabatic parameter is below a critical value. In the strongly correlated regime and in the adiabatic limit, the region in which the weak-coupling solution is stable is sizeably enlarged with respect to the weakly correlated system and the Mott metal-insulator transition is found to be robust with respect to e-ph interaction.

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I. INTRODUCTION

Experimental indications of noticeable electron-phonon (e-ph) effects in the superconducting cuprates have revived the discussion of the interplay of e-ph and electron-electron (e-e) interactions. This issue has obviously a broader relevance, as both interaction mechanisms are important also in materials like fullerenes and manganites. The wealth of experiments available for the cuprates underscores quite a puzzling scenario where the fingerprints of e-ph interaction are strikingly different than in weakly correlated materials. In fact, while some quantities seem to be affected by phonons even more than in ordinary metals, particularly in the underdoped regime (photoemission spectra even more than in ordinary metals, particularly in the underdoped regime), while some quantities seem to be affected by phonons while some quantities seem to be affected by phonons, like resistivity. Such a situation is ultimately related to the presence of several energy scales in strongly correlated materials, which makes it compelling the use of nonperturbative approaches. Several nonperturbative methods have been indeed applied to different models with both e-e and e-ph interactions. Among those, we can count fully numerical approaches such as various kinds of Quantum Monte Carlo and exact diagonalization, the semi-analytical dynamical mean-field theory (DMFT), and approximate analytical results based on large-N expansions. Each of this approaches has its own advantages, and typical range of validity. An analysis of the recent literature seems to uncover an unclear scenario, since some calculations conclude an enhanced role of e-ph interaction in the presence of correlations and others suggest exactly an opposite situation. An important part of those discrepancies can be attributed to the different physical regimes in which the investigations have been performed (e.g., antiferromagnetic or paramagnetic phase), but another part is probably due to the numerical character of the previous analyses which does not elucidate enough the underlying physical mechanisms. In the present paper, we try to build a more analytical understanding for the correlated metal at and near half-filling and compare with the results obtained using DMFT in the same regime near the Mott transition. DMFT is the quantum version of mean-field theories, that freezes spatial fluctuations but fully retains local dynamics. The method has been recently used to study the effects of e-ph interaction close to the Mott metal-insulator transition in the Hubbard-Holstein model. In particular in Ref. 14, it has been shown that, close to the Mott transition, e-ph interaction manifests in a different way in low- and high-energy properties. While the high-energy Hubbard bands are affected by e-ph coupling, the low-energy quasiparticle physics is to some extent “protected” against the phonon effects by e-e correlation. The main effect of e-ph interaction is indeed the reduction of the repulsive $U$ leading to an effective interaction which can be parameterized in a simple way. Since DMFT still requires numerical calculations which sometimes make it difficult to disentangle different effects, it is instructive to compare approximate analytical methods with DMFT in order to gain insight into the physical picture arising from the latter method.

To this purpose we present here a mean-field picture of the Hubbard-Holstein model, following a recent suggestion by Perroni et al. From one side we exploit the ability of the slave-boson mean-field approach to capture the main features of the Hubbard model in the strongly correlated regime. To treat the phonon degrees of free-
dom we use a variational Lang-Firsov transformation\textsuperscript{21}, that has been introduced to describe the effects of e-ph interaction both in the weak- and strong-coupling regimes.\textsuperscript{20} To this end one introduces a “rotation” parameter \( \eta \), defined below, which measures the degree of polaron formation.

Slave-boson approaches have been recently performed\textsuperscript{21,22}, in a similar spirit of the present paper, to gain insight on the Quantum Monte Carlo results of Ref. \textsuperscript{[3]}, proposing that, in a range of correlation values, the small momentum e-ph vertex can be enhanced by increasing the repulsion (yet being smaller than the bare one). The studies of Refs. \textsuperscript{21,22} suggest that the enhancement of the vertex could be related to a finite-temperature signature of a zero-temperature phase separation. Our approach here follows the spirit of those calculations (namely the use of simplified approaches to gain insight into more involved calculations) but focuses on a slightly different subject, such as the “protection” of low-energy degrees of freedom from e-ph effects.

The paper is organized as follows: in Section II we introduce the model and derive the general mean-field equations for the paramagnetic homogeneous phase. In Section III, after a brief summary of the most important results for the half-filling case within the present approach\textsuperscript{12}, we extend the analysis of the mean-field solutions to the strongly correlated small-doping regime and discuss the evolution from weak to strong e-ph coupling, with particular attention to the way electronic properties are modified. The last Section is devoted to conclusions and acknowledgments.

II. MEAN-FIELD ANALYSIS OF THE HUBBARD-HOLSTEIN MODEL

The Hamiltonian of the Hubbard-Holstein model reads:

\[
H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \omega_0 \sum_i n_{i\uparrow} \bar{a}_i + \alpha \omega_0 \sum_i (a_i^\dagger + a_i) n_i
\]  

(1)

where \( t \) is a nearest-neighbor hopping term, \( c_{i\sigma}^\dagger \) (\( c_{i\sigma} \)) is the creation (annihilation) operator for an electron with spin \( \sigma \) at the site \( i \) while \( n_i = n_{i\uparrow} + n_{i\downarrow} \) is the local density operator. The operator \( a_i^\dagger \) (\( a_i \)) creates (destroys) a phonon at the site \( i \) with energy \( \omega_0 \) and \( \alpha \) parameterizes the coupling between electrons and local displacements. In what follows we will introduce the adiabaticity parameter \( \gamma = \omega_0 / C_d t \) and the dimensionless parameter \( \lambda = \alpha^2 \omega_0 / C_d t = \alpha^2 \gamma \), which measures the strength of the e-ph interaction. Here \( C_d \) is a factor depending only on the dimensionality and the topology of the lattice defined by the expression of the non-interacting kinetic energy at half filling, \( \varepsilon_0 = C_d \).

As mentioned above, we treat the e-ph interaction by means of a variational Lang-Firsov transformation \( U = e^S \), with:

\[
S = \alpha \sum_i [(n_i + f_i (n_i - (n_i))] (a_i - a_i^\dagger).
\]  

(2)

\( f_i \) are variational parameters which measure the coupling between phonon displacements and density fluctuations for any value of the adiabaticity parameter. We expect \( f_i \) to be equal to one in the antiadiabatic regime, where the standard Lang-Firsov transformation applies, and equal to zero in the adiabatic regime where the Born-Oppenheimer approximation holds. Averaging \( H_{\text{eff}} = e^{-S} H e^S \) on the vacuum state of the transformed phonons we obtain a purely fermionic Hubbard-like model with phonon-dependent renormalizations of the kinetic and correlation terms and with a rescaling of the chemical potential, all of which are controlled by the variational parameters \( f_i \).

The effective electronic model is then solved within the Kotliar-Ruckenstein slave-bosons technique\textsuperscript{12}. For each site we introduce four bosons \( e_i, d_i, p_{i\sigma}, \) representing the four possible states on site \( i \) (zero, two and one \( \sigma \) electron state), and a fermionic operator \( \tilde{c}_{i\sigma} \) which is connected to the original electron operator by the relation \( c_{i\sigma} = \tilde{c}_{i\sigma} \), where

\[
\tilde{z}_{i\sigma} = \frac{\langle e_i^\dagger p_{i\sigma} + p_{i\sigma}^\dagger d_i \rangle}{\sqrt{1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma}}}. 
\]  

(3)

The equivalence with the original Hilbert space is guaranteed by the constraints

\[
c_{i\sigma}^\dagger c_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i \quad (\forall i, \sigma), \quad 1 = \sum_{\sigma} p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i + e_i^\dagger e_i \quad (\forall i)
\]

which can be enforced introducing three Lagrange multipliers \( \lambda_1^{(1)}, \lambda_1^{(2)} \). The mean-field solution at a given value of density \( n \) in the paramagnetic homogeneous phase is obtained by taking the saddle-point value for the Bose fields ((\( e_i = e_0, d_i = d_0, p_{i\sigma} = p_0 \)) and assuming translation invariance, so that \( f_i = f \) and \( \lambda_1^{(1)} = \lambda_2^{(1)} \), \( \lambda_2^{(2)} = \lambda_0^{(2)} \). Following closely Ref. \textsuperscript{23} we minimize the resulting variational energy with respect to the Lagrange multipliers and use the constraints to get

\[
E_0 = -\varepsilon [q e^{-\alpha^2 f^2} + d_0^2 \frac{1}{(1 + \delta) (1 - \delta)}, \quad 1 - \delta (1 - f^2)]
\]

(4)

where \( \varepsilon \) is the kinetic energy per site in the uncorrelated case and \( n = 1 - \delta \); by introducing the standard notation \( x = e_0 + d_0^2 \), one can express the double occupancy as \( d_0^2 = (x^2 - \delta^2) / 4x^2 \) and \( q = z_0^2 \), i.e. the reduction of the kinetic energy due to the electronic correlation, as \( q = (2x^2 - x^4 - \delta^2) / (1 - \delta^2) \). In the absence of
e-ph coupling, when \( \alpha = 0 \), Eq. (4) reduces to the well-known Gutzwiller energy for the pure Hubbard model. On the other hand, taking the limit \( f = 1 \), one recovers the standard Lang-Firsov result, being the kinetic energy exponentially renormalized with the electron energy level and the Hubbard term shifted respectively by \(-\alpha^2\omega_0\) and \(-2\alpha^2\omega_0\).

In order to determine the mean-field solutions we minimize (4) with respect to the remaining variational parameters \( x^2 \) and \( f \). One gets:

\[
8 \frac{1 - x^2}{1 - \delta^2} e^{-\alpha^2 f^2} = \left[ U + 2\alpha^2\omega_0(f^2 - 2f) \right] \frac{x^4 - \delta^2}{x^4}
\]

\[
q(\varepsilon) f e^{-\alpha^2 f^2} = \omega_0(1 - f) \left[ \frac{(x^2 - \delta)^2}{2x^2} + \delta(1 - \delta) \right].
\]

For small doping \( \delta \) the kinetic energy can be expanded around the half-filling value \( |\varepsilon_0| \) as \( |\varepsilon| = |\varepsilon_0|(1 - \alpha\delta^2) \) (with \( \alpha \) depending on the specific shape of the uncorrelated band), and the mean-field equation (5) can be conveniently rewritten as:

\[
(1 - x^2) \frac{x^4}{x^4 - \delta^2} = \tilde{u} \frac{1 - \delta^2}{1 - \alpha\delta^2}
\]

where \( \tilde{u} = \left[ \frac{U}{U_c} + \lambda(f^2 - 2f)/4 \right] / e^{-\alpha^2 f^2} \), in which \( U_c = 8|\varepsilon_0| \) is the Brinkmann-Rice critical value for the Mott transition in the absence of phonons. Eq. (4) coincides with the result for the Hubbard model once \( U/U_c \) is replaced by \( \tilde{u} \) (cfr. Eq. (8) of Ref. 23). This finding is easily interpreted in terms of renormalized interaction \( U_{eff} = U + 2(f^2 - 2f)\alpha^2\omega_0 \) and renormalized kinetic energy \( \varepsilon_{eff} = \varepsilon e^{-\alpha^2 f^2} \), showing that the value of the parameter \( f \) determines to what extent the electronic properties are affected by phonons. Furthermore, being Eq. (5) a transcendental equation, it can be useful to separate the exponential from the algebraic dependence on \( f \), obtaining:

\[
f = \left[ \frac{2(1 - \alpha\delta^2)}{\gamma(1 - \delta^2)} \frac{x^2(2x^2 - x^4 - \delta^2)}{x^4 + \delta^2(1 - 2x^2)} e^{-\alpha^2 f^2} \right]^{-1}
\]

This form, as we shall see in the next Section, is more suitable for a graphical analysis.

III. RESULTS

We are now in the position to discuss the effect of e-ph interaction on the correlation-driven Mott transition at \( \delta = 0 \). The transition occurs for \( \tilde{u} = 1 \), which implies \( x^2 = 0 \). In the small \( \gamma \) adiabatic regime if we plug this condition into Eq. (5), we find \( f = \gamma/4\tilde{u} \), while \( f = 1 \) is recovered for large \( \gamma \). Therefore, while in the adiabatic limit the e-ph coupling strongly reduces both the Coulomb repulsion and the kinetic term, in the adiabatic regime, the small value of \( f \) makes the effect of e-ph smaller on both quantities. In this regime the exponential factor is closer to one, since the phonons are less effective in reducing the electron mobility, and, noticeably, \( (U/\varepsilon_0)_{eff} = (U/\varepsilon_0)(1 - \frac{\gamma\alpha^2\omega_0}{U}) \), in remarkable quantitative agreement with DMFT results. For small \( \gamma \) the line marking the Mott transition in the \( \lambda-U \) diagram is then given by \( \lambda = (16/\gamma)(U/U_c - 1) \), and reproduces accurately previous diagrams obtained by DMFT. The increase of the critical \( U \) as a function of e-ph interaction results from the two renormalizations of \( U_{eff} \) and \( \varepsilon_{eff} \). Because both effects are essential to get the agreement with the DMFT result at \( \delta = 0 \), we expect them to be important also at finite \( \delta \).

Let us now move away from half-filling, and consider the large \( U \) limit. Here we expect \( x^2 = |\delta|/\zeta \) (being \( x^2 = 0 \) at half-filling for \( u \equiv U/U_c > 1 \)). Expanding (5) to second order in \( \delta \) we obtain \( \zeta = \sqrt{1 - 1/\tilde{u}} \) that again coincides with the expression for the Hubbard model, with renormalized parameters depending on \( f \). The value of \( f \) at small doping is then found by solving the self-consistent equation (derived from Eq. (5))

\[
f = \frac{1}{1 + B_2 e^{-\frac{\gamma f^2}{2}}}
\]

with \( B = 2\tilde{u}/(2\tilde{u} - 1) \). In the limit \( \tilde{u} \gg 1 \) (which is equivalent to \( u \gg 1 \) if \( \lambda \) is not too large) the prefactor \( B \) goes to 1, thus simplifying the analysis of Eq. (5).

![FIG. 1: Evolution with \( \lambda \) of the numerical solution of the mean-field equations for \( u = 4 \) and various values of \( \gamma \).](image-url)
small $f$, so that $h(f)$ crosses $f$ in three points, while for larger $\gamma$ only one intersection survives as the inflection point moves toward large $f$. $\gamma$ clearly plays a role similar to the temperature, with a critical value $\gamma_c$ which separates the two regimes. The critical point $(f_c, \gamma_c, \lambda_c)$ may be evaluated analytically by imposing $f_c = h(f_c; \lambda_c, \gamma_c)$, and $0 = \frac{d}{df} h(f_c; \lambda_c, \gamma_c)$, which in the limit $B=1$ give the critical values $f_c = \frac{4}{\gamma}$, $\gamma_c = 4e^{-\frac{f}{\lambda}} \simeq 0.8925$, and $\lambda_c = \frac{d}{df} \gamma_c \simeq 3.0123$. When three solutions exist, we find two locally stable solutions $f_-$ and $f_+$ associated to weaker and stronger effective e-ph interaction. The two solutions correspond to negative and positive magnetization in the ferromagnetic terminology. Notice that the variational nature of our treatment of phonon degrees of freedom implies that only the lowest energy state is a valid result of our approach, even if the equations allow for more solutions. The parameter $\lambda$ (or more precisely the deviation from $\lambda_c$) acts as a magnetic field in determining the existence of the two potential solutions and which one is the ground state. For small (large) $\lambda$ only $f_-(f_+)$ exists, and the energies of the two solutions cross in a first order line $\lambda_c(\gamma)$, ending in a critical point. To summarize, in the anti-adiabatic limit (large “temperature”) regime, we have a single solution smoothly evolving with the “magnetic field” $\lambda$. When $\lambda$ is large, lowering the “temperature” going from the anti-adiabatic to the adiabatic regime does not imply a dramatic change in the value of $f$. On the other hand for small $\lambda$ $f$ changes from $f \approx 1$ to $f \approx \gamma$ moving from large to small $\gamma$.

The above “Curie-Weiss” scenario is recovered also for finite yet large $u = 4$, by solving numerically the mean-field equations. In Fig.1 we plot $f$ as a function of $\lambda$ for selected value of $\gamma$. As in the $u \gg 1$ limit, the evolution from weak to strong coupling is smooth for $\gamma > \gamma_c \simeq 0.9$, while for $\gamma < \gamma_c$ the two solutions with small and large $f$ coexist. Again for large $\lambda$ $f \approx 1$ for any value of the adiabaticity parameter, while for small values of the e-ph coupling $f \propto \gamma$ in the adiabatic regime and is $f \approx 1 - 1/\gamma$ when $\gamma \gg 1$. In Fig.2 we report the first-order transition line between weak-coupling and strong-coupling solution, as well as the lines $\lambda_{c1}$ and $\lambda_{c2}$ marking the existence of the two solutions $f_+$ and $f_-$. For large $\gamma$ the line of first-order transitions ends in a second-order end-point, where also $\lambda_{c1}$ and $\lambda_{c2}$ collapse. The main effect of a finite $u$ compared to the infinite $u$ limit is to move the critical point to slightly larger values of $f, \gamma$ and $\lambda$. The strong-coupling solutions always show a full renormalization of $U$, while the kinetic energy is strongly suppressed moving from large to small values of $\gamma$. On the other hand, the weak-coupling solutions are characterized by a smooth renormalization of the correlation term that goes from its bare value in the adiabatic limit to the fully renormalized value $U - 2a^2U_0$ as $\gamma \to \infty$; however the renormalized kinetic energy $\varepsilon_{ef}$, dominated by the exponential term $\exp(-\lambda f^2/\gamma)$, is always $\simeq 1$.

The phase diagram in Fig. 2 is not changed much as function of doping. This result may be understood in the following way. The phase transition line is obtained by comparing the values of the energies for the solution for $f_-$ and $f_+$. As it can be inferred from Eq. (4), both the kinetic energy and the polaron energy differ by a quantity of order $\delta$ in the two solutions, so that the critical values of $\lambda$ depend on doping through subleading corrections in $\delta$ which are quite small at $u = 4$. The physics underlying the phase diagram of Fig.2 is that by increasing $\lambda$ a small number $\delta$ of localized holes strongly coupled to phonons have a lower energy ($\sim -\delta \lambda |\varepsilon_0|$, i.e., the energy of $\delta$ polaronic holes) than a bad metal that has a reduced kinetic energy, again of order $\delta (\varepsilon_{eff} \sim -\delta |\varepsilon_0|)$ due to the large effective mass ($m^* \sim 1/\delta$).

We now consider the fate of the two solutions $f_-$ and $f_+$ as we approach the Mott transition by letting both $\delta \to 0$ and $U \to U_c$. In the adiabatic regime the mean field equations can be solved analytically and the polaron solution only establishes at $\lambda_{pol} = 4(U/U_c)(1 - \sqrt{1 - U_c/U})$. At $U \approx U_c$ this gives $\lambda_{pol} = 4$, which is reduced to 2 in the large $U$ limit. We can translate these values of the dimensionless coupling in terms of the dimensional phonon-mediated attraction at the zero-frequency, $V_{ph} = 2\lambda |\varepsilon_0|$. We obtain $V^{pol}_{ph} = 8|\varepsilon_0| = U_c$ close to the Mott transition and $V^{ph}_{pol} = 4|\varepsilon_0| = U_{c}/2$ in the large-$U$ limit. We therefore find that, for $U$ close to $U_c$, the weak-coupling solution $f_-$ is always the stable one even for quite large e-ph coupling up to $V_{ph} \approx U$, thus showing that the Mott transition is robust with respect to e-ph interaction and polaron formation. Through the stabilization of the $f_-$ solution the strong correlations close to the Mott transition also protect the quasiparticles from a strong mass renormalization due to phonon effects. Considering the fluctuations around the mean-field solution one recovers the high-energy Hub-
We expect that phonon effects will contribute significantly to them. As it is well known, the mean-field treatment may be incorrect in reproducing the order of a phase transition, and in this sense the polaronic transition discussed above may be turned to a crossover when fluctuations are included, as it happens in DMFT. On the other hand, the comparison with the DMFT results shows that the mean-field description captures the basic qualitative features of how the polaron formation is affected by the presence of the e-e interaction.

We gain further information on the way the system evolves when the Mott insulator is approached by considering the compressibility \(\kappa = \partial n / \partial \mu\), or equivalently the Landau parameter \(F_0^S\), related to \(\kappa\) by the relation \(\kappa = 2N^*/[1 + F_0^S]\), where \(N^*\) is the quasiparticle density of states per spin at the Fermi level. To leading order in \(\delta\) we obtain

\[
\frac{F_0^S}{N_0/2\delta} \approx 4|\varepsilon_0| \frac{-2u - 1}{\sqrt{u(u - 1)}} - 16|\varepsilon_0|\alpha^2 f(1 - f) \frac{\sqrt{u(u - 1)}}{2u - 1}
\]

where \(N_0\) is the free DOS (per spin) at the Fermi level. The second term in Eq. \(10\) represents the phononic contribution to the Landau parameter dressed by the e-e interaction. The first term describes the electronic contribution to \(F_0^S\) dressed by the e-ph correlation; once more we find the same expression of the Hubbard model with phonon-renormalized parameters\textsuperscript{22}. The attractive phononic contribution to \(F_0^S\) increases the compressibility, and could eventually lead to a phase separation\textsuperscript{13,22}. This term is indeed only effective for the weak coupling \(f\) solutions. However the compressibility of \(f\) solutions diverges only for values of the parameters \(\lambda, \gamma\) for which the \(f\) solution is energetically favored. This finding is closely reminiscent of the DMFT analysis of Ref. \textsuperscript{13}, where the insulating behavior is favored by the e-ph interaction, but the divergence of the compressibility in the metal is prevented by the stabilization of the insulator. To verify the accuracy of our approach, we compare our compressibility \(10\) to the predictions of large-N expansion\textsuperscript{26} and DMFT\textsuperscript{12}. To compare with Ref. \textsuperscript{13}, we take the large-\(U\) and small-\(\gamma\) limit; then \(10\) acquires a simple random-phase approximation form

\[
\kappa(\lambda) = 2N^*(0)/[1 + (F_0^S)_e + (F_0^S)_{ph}],
\]

where \(N^*(0) = N_0/2\delta\) is the density of states per spin in the large-\(U\) limit in the absence of e-ph interaction and the phononic contribution to the symmetric Landau amplitude is simply given by \(F_0^S)_{ph} = -4N^*(0)\alpha^2 \omega_0\), in excellent agreement with \textsuperscript{10}. Relaxing the large-\(U\) limit we obtain

\[
\frac{\kappa(\lambda)}{\kappa(0)} = \frac{1}{1 - 2\alpha^2 \omega_0 \beta \kappa(0)}
\]
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