Stability of correlated electronic systems under the influence of the electron-phonon interaction

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Abstract

We have used an exact diagonalization technique to study the stability of the $t-J$-Holstein and Hubbard-Holstein models under the influence of the electron-phonon interaction. Previous results have been obtained using frozen-phonon technique or introducing only a few dynamical phonon modes due to the large Hilbert space. To check these results we have done exact diagonalization in a small cluster (four sites) including all the phonon modes allowed by symmetry. We compare our results with those obtained by using the adiabatic approximation.
I. INTRODUCTION

Strong correlation and electron-phonon interaction are two important features of High Tc (HTC) Superconductors. This situation motivates the study of electron-phonon (e-ph) interaction in strongly correlated electronic systems. One important question is how stable the system is in the presence of the e-ph interaction. If the system has a robust stability, it is possible to use BCS-like theories, but if the system has a tendency to instability, polaronic and bipolaronic theories play an important role.

Many analytical and numerical works have been done to answer this question. Most of the numerical works use the frozen-phonon (adiabatic) approximation and neglect dynamical effects.

In a previous paper we studied the role of dynamical phonons in the $t - J$ model with clusters of 10 and 16 sites including the phonon Hilbert space. We found an instability to a charge density wave (CDW) for moderate e-ph interactions. However, due to the large size of the Hilbert space, only a few phonon modes were included in the calculation. In this case the sensibility of our results with respect to the number of phonon modes is a matter of debate.

In order to check the validity of the truncation of the Hilbert space in the number of phonon modes, we consider, as in other works, a small cluster (four sites) including all the phonon modes allowed by symmetry. In section II we present models, approximations and results; while in section III we discuss the main conclusions of this study.

II. MODELS AND RESULTS

The Hamiltonian of the $t - J$-Holstein ($t - J$-H) model is:

$$H = -t \sum_{i,j,\sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + H.c.) + J \sum_{i,j} (S_i S_j - n_i n_j/4) +$$

$$\sum_i (\frac{P_i^2}{2M} + K/2u_i^2 - \alpha u_i n_i)$$  (1)
where the first two terms correspond to the usual $t - J$ model, $t$ is the hopping term and $J$ is the antiferromagnetic exchange interaction. $\tilde{c}$ and $\tilde{c}^\dagger$ are the creation and destruction operators of a hole in a simple occupied Hilbert space, respectively. The following two terms are the kinetic and elastic energy of ions with mass $M$, and elastic force constant $K$. Finally, the last term is the Holstein-type interaction between electrons and ions with strain $\alpha$. In this interaction the movement of the internal molecular degrees of freedom ($u$) affect the electron density at a given site. This kind of interaction is important in HTC superconductors\(^8\). For the case of cuprates, this internal degree of freedom simulates the breathing mode, where the oxygens of the unit cell move toward the Cu ion\(^9\). Hereafter, we are going to study the dynamics of one hole in a 4-sites cluster.

### a) Adiabatic phonon calculation

In this approximation the kinetic energy of the ions is negligible with respect to the other terms in the Hamiltonian. This approximation is exact when the mass of the ions are infinite.

We have a quantum problem with a classical variable $u$. We minimize, iteratively, the adiabatic potential $E_e[\{u\}]$ starting from an initial displacement configuration $\{u\}$. In each step of the iteration, we evaluate the ground state of the electronic system and the site electron density $< n_i >$. Using $< n_i >$ and the relation $u_i^{\text{new}} = -\frac{\alpha}{K} < n_i >$, a new displacement set is obtained; if it falls within a predetermined threshold from the initial, we stop the calculation, otherwise we iterate the procedure.

We define the dimensionless electron-phonon constant $\lambda = \frac{\alpha^2}{Kt}$. With this definition and rescaling $\alpha u_i \rightarrow u_i$ all the results can be written in terms of $\lambda$ for a given set of electronic parameters $t$ and $J$. We choose $t$ as unit of energy.

We show in Fig.1 the equilibrium displacement of a given site as a function of $\lambda$, for different values of $J$. In order to describe our results we choose the most representative site displacement. We can distinguish two different regimes: $0.0 < J < J_N$ and $J > J_N$, where $J_N = 0.28$ for our cluster\(^{12}\).

For $J$ smaller than $J_N$ the electronic model has a ferromagnetic ground state (Nagaoka
regime). The hole moves as a free spinless fermion. Therefore, like in the Holstein model, we expect a transition towards a localized state at a critical value of $\lambda(\lambda_c)$. It is possible to see in Fig.1 that the transition occurs for $\lambda \sim 2.2$ and this value is practically independent of $J$. For $\lambda < 2.2$ the system presents a homogeneous phase, while for $\lambda > 2.2$ an abrupt transition towards a localized state occurs. In this state the hole is principally located in a given site and the equilibrium displacement associated with this site is larger than the other ones. In the figure we show the biggest displacement $u_i$. There is also an increase of the hole occupation in this site, which shows the localization of the hole. This phase was previously interpreted as a ”polaronic” state of the system. We call this state ”polaronic” even, at this stage of the calculation, the adiabatic condition is not broken down and a true polaron formation implies a mixing between the electronic and phononic degrees of freedom.

For $J > J_N$ the transition towards a localized phase occurs at smaller $\lambda$, due to the preexisting self-localization of the hole in the antiferromagnetic background and the resulting band narrowing. We can also see that the transition is smoother, and before going to a ”polaronic” state the system undergoes a breathing type of deformation. This kind of phase is due to the nontrivial momentum value of the ground state of the system for $\lambda = 0.0$.

b) Full dynamics phonon calculation

In the momentum space for the phononic degrees of freedom, the Hamiltonian (1) is:

$$H = -t \sum_{i,j,\sigma}(\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + H.c.) + J \sum_{i,j}(S_i S_j - n_i n_j/4) + \sum_q ((\omega(a_q^\dagger a_q + 1/2) + gn_i(a_q^\dagger + a_{-q})))$$

At this stage the Hamiltonian operates over the Hilbert space of fermionic and bosonic variables. Since the bosonic levels could be infinitely populated, we must adopt some criteria to render finite the dimension of our Hilbert space. In the calculation we include all the phonon modes (the zero mode is excluded because it represents only a change in the total energy). We populate each mode with the minimum number of states for which we converge the observable under consideration. We find that 15-phonon states for each mode is enough,
at least for not very large electron-phonon interaction.

For small frequencies and for $J < J_N$ the system has an abrupt transition characterized by a rapid increases of the phonon occupation number $< n_{ph} >$ for each mode. Fig. 2a shows the occupation number of the phonon $(\pi, \pi) \ n_{\pi,\pi}$ as a function of $\lambda$ for different values of $J$ and for $\omega = 0.1$. When $J > J_N$ the transition is smoother and it takes place at small $\lambda$ values. One important difference with the adiabatic case is that here the transition depends on $\lambda$ even for $0 < J < J_N$. We have seen that the static phonon calculation always gives rise to a localization for $\lambda > \lambda_c$. The localization is not obvious in the dynamical calculation, but the behaviour of the phonon occupation as a function of $\lambda$ and the close agreement between $\lambda_c$ obtained with both methods suggest that for $\omega = 0.1$ the instability is similar to that observed in the static case. We think that the adiabatic calculation is still valid for small values of $\omega$.

For small $\lambda$ the phonon occupation is rather small indicating that the system is formed by renormalized electron and phonons.

When the frequency increases the system is more stable as it is shown in Fig.2b for $\omega = 1.0$. The transition towards a polaronic state is less evident than that for smaller $\omega$. We conclude that the hole moves, as in a pure $t - J$ model, but with a bigger effective mass.

It is important to point out that the static calculation underestimates the critical value of $\lambda$, which in our calculation seems to be large. Thus the polaron occurs only for large $\lambda$ and small $\omega$ values.

We finish the section showing some results on the Hubbard-Holstein (HH) model. It is well known that the Hubbard model could be mapped on the $t - J$ model with $J = 4t^2/U$ for $U/t \gg 1$. Moreover, for $U = 0$ the HH model has become the usual Holstein model. Therefore, for the HH model, it is interesting to study the crossover from the small polaron of the uncorrelated electron-phonon system to the one in the $t - J$ Holstein model.

The Hamiltonian of the HH model is:
\[
H = -t \sum_{i,j,\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma}^\dagger + H.c.) + U \sum_{i} n_i n_j + \\
\sum_{i} \left( \frac{P_{i}^2}{2M} + K/2u_{i}^2 - \alpha u_i n_i \right)
\]  

(3)

Similarly to the \(t-J-H\) case we are going to study the HH model using static and dynamic phonon approximations. The notation in the Hamiltonian is standard. Note that we are studying the one hole doped system (3 electrons in our cluster). This is different from the one particle problem previously studied by different authors.\[3\[4\]

In Fig. 3 we show the adiabatic calculation of a site deformation (the biggest deformed one) as a function of \(\lambda\) for different values of \(U\) (the analogue of Fig. 1 for the \(t-J-H\) model). In Fig. 4 we show the occupation of the \((\pi, \pi)\) mode (dynamic calculation).

For a very large \(U\) \((U > U_c\), where \(U_c\) is of order of 40) the model behaves like the \(t-J-H\) model. That means: we obtain an abrupt transition from a totally delocalized state to a full localized state. This transition occurs for \(\lambda \sim 2\). This is exactly what happens for the \(t-J-H\) model for \(J < J_N\). When \(U\) decreases \(\lambda_c\) also decreases and the transition is less abrupt. We found, like for the \(t-J\) model case, that before going to the polaron state the system has the breathing-type state for \(U < U_c\). Note the following different behaviour between the \(t-J-H\) and HH model: in the former \(\lambda_c\) always decreases as \(J\) increases showing the strong self-localization of the hole in the antiferromagnetic background. In the HH model case \(\lambda_c\) goes to a finite value when \(U\) goes to zero, this is precisely the threshold for the appearance of the polaronic band in the pure Holstein model.

For small \(\omega\) and large \(U\) the average of the phonon occupation presents an abrupt transition at a given value of \(\lambda\) which is close to the \(\lambda_c\) obtained using adiabatic approximation. Moreover, for small \(U\) and large \(\omega\) the transition is smoother and occurs at smaller \(\lambda\). Therefore, stability of the system is reinforced when both \(\omega\) and \(U\) increase.
III. DISCUSSIONS AND CONCLUSIONS

In this paper we have studied the stability of correlated electronic systems under the influence of a Holstein electron-phonon interaction. Both $t - J$ and Hubbard models have been analyzed using adiabatic and dynamical phonon approximations.

The important features found in the adiabatic calculation on the $t - J$-H model are:

- Polaronic instability for the electron-phonon couplings $\lambda > \lambda_c$.
- The critical value of the electron-phonon interaction decreases as $J$ increases. This is a consequence of the preexisting self-localization for the pure $t - J$ model case.
- The critical electron-phonon coupling is $J$-independent in the Nagaoka regime ($0.0 < J < J_N$).
- In the Nagoka regime the transition towards a polaron is rather abrupt while it is smoother when $J > J_N$.

Treating the phonon dynamically we found that most of the results obtained adiabatically are still valid for finite but small $\omega$ values. A difference is that the value of $\lambda_c$ obtained in the dynamical case is not independent of $J$ for the $0.0 < J < J_N$ regime.

Increasing $\omega$, the transition towards the polaron state is less evident and the system behaves like a liquid formed by renormalized electrons and phonons.

It is important to point out that the adiabatic calculation underestimates the stability of the system. The system is more stable when $J$ decreases and $\omega$ increases.

We have also performed a calculation for the Hubbard model. In this model most of conclusions made for the $t - J$ model were recovered for large $U$. For small $U$ the stability of the system tends to that of the pure Holstein model and the critical $\lambda$ goes to a finite value when $U$ goes to zero.

When this paper has been finished we received a preprint of Wellein, Roeder and Fehske where the Holstein Hubbard and $t - J$ Holstein models were studied on finite cluster up to
ten sites by an exact diagonalization technique. The main results of this paper are consistent with the ones obtained here. Moreover, for one hole doped $t-J$ model they found evidence for the appeareance of a polaronic state from a critical value of electron-phonon coupling. As this value is similar to the one obtained in our paper, we believe that finite size effect are not very important. We thank Dr. Fehske for sending us a copy of his paper prior its publication.

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REFERENCES

1 A.B. Alexandrov and J. Ranninger, Phys. Rev.B 23,1796 (1981); 24,1164 (1981).

2 V.V. Kabanov and O. Yu. Mashtakov; Phys Rev B 47 6060 1993; U. Trapper, H.Fehske, M. Deeg and H. Buttner; Z.Phys B 93,465 (1994).

3 H. Roder, et al; Phys. Rev.B 47,12420 (1993).

4 A. Dobry, A. Greco, J. Lorenzana and J. Riera; Phys. Rev.B 49,505 (1994).

5 J. Zhong and H. Schuttler; Phys. Rev.Lett 69 ,1600 (1992).

6 R. T. Scalettar,N.E.Bickers and D.J.Scalapino Phys. Rev. B 40 197 (1989); R. M. Noack, D.J. Scalapino and R.T. Scalettar;Phys. Rev. Lett. 66 778 (1991).

7 A. Dobry, A. Greco, S. Koval and J. Riera; Phys. Rev.B,in press (1995).

8 D.Poilblanc, D.J. Scalapino and W. Hanke; preprint (1995).

9 A. Alexandrov, V. Kabanov and D. Ray; Phys. Rev.B 49 ,9915 (1994).

10 R. Zeyher; Z.Physik B80,187 (1990).

11 L. Pintschovius et al, in Physical Properties of High Temperature Superconductors IV, ed D.M. Ginsberg, World Scientific (1994).

12 E. Dagotto,et al; Phys. Rev.B 40 ,6721(1989).

13 G.Wellein, H.Röder and H.Fehske; preprint
Figure Captions:

**Figure 1**: Displacement of one of the ions (the one who’s shift from the equilibrium position is maximum) obtained with the iterative method described in the text for the $t-J$ Holstein model.

**Figure 2**: Occupation of the phonon of $k = (\pi, \pi)$ as a function of $\lambda$, in the full quantum calculation including 15 state for each phonon mode. a) $\omega = 0.1$; b) $\omega = 1$.

**Figure 3**: The same as fig. 1 but for the Hubbard-Holstein model

**Figure 4**: The same as fig. 2 but for the Hubbard-Holstein model
(a) $\omega=0.1$

\[ n_{\pi,\pi} \]

\[ \lambda \]

(b) $\omega=1.$

\[ n_{\pi,\pi} \]

\[ \lambda \]