Suppression of superconductivity in the Hubbard model by buckling and breathing phonons

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Abstract

We study the effect of buckling and breathing phonons, relevant for cuprate superconductors, on the d-wave superconductivity in the two-dimensional Hubbard model by employing dynamical cluster Monte Carlo calculations. The interplay of electronic correlations and the electron–phonon interaction produces two competing effects: an enhancement of the effective d-wave pairing interaction, which favors d-wave superconductivity, and a strong renormalization of the single-particle propagator, which suppresses superconductivity. In the region of the parameter space relevant for cuprate superconductors, we find that the buckling and the breathing phonons suppress the superconductivity.

(Some figures may appear in colour only in the online journal)

1. Introduction

While it is widely accepted that electronic correlations play a fundamental role in the mechanism of high temperature superconductivity of cuprates, the role of electron–phonon (EP) interaction is under hot debate. Nevertheless, many experiments, including Raman [1], neutron scattering [2–4] and photoemission [5, 6] find clear evidence of electron–phonon (EP) interaction in high \(T_c\) materials.

In the recent years a large theoretical effort was undertaken by numerous authors to study the role of phonons in cuprates. The photoemission features were addressed by investigating the spectral properties of one hole in a \(t-J\) model with optical phonons [7–9]. The interplay between electronic correlations and electron–phonon coupling was found [10–15] to affect significantly both the electron and the phonon propagators indicating enhanced polaron formation and phonon softening in the underdoped regime. Dynamical cluster approximation (DCA) calculations [16, 17] show noticeable isotope effect in many properties such as superconducting \(T_c\), pseudogap, antiferromagnetic and charge susceptibilities.

The phonons believed to be the most relevant to the cuprates are the buckling (BC) and the breathing (BR) modes [1–5, 18–21], defined, respectively, by the out-of-plane and in-plane displacement of the oxygen ions. Previous investigations suggest that the symmetry of these phonon modes is significant. There are arguments suggesting that coupling to the out-of-plane oxygen BC or the local Holstein (H) phonons, enhance the d-wave pairing interaction [22–26], whereas, the BR mode has been found to suppress the interaction [23–25]. It also was shown that the electronic correlations in the presence of EP coupling strongly enhance polaron formation [10–12] and renormalize the quasiparticle (QP) weight, an effect which suppresses superconductivity.

In this paper we employ the dynamical cluster approximation [27, 28] to study two models relevant for cuprates, the Hubbard model with BC and BR phonons. We also extend the work on superconductivity in the Hubbard–Holstein model [12]. DCA has proved to be one of the few techniques able to capture the superconducting
properties of strongly correlated systems [28]. We investigate the role of phonons on superconductivity in the region of small and intermediate doping where the antiferromagnetic (AF) correlations are strong. In agreement with previous investigations, we find enhancement of the d-wave pairing interaction by H [12, 22] and BC [23–26] phonons. Moreover we find an enhancement of the d-wave pairing interaction even for BR phonons contrary to some predictions [23–25]. However, despite the enhancement of the d-wave pairing, we find a suppression of the superconducting $T_c$ for all three modes, due to the strong renormalization of the electronic single-particle propagator.

2. Formalism

The Hamiltonian for each model, Hubbard–Holstein (HH), Hubbard-buckling (HBC) and Hubbard-breathing (HBR), can be written as

$$H = H_U + H_{ph} + H_{ep}$$

(1)

where

$$H_U = -t \sum_{\langle ij \sigma \tau \rho \rho' \sigma' \tau' \sigma'' \tau'' \sigma'''} (-c_{i \sigma}^\dagger c_{j \sigma'}^\dagger e_{\rho \rho'}^{\sigma \sigma'} + c_{j \sigma'}^\dagger c_{i \sigma'}^\dagger) + U \sum_i n_{i \uparrow} n_{i \downarrow},$$

(2)

is the Hubbard part with nearest-neighbor hopping $t$ and on-site repulsion $U$. For H phonons, described as a set of independent oscillators at every site $i$ which couple locally to the electronic density,

$$H_{ph}^H + H_{ep}^H = \sum_i \frac{p_i^2}{2M} + \frac{1}{2} M \omega_0^2 u_i^2 + g \mu_i u_i,$$

(3)

where $\{u_i, p_i\}$ are canonical conjugate coordinates for each oscillator with characteristic frequency $\omega_0$. The BC (BR) phonons are independent out-of-plane (in-plane) oscillators on each bond $i + \hat{\gamma}/2$, with $\hat{\gamma} = \hat{i}, \hat{j}$, such that

$$H_{ph}^{BC, BR} + H_{ep}^{BC, BR} = \sum_{i, \gamma} \frac{p_{i,\gamma}^2}{2M} + \frac{1}{2} M \omega_0^2 u_{i,\gamma}^2 \pm g (n_i \pm n_{i+\hat{\gamma}}) u_{i,\gamma}/2$$

(4)

where the last term of equation (4) with plus (minus) describes the coupling to the BC (BR) phonons. The dimensionless EP coupling, defined as the ratio of the single-electron lattice deformation energy to half of the electronic bandwidth $W/2 = 4t$, is $\lambda^H = 2g^2/(2M\omega_0^2W)$ and $\lambda^{BC, BR} = 4 \times 2g^2/(2M\omega_0^2W)$, with an extra factor of four in $\lambda^{BC, BR}$ due to local coordination. Note that in general the coupling to the BC mode implies both modulation of orbital energy and hopping integrals [21]. However, due to the technical difficulties associated with off diagonal EP coupling, we consider here only the former effect as was done previously in [23, 24].

To study the Hamiltonian (1) we employ the DCA, a cluster mean-field theory which for a two-dimensional system maps the original lattice model onto a periodic cluster of size $N_c = L_c^2$ embedded in a self-consistent host. Correlations up to a range $L_c$ are treated explicitly, while those at longer length scales are described at the mean-field level. With increasing cluster size, the DCA systematically interpolates between the single-site dynamical mean-field result and the exact result, while remaining in the thermodynamic limit. Cluster mean-field calculations on the simple Hubbard model successfully reproduce many of the features of thecuprates, including a Mott gap and strong AF correlations, d-wave superconductivity and pseudogap behavior [28].

We solve the cluster problem using a quantum Monte Carlo (QMC) algorithm [31] modified to perform the sum over both the discrete field used to decouple the Hubbard repulsion, as well as the phonon field $u$. The space of configurations of the latter field is significantly larger than the former. In part, this is offset by the strong correlations of the phonon field in Matsubara time. Therefore, in the QMC Markov process, correlated changes, in which adjacent phonon fields in time are moved together, are mixed in with local moves to reduce the autocorrelation time. Nevertheless, the present code including the effect of phonons requires significantly more CPU time than required for the Hubbard model. Thus, most of the present calculations are restricted to clusters of size $N_c = 4$. Nevertheless we check the robustness of our conclusions by employing calculations on larger clusters of size $N_c = 16$.

3. Results

In a previous paper, addressing the HH model [12], we show that the synergistic interplay of AF correlations and the EP interaction strongly enhances both polaron formation and antiferromagnetism. Since the effective EP coupling is inversely proportional to the kinetic energy of the holes, the AF correlations, which reduce the mobility of the holes, enhance the effective EP coupling. On the other hand, since at finite doping the antiferromagnetism is suppressed by the hole motion, the decrease in hole mobility due to EP coupling increases the antiferromagnetism. Considering the BC and the BR phonons we find a similar behavior indicative of enhanced polaron formation. In figure 1(a) we show that the AF susceptibility at 5% doping is strongly enhanced by coupling with any of the three phonon modes. The EP coupling also reduces the Matsubara QP weight, $Z_0(T) = 1/(1 - \text{Im} \Sigma(K, i\pi T) / \pi T)$ (figure 1(b) for momentum $K = (0, \pi)$), and increases the kinetic energy (figure 1(c))\footnote{\footnote{This definition of $\lambda$, common in polaron studies and used also in [29] for cuprates, does not always coincide with the Migdal–Eliashberg definition [30].}}. For all three models the local moment, $\mu^2 = \langle (n_{i \uparrow} - n_{i \downarrow})^2 \rangle$, at low temperature has a large value, close to that corresponding to the $\lambda = 0$ case (figure 1(d)), due to reduction of the effective hole hopping. However, aside from the similarities between the three models, there are also significant differences. We find that for the HBC model the same value of EP coupling produce much stronger effects than the HH and HBR models. For example at 5% doping a value of $\lambda^{BC} = 0.3$
However, an increase of the interaction which favors d-wave coupling with BC or H phonons is considered \cite{22, 23}. 

The phonon contribution to the d-wave pairing interaction when $T$ for HH, HBC and HBR models at 5\% doping. All three modes show enhanced polaron formation at low $T$.

Figure 1. (a) AF susceptibility $\chi_{AF}$. (b) Matsubara QP fraction $Z_0 = 1/(1 - \text{Im} \Sigma(K, \pi T)/\pi T)$ at $K = (0, \pi)$. (c) kinetic energy $E_{kin} = \sum_\omega \epsilon(k)n_{\omega}$ and (d) local moment $\mu^2 = \langle (n_+ - n_-)^2 \rangle$ versus $T$ for HH, HBC and HBR models at 5\% doping. All three modes show enhanced polaron formation at low $T$.

Figure 2. $T_c$ versus $\lambda$ for HH, HBC and HBR models at (a) 5\% and (b) 15\% doping for $\omega_0 = 0.3t$, $U = 8t$ and $N_c = 4$.

Figure 3. d-wave eigenvalue of pairing matrices $M = \Gamma \chi_0$ and $M_0 = \Gamma z_{00}$ versus $T$ on $N_c = 4$ cluster for HH (a), HBC (b) and HBR (c) models at 5\% doping and HBC (d) at 15\% doping. Despite the overall reduction of $T_c$ shown by the eigenvalues of $M_0$ increase strongly with decreasing $T$, showing that EP coupling enhances the effective pairing interaction.

produces effects similar to $\lambda_c^{H, BR} = 0.5$. The temperature dependence of the local moment (figure 1(d)) as well as of other quantities such as DOS (not shown) is much stronger in the HBR model.

In figure 2 we show the dependence of superconducting $T_c$ versus EP coupling for the three models for $\omega_0 = 0.3t$ at 5\% and 15\% doping. We find $T_c$ decreases with increasing $\lambda$, weakly for small $\lambda$ and then quite abruptly for $\lambda > \lambda_c$. We find that $\lambda_c^{H, BC, BR} \approx 0.5, 0.25, 0.4$.\footnote{\lambda_c here should not be understood necessarily as the critical EP coupling which indicates the transition to the polaron regime.} Notice that the decrease of $T_c$ with $\lambda$ for HBC model is much sharper once $\lambda > \lambda_c^{H, BC}$.

Previous investigations predict an enhancement of the phonon contribution to the d-wave pairing interaction when the coupling with BC or H phonons is considered \cite{22, 23}. However, an increase of the interaction which favors d-wave pairing does not necessarily imply an increase of $T_c$, since the reduction in the charge carriers mobility associated with polaron formation has the opposite effect. We find for all three models an increase of the d-wave pairing interaction. However, in spite of this, the $T_c$ is reduced as shown in figure 2. To understand this dichotomy, we must disentangle the effects of the pairing interaction from renormalization of the single-particle propagator.

A divergent pairing susceptibility indicates the superconducting transition and hence $T_c$. At this instability the leading eigenvalue of the pairing matrix becomes 1. The pairing matrix $M = \Gamma \chi_0$ enters in the Bethe–Salpeter equation of the two-particle Green’s function,

$\chi = \chi_0 + \chi_0 \Gamma \chi = \chi_0 (1 - M)^{-1} M$ \hfill (5)

where $\chi_0 = G \ast G$ (the bubble diagram) describes propagation of the two particles without mutual interaction, a product of the fully renormalized single-particle propagators $G(k, i\omega_n) = (i\omega_n - \epsilon(k) + \mu - \Sigma(i\omega_n, k))^{-1}$. $\Gamma_{\omega_0, i\nu} = \chi_0^{-1}(K, i\omega_n, K') \Sigma_{\omega_0, i\nu}$ is the irreducible interaction vertex in the particle–particle channel and can be regarded as the effective renormalized interaction. We find that for all three models the leading eigenvector $\Phi_{\omega}(K, i\omega_n)$ of the pairing matrix $M$ has d-wave symmetry.

The phonons affect the pairing matrix by modifying both the effective interaction $\Gamma$ and the single-particle propagator $G$, or implicitly $\chi_0$. To separate these effects we compare, in figure 3, the eigenvalues of two different pairing matrices: $M$ and $M_0$. $M_0$ was defined above and we define $M_0 = \Gamma z_{00}$ with $z_{00} = G \ast G, G^0(k, i\omega_n) = (i\omega_n - \epsilon(k) + \mu + \Sigma_{\omega_0, i\nu})^{-1}$ is a single-particle propagator which does not account for the renormalization resulting from the EP interaction, i.e. $\mu$ and $\Sigma_{\omega_0, i\nu}$ are the obtained by setting $\lambda = 0$. Note that the effective interaction $\Gamma_{\omega_0}$ in $M_0$ is, however, fully renormalized by phonons.

The leading eigenvalue of $M$ increases with decreasing $T$ and reaches a value of 1 at the transition temperature $T_c$. This transition occurs at lower temperature when $\lambda$ is finite, thus indicating a reduction in $T_c$ in accordance with the phase diagram shown in figure 2. However, the d-wave eigenvalue of the matrix $M_0$ increases much faster and reaches 1 at a temperature much larger than without phonons. Since the
always reduces when larger clusters are considered. We find that EP coupling
exemplify this by showing in figures 4(c)–(e) the inverse of the d-wave pairing susceptibility \(\chi_d\) for some particular cases.

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4. Conclusions

By employing DCA with a QMC algorithm we investigate the Hubbard model with H, BC and BR phonons. We find that the interplay of EP interaction and electronic correlations in HBC and HBR models leads to synergistic enhancement of both polaron formation and AF correlations, similar to previous findings for the HH model [12]. Regarding superconductivity, all three modes produce two competing effects: a strong renormalization of the single-particle electronic propagator which suppresses superconductivity and an enhancement of the effective pairing interaction which favors d-wave superconductivity. In the region of parameter space relevant for cuprates, we find that the combination of these two effects leads to a reduction in superconducting \(T_c\).

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