Polaron and bipolaron formation in the Hubbard-Holstein model: Role of next-nearest-neighbor electron hopping

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The influence of next-nearest-neighbor electron hopping t' on the polaron and bipolaron formation in a square Hubbard-Holstein model is investigated within a variational approach. The results for electron-phonon and electron-electron correlation functions show that a negative value of t' induces a strong anisotropy in the lattice distortions favoring the formation of nearest-neighbor intersite bipolaron. The role of t', electron-phonon and electron-electron interactions is briefly discussed in view of the formation of charged striped domains.

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I. INTRODUCTION

In recent years the experimental evidence in favor of polaronic carriers in doped cuprates and in manganese oxide perovskites has grown. In manganites a large amount of experimental results, ranging from extended x-ray-absorption fine structure (EXAFS) (Ref. 1) measurements of lattice distortions to giant isotope shift of the Curie temperature[2] and to frequency shifts of the internal phonon modes,[3] have pointed out the relevance of the Jahn-Teller polaron formation[4] beside the double and superexchange magnetic effects.[5] Also in cuprates there is strong experimental evidence supporting a relevant role of the interaction between charge carriers and lattice distortions in addition to the strong electron correlations. Optical experiments in the midinfrared frequency region,[6] atomic pair distribution function analysis of the neutron powder-diffraction data[7] and of the EXAFS signals[8] due to the Cu–O bond distances have shown polaronic effects in doped cuprates pointing out a strong response of the local structure to the charge state.

This large amount of experimental data has renewed the interest in studying problems of electrons interacting with the lattice degrees of freedom. In literature several models have been introduced to treat the electron-electron (el-el) and electron-phonon (*e*-ph) interactions in these compounds.[9,10] In this paper we will restrict our attention to one of the most simple and frequently considered models for the polaron and bipolaron formation: the Holstein-Hubbard model. The problem of a single tight binding electron coupled to an optical local phonon mode has been analyzed in several ways: Monte Carlo simulations,[11] numerical exact diagonalization of small clusters,[12] dynamical mean-field theory,[13] density-matrix renormalization group,[14] and variational approaches.[15–17] As a common result the ground-state energy and the effective mass in the Holstein model are continuous functions of the *e*-ph coupling constant and this one-body system does not have phase transition.[18] Depending on the adiabatic parameter the ground-state properties can change more or less significantly but without breaking the translational symmetry. Recently the influence of the Hubbard repulsion on bipolaron formation has been investigated[19,20] by variational and exact diagonalization methods in one and two dimensions. In the adiabatic regime the possibility of formation of intersite bipolarons has been suggested and it has been shown that their mass is significantly reduced with respect to the on-site bipolaron.

On the other hand, accurate investigations on high-temperature superconducting materials have shown that some properties of cuprates compounds, such as the shape of the Fermi surface or the band structure, can be explained introducing a next-nearest-neighbor (NNN) electron hopping term.[21] This term is essential for reproducing the experimentally observed behavior of the electron band near the *M* points of the Brillouin zone and it allows to handle the differences between electron and hole doped materials. The inclusion of NNN electron hopping is expected to affect significantly the behavior of the system. For instance, it has been shown that t' may deeply modify the properties of the $t-j$ and Hubbard models and that the renormalization of the bare parameters, t and t', can be very strong also for moderate values of the electron correlations.[22]

In this paper we investigate, within a variational approach, the influence of NNN transfer integral on the polaron and bipolaron formation in the two-dimensional Hubbard-Holstein model. In particular for the single electron we use a recently proposed variational approach[15] based on a linear superposition of Bloch states that describe large and small polaron wave functions. This approach provides a very good description of the polaron features in any regime of the parameters of the Holstein model and it does not involve a truncation of the boson Hilbert space as required by all the numerical techniques. The computational effort is very little involving few variational parameters. A variational approach is used also to study the ground-state bipolaron features. In this case we use a single wave function able to interpolate between large and small bipolaron regimes. In order to check the validity of the proposed wave function we compare our results for the one-dimensional Hubbard-Holstein model with those recently published by Bonca *et al.*,[19] which are the most accurate bipolaron available calculations. In the most interesting regime, characterized by electron and phonon energy scales not well separated, the difference between the bipolaron ground-state energy estimations of the two methods is about 0.1%: this makes us confident of the accuracy of the proposed approach. Next we apply the variational

method to the two-dimensional extended Holstein-Hubbard model.

In this paper we show that a negative value of t' induces a relevant anisotropy in the lattice displacements associated to the polaron formation. A decreasing of t', in the range of parameters of physical interest, strengthens the e-ph correlations along the (1,0) and (0,1) directions and reduces the lattice displacements along the (1,1) and (1,−1) directions. Moreover, a negative value of t' favors the mobile intersite bipolaron formation along the (1,0) and (0,1) directions and, when this does not happen, the el-el effective potential shows a strong dependence on the spatial directions. Although these results concern the case of only two electrons interacting with local phonon modes, we believe that the formation of intersite bipolaron in the (1,0) direction suggests the possibility that, at physical relevant doping in the manganites and cuprates, the *e*-ph interaction together with anisotropy can favor the formation of charged stripes. Of course, further investigation is needed to support this idea in specific materials.

The paper is organized in the following way. In Sec. II the model is introduced. In Sec. III the variational approach for a single polaron is discussed. In Sec. IV the bipolaron properties within the one-dimensional Holstein-Hubbard model are analyzed by means of a variational method and are successful compared with the best available results recently published by Bonca *et al.*[19] Successively the variational approach is extended to study the bipolaron features within the two-dimensional Hubbard-Holstein model. In Sec. V the numerical results are presented and the role of t', *e*-ph, and el-el interactions is briefly discussed in view of the formation of charged striped domains.

II. MODEL

The two-dimensional extended Hubbard-Holstein model is described by the Hamiltonian

$$H=-t\sum_{i,\delta,\sigma} c^{\dagger}_{i+\delta,\sigma}c_{i,\sigma}-t'\sum_{i,\delta',\sigma} c^{\dagger}_{i+\delta',\sigma}c_{i,\sigma}+\omega_0\sum_{\vec{q}} a^{\dagger}_{\vec{q}}a_{\vec{q}} + \frac{g\omega_0}{\sqrt{N}}\sum_{i,\sigma,\vec{q}} c^{\dagger}_{i,\sigma}c_{i,\sigma}(a_{\vec{q}}e^{i\vec{q}\cdot\vec{R}_i}+a^{\dagger}_{\vec{q}}e^{-i\vec{q}\cdot\vec{R}_i}) + U\sum_i n_{i,\uparrow}n_{i,\downarrow}. \quad (1)$$

In Eq. (1) $c^{\dagger}_i$ denotes the electron creator operator at site i, whose position vector is indicated by $\vec{R}_i$, $a^{\dagger}_{\vec{q}}$ represents the creation operator for phonon with wave number $\vec{q}$, t and t' are, respectively, the transfer integral between nearest- and next-nearest-neighbor sites $\vec{\delta}$ and $\vec{\delta}'$ indicate, respectively, the nearest- and next-nearest-neighbors, ω_0 is the frequency of the optical local phonon mode, U represents the Hubbard interaction for electrons on the same site, and M_q indicates the *e*-ph matrix element. In the Holstein model (short-range *e*-ph interaction) M_q assumes the form

$$M_q=\frac{g}{\sqrt{N}}\omega_0. \quad (2)$$

Here N is the number of lattice sites.

III. POLARON VARIATIONAL APPROACH

In previous papers,[15] we have developed a variational approach based on a linear superposition of Bloch states that represent the large and small polaron wave functions. These two wave functions are chosen as translationally invariant Bloch states, they are obtained from localized states centered on different lattice sites, just like a band state is related to atomic orbitals, and they provide a very accurate description of the two asymptotic regimes of weak and strong *e*-ph coupling:

$$|\psi^{(\alpha)}_{\vec{k}}\rangle=\frac{1}{\sqrt{N}}\sum_n e^{i\vec{k}\cdot\vec{R}_n}|\psi^{(\alpha)}_{\vec{k}}(\vec{R}_n)\rangle, \quad (3)$$

where

$$|\psi^{(\alpha)}_{\vec{k}}(\vec{R}_n)\rangle=e\sum_{\vec{q}}[f^{(\alpha)}_{\vec{q}}(\vec{k})a_{\vec{q}}e^{i\vec{q}\cdot\vec{R}_n}-\text{H.c.}]\sum_m \phi^{(\alpha)}_{\vec{k}}(\vec{R}_m)c^{\dagger}_{n+m}(|0\rangle_{el} \otimes|0\rangle_{ph}). \quad (4)$$

In Eqs. (3) and (4) the apex α indicates the large ($\alpha=l$) and small ($\alpha=s$) polaron wave function, $|0\rangle_{el}$ and $|0\rangle_{ph}$ denote the electron and boson vacuum states, and $\phi^{(\alpha)}_{\vec{k}}(\vec{R}_m)$ are variational parameters such that $\Sigma_m|\phi^{(\alpha)}_{\vec{k}}(\vec{R}_m)|^2=1$. These two wave functions are characterized by different phonon distribution functions:

$$f^{(l)}_{\vec{q}}(\vec{k})=\frac{g\omega_0/\sqrt{N}}{\omega_0+E_b(\vec{k}+\vec{q})-E_b(\vec{k})} \quad (5)$$

and

$$f^{(s)}_{\vec{q}}(\vec{k})=\frac{g}{\sqrt{N}}\sum_i e^{i\vec{q}\cdot\vec{R}_i}|\phi^{(s)}_{\vec{k}}(\vec{R}_i)|^2. \quad (6)$$

Here $E_b(\vec{q})$ is the free-electron band energy and the variational parameters $\phi^{(\alpha)}_{\vec{k}}(\vec{R}_m)$ take into account the broadening of the electron wave function. In this paper we restrict the sum in Eq. (4) to fifth neighbors. It is evident that the large polaron wave function takes into account the average effect of the correlation introduced by the electron recoil [Eq. (5)] effect absent in the small polaron phonon distribution function.

We have shown[15] that these wave functions, far away from the two asymptotic regimes, are not orthogonal and the off-diagonal matrix elements of the Holstein Hamiltonian are not zero. This suggests that the lowest state of the system is made of a mixture of the large and small polaron solutions and so justifies the idea to use a variational method to determine the ground-state energy by considering as trial state a linear superposition of the wave functions describing the two

types of previously discussed polarons. At $t'=0$ the comparison of the numerical results with the data of the density-matrix renormalization-group[14] and global local variational[16] methods has shown the great accuracy of the proposed approach.

IV. BIPOLARON VARIATIONAL APPROACH

A. One-dimensional case

Regarding the bipolaron, the most general wave function of two electrons in a periodic potential interacting with the longitudinal optical phonons and with each other through the Coulomb force can be written as

$$|\psi_{\vec{k}}\rangle=\frac{1}{N}\sum_{n_1,n_2} e^{i\vec{k}\cdot[(\vec{R}_{n_1}+\vec{R}_{n_2})/2]}]|\psi_{\vec{k}}(\vec{R}_{n_1},\vec{R}_{n_2})\rangle. \qquad (7)$$

$|\psi_{\vec{k}}\rangle$ is a state that is multiplied by the factor $e^{i\vec{k}\cdot\vec{R}_m}$ under a lattice vector $\vec{R}_m$ translation and $\vec{k}$ is the Bloch state wave number. Equation (4), i.e., the polaron wave-function component describing the charge carrier distributed around the site $\vec{R}_n$, is the key ingredient to build the bipolaron wave-function component $|\psi_{\vec{k}}(\vec{R}_{n_1},\vec{R}_{n_2})\rangle$. Fixed the relative distance between the centers of the two electrons $(\vec{R}_{n_1}-\vec{R}_{n_2})$, we adopt a trial wave function for the singlet state that is proportional to the product of two polaron wave functions centered on $\vec{R}_{n_1}$ and $\vec{R}_{n_2}$ sites:

$$\begin{aligned}|\psi_{\vec{k}}(\vec{R}_{n_1},\vec{R}_{n_2})\rangle=\gamma_{\vec{k}}(\vec{R}_{n_1}-\vec{R}_{n_2})e\sum_{\vec{q}}\{h_{\vec{q}}(\vec{k},\vec{R}_{n_1}&\\ -\vec{R}_{n_2})a_{\vec{q}}[e^{i\vec{q}\cdot\vec{R}_{n_1}}+e^{i\vec{q}\cdot\vec{R}_{n_2}}]&\\ -\mathrm{H.c.}\}\sum_{m_1}\phi_{\vec{k}}(\vec{R}_{m_1},\vec{R}_{n_1}&\\ -\vec{R}_{n_2})c^{\dagger}_{n_1+m_1,\uparrow}\sum_{m_2}\phi_{\vec{k}}(\vec{R}_{m_2},\vec{R}_{n_1}&\\ -\vec{R}_{n_2})c^{\dagger}_{n_2+m_2,\downarrow}(|0\rangle_{el}\otimes|0\rangle_{ph})&\end{aligned}$$

where ϕ, γ, and h are variational functions. In particular, $\gamma_{\vec{k}}(\vec{R}_{n_1}-\vec{R}_{n_2})$ gives the weight of the bipolaron wave-function component with the centers of the two charge carriers at distance $|\vec{R}_{n_1}-\vec{R}_{n_2}|$. For the phonon distribution function h we assume the following form:

$$h_{\vec{q}}(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})=\frac{g\omega_0 d(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})/\sqrt{N}}{\omega_0+h_1(\vec{k})[E_b(t,\vec{k}+\vec{q})-E_b(t,\vec{k})]},$$

that is able to interpolate between the asymptotic expressions of large ($h_1=d=1$) and small ($h_1=0$ and $d=1$) polaron. Here $E_b(t,\vec{q})=-2t\cos(q_x a)$ is the free-electron band energy, a is the lattice constant, and $d(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})$ and $h_1(\vec{k})$ are variational functions. We note that we have not used a linear superposition of polaron wave functions to build the bipolaron wave function, but, following Toyozawa,[23] a single wave function able to interpolate between the two asymptotic regimes, as shown by Romero *et al.*[16] This approach allows us to reduce the number of variational parameters, it requires, to be implemented, a very little computational effort and it provides a very good description of the bipolaron ground-state properties as will be shown in the following.

The coefficient ϕ has been chosen such that it takes into account the broadening of the electron wave function to third neighbors. Therefore, for any fixed relative distance between the centers of the two charge carriers, we introduce three independent variational parameters:

$$\phi_{\vec{k}}(\vec{R}_m,\vec{R}_{n_1}-\vec{R}_{n_2})=\begin{cases}\alpha(|\vec{R}_{n_1}-\vec{R}_{n_2}|) & \text{if } |\vec{R}_m|=0\\ \beta(|\vec{R}_{n_1}-\vec{R}_{n_2}|) & \text{if } |\vec{R}_m|=a\\ \gamma(|\vec{R}_{n_1}-\vec{R}_{n_2}|) & \text{if } |\vec{R}_m|=2a\\ \delta(|\vec{R}_{n_1}-\vec{R}_{n_2}|) & \text{if } |\vec{R}_m|=3a\\ 0 & \text{otherwise}\end{cases}$$

with $\alpha^2+2(\beta^2+\gamma^2+\delta^2)=1$. In this paper, to simplify the numerical calculations, we have chosen α, β, γ, δ independent on $|\vec{R}_{n_1}-\vec{R}_{n_2}|$ for $|\vec{R}_{n_1}-\vec{R}_{n_2}|\geqslant 3a$. Likewise the function $d(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})$ assumes the following form:

$$d(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})=\begin{cases}d_0(\vec{k}) & \text{if } |\vec{R}_{n_1}-\vec{R}_{n_2}|=0\\ d_1(\vec{k}) & \text{if } |\vec{R}_{n_1}-\vec{R}_{n_2}|=a\\ d_2(\vec{k}) & \text{if } |\vec{R}_{n_1}-\vec{R}_{n_2}|=2a\\ d_3(\vec{k}) & \text{otherwise,}\end{cases}$$

where $d_0(\vec{k})$, $d_1(\vec{k})$, $d_2(\vec{k})$ and $d_3(\vec{k})$ are variational parameters. Finally we choose the following form for the function $\gamma_{\vec{k}}(\vec{R}_{n_1}-\vec{R}_{n_2})$:

$$\gamma_{\vec{k}}(\vec{R}_{n_1}-\vec{R}_{n_2})=\begin{cases}\gamma_0(\vec{k}) & \text{if } |\vec{R}_{n_1}-\vec{R}_{n_2}|=0\\ \gamma_1(\vec{k}) & \text{if } |\vec{R}_{n_1}-\vec{R}_{n_2}|=a\\ \gamma_2(\vec{k}) & \text{if } |\vec{R}_{n_1}-\vec{R}_{n_2}|=2a\\ \gamma_3(\vec{k})e^{-\gamma_4(\vec{k})|\vec{R}_{n_1}-\vec{R}_{n_2}|} & \text{otherwise,}\end{cases}$$

where $\gamma_0(\vec{k})$, $\gamma_1(\vec{k})$, $\gamma_2(\vec{k})$, and $\gamma_3(\vec{k})$ are variational parameters. The minimization of the quantity $\langle\psi_{\vec{k}}|H|\psi_{\vec{k}}\rangle/\langle\psi_{\vec{k}}|\psi_{\vec{k}}\rangle$ has been performed by making use of a routine based on a standard Newton algorithm.

In Fig. 1 we plot the energy difference between the two-particle ground state and twice the one-particle ground state as a function of the Hubbard repulsion U at $t=\omega_0$ and $g=1$. The comparison with the numerical results recently published by Bonca *et al.*[19] shows the accuracy of the proposed variational approach. For example, the present method's estimate of the bipolaron ground-state energy for $g=1$, $t=\omega_0$, and $U=0$ in the thermodynamic limit is $E_0=$

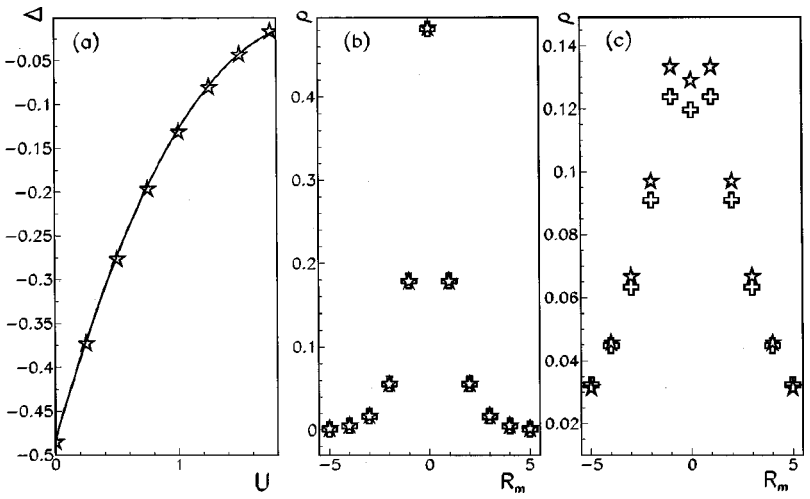

FIG. 1. (a) The bipolaron binding energy is plotted as function of U for a one-dimensional lattice of 36 sites with periodic boundary conditions. The values of the parameters are $t=\omega_0$ and $g=1$. The stars indicate the data kindly provided by J. Bonca; (b) and (c): the electron-electron correlation function is plotted at $g=1$ and $t=\omega_0$ for two different values of U: $U=0$ in (b) and $U=1.5$ in (c). The energies are given in units of ω_0. The stars represent the data kindly provided by J. Bonca.

-5.4185 that is in excellent agreement with the Bonca's result: $E_0=-5.4246$, the difference being about 0.1%. In Figs. 1(b) and 1(c) the electron-electron correlation function $\rho(\vec{R}_m)=\langle\psi_{\vec{k}=0}|\Sigma_i n_{i,\uparrow}n_{i+m,\downarrow}|\psi_{\vec{k}=0}\rangle/\langle\psi_{\vec{k}=0}|\psi_{\vec{k}=0}\rangle$ is plotted for two different values of U at $t=\omega_0$ and $g=1$. The results are compared with the data reported by Bonca *et al.*[19] The comparison shows that the used wave function provides not only an excellent estimation of the ground-state energy but gives a high accurate description of the bipolaron ground-state properties. In the next subsection we extend the proposed approach to the two-dimensional case.

B. Two-dimensional case

Here we extend the variational approach to explore the bipolaron features for electrons interacting with longitudinal optical phonons and with each other in a two-dimensional lattice. As in the one-dimensional case, we adopt a trial wave function for the singlet state which is a boson coherent state multiplied by the product of linear superpositions of Wannier wave functions:

$$|\psi_{\vec{k}}(\vec{R}_{n_1},\vec{R}_{n_2})\rangle=\gamma_{\vec{k}}(\vec{R}_{n_1}-\vec{R}_{n_2})e^{\sum_{\vec{q}}\{h_{\vec{q}}(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})a_{\vec{q}}^{\dagger}[e^{i\vec{q}\cdot\vec{R}_{n_1}}+e^{i\vec{q}\cdot\vec{R}_{n_2}}]-\text{H.c.}\}}\sum_{m_1}\phi_{\vec{k}}(\vec{R}_{m_1},\vec{R}_{n_1}-\vec{R}_{n_2})c_{n_1+m_1,\uparrow}^{\dagger}$$

$$\times\sum_{m_2}\chi_{\vec{k}}(\vec{R}_{m_2},\vec{R}_{n_1}-\vec{R}_{n_2})c_{n_2+m_2,\downarrow}^{\dagger}(|0\rangle_{el}\otimes|0\rangle_{ph}),$$

where ϕ, χ, γ, and h are variational functions, with $\chi_{\vec{k}}(\vec{R}_m,\vec{R}_{n_1}-\vec{R}_{n_2})=\phi_{\vec{k}}(\vec{R}_m,\vec{R}_{n_2}-\vec{R}_{n_1})$. For the phonon distribution function we assume the following form:

$$h_{\vec{q}}(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})=\frac{g\omega_0 d(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})/\sqrt{N}}{\omega_0+h_1(\vec{k})[E_b(t,\vec{k}+\vec{q})-E_b(t,\vec{k})]+h_2(\vec{k})[E_b(t',\vec{k}+\vec{q})-E_b(t',\vec{k})]}$$

that is able to interpolate between the asymptotic expressions of large ($h_1=h_2=d=1$) and small ($h_1=h_2=0$ and $d=1$) polaron. Here $E_b(t,\vec{q})=-2t[\cos(q_x a)+\cos(q_y a)]$, $E_b(t',\vec{q})=-4t'\cos(q_x a)\cos(q_y a)$ and $d(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})$, $h_1(\vec{k})$ and $h_2(\vec{k})$ are variational functions. The coefficients ϕ and χ have been chosen such that they take into account the broadening of the electron wave function to next-nearest neighbors, i.e., the sums in the expression of $|\psi_{\vec{k}}(\vec{R}_{n_1},\vec{R}_{n_2})\rangle$ are restricted to next-nearest neighbors. Furthermore ϕ and χ have the bipolaron symmetry for relative distances $|\vec{R}_{n_1}-\vec{R}_{n_2}|\leqslant 2\sqrt{2}a$ (fifth neighbors), while for $|\vec{R}_{n_1}-\vec{R}_{n_2}|>2\sqrt{2}a$ we assume, in analogous way to the one-dimensional case, the following form for ϕ:

$$\phi_{\vec{k}}(\vec{R}_m,\vec{R}_{n_1}-\vec{R}_{n_2})=\begin{cases}\alpha & \text{if } |\vec{R}_m|=0\\ \beta & \text{if } \vec{R}_m=\vec{\delta}\\ \gamma & \text{if } \vec{R}_m=\vec{\delta}'\\ 0 & \text{otherwise}\end{cases}$$

with $\alpha^2+4(\beta^2+\gamma^2)=1$ and α, β, γ independent on $(\vec{R}_{n_1}-\vec{R}_{n_2})$. The on site, nearest neighbor and next-nearest-

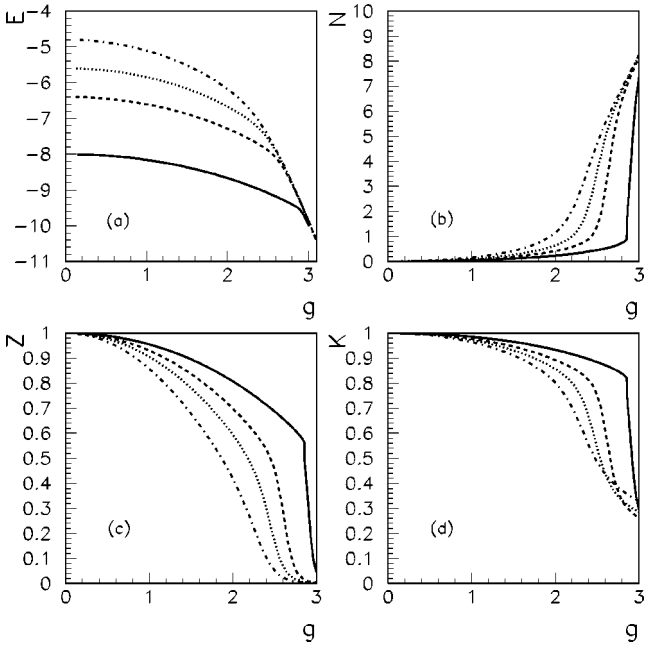

FIG. 2. The polaron ground-state energy (a), the mean phonon number (b), the spectral weight (c), and the mean value of the hopping term, in units of the bare electron kinetic energy (d), are reported, for a two-dimensional lattice in the thermodynamic limit ($N\to\infty$), at $t/\omega_0=2$ for different values of t': $t'/\omega_0=0$ (solid line), $t'/\omega_0=-0.4$ (dashed line), $t'/\omega_0=-0.6$ (dotted line), $t'/\omega_0=-0.8$ (dashed-dotted line). The energies are given in units of ω_0.

neighbor values of the functions $\gamma_{\vec{k}}(\vec{R}_{n_1}-\vec{R}_{n_2})$ and $h_{\vec{q}}(\vec{k},\vec{R}_{n_1}-\vec{R}_{n_2})$ have been determined variationally whereas for relative distances between the centers of the two charge carriers such that $|\vec{R}_{n_1}-\vec{R}_{n_2}|>\sqrt{2}a$ (next-nearest neighbors) we have used asymptotic expressions with parameters fixed by the variational approach as in the above-introduced one-dimensional case. Here we take into account the polaron and bipolaron ground state ($\vec{k}=0$).

V. RESULTS

In Fig. 2 we plot the polaron ground-state energy E, the mean phonon number N, the spectral weight Z, and the polaron kinetic energy K, in units of the bare electron kinetic energy, as a function of the e-ph coupling constant, at $t/\omega_0=2$, for different values of NNN transfer integral t'. At $t'=0$ there is a sharp transition between the large and small polaron solutions for $\lambda\simeq 1$, where $\lambda=g^2\omega_0/4t$ is the ratio between the small polaron binding energy and the energy gain of an itinerant electron on a rigid lattice. In the weak-coupling regime K is $\simeq 1$ and N is $\simeq 0$ so that the electron is slightly affected by the interaction with the phonons: its bare mass presents weak renormalization. In the opposite regime the polaron band collapses: the average number of phonons increases, the kinetic energy reduces, and asymptotically tend to the values predicted by the strong-coupling perturbation theory ($N\to g^2$, $K\to e^{-g^2}$). The ground-state spectral weight shows a sharp transition at $\lambda\simeq 1$ but it is evident the presence of a wide range of values of the e-ph coupling constant where Z is significantly smaller than the unity but not negligible: here the ground-state properties are those characteristic of an electron weakly affected by the e-ph interaction but a large part of the single-particle spectral weight lies at higher energies (intermediate polaron phase[15]). Decreasing the value of t' ($t'<0$), this intermediate regime becomes more important with respect to the small and large polaron phases: the spectral weight is equally distributed between ground and all the excited states and the polaron ground-state features are well described by a linear superposition of $|\psi_{\vec{k}}^{(l)}\rangle$ and $|\psi_{\vec{k}}^{(s)}\rangle$. In the weak-coupling regime, for a fixed value of the e-ph coupling constant, decreasing t' the mean phonon number grows, the ground-state spectral weight and the kinetic energy decrease indicating a greater polaron localization. The strong-coupling regime shows, instead, a nonmonotonous behavior as function of t' that can be explained in terms of the third order of the strong-coupling perturbation theory. In fact, at this order the small polaron binding energy is the sum of three contributions: the first term is $-g^2\omega_0$, the second and the third ones are proportional, respectively, to $-(t^2+t'^2)/g^2\omega_0$ and $-t^2t'/g^3\omega_0^2$.

The effect of NNN transfer integral on the lattice displacements associated to the polaron formation, $S(\vec{R}_m)=\langle\Sigma_i n_i(a_{i+m}+a_{i+m}^\dagger)\rangle$, is particularly interesting. A negative value of t' induces a strong anisotropy in the lattice distortions along the (1,1) and (1,0) directions as it results from Fig. 3. In the range of parameters of physical interest, for a fixed value of the e-ph interaction, $S(1,0)/S(0,0)$ and $S(1,1)/S(0,0)$ decrease in a very different way with t'. In fact, the ratio $S(1,1)/S(1,0)$ reduces in a dramatic way indicating very strong correlations between electron positions and lattice displacements along the symmetry axes of the crystal.

A similar trend is revealed by correlation functions of two interacting electrons. We have investigated the bipolaron formation in the adiabatic regime where the retardation effect of the e-ph interaction may favor the rise of more extended electron bound states and in particular the mobile intersite bipolaron formation.[19,20] Figure 4(a) shows the phase diagram for the transition from unbound polarons to bipolarons at fixed t and U. We stress that the presence of a negative NNN electron hopping extends the region of g values where the intersite mobile bipolaron formation is favored. In Fig. 4(b) the density-density correlation function $\rho(\vec{R}_m)=\langle\psi|\Sigma_i n_{i,\uparrow}n_{i+m,\downarrow}|\psi\rangle/\langle\psi|\psi\rangle$ is plotted. When the intersite bipolaron formation takes place, the probability to find the two interacting electrons along the (1,0) and (0,1) directions exceeds the 90% and the maxima of $\rho(\vec{R}_m)$ are located at $\vec{R}_m=\{(\pm 1,0),(0,\pm 1)\}$. When the bipolaron does not form, both along (1,0) and (1,1) directions $\rho(\vec{R}_m)$ does not show any structure and the typical distance between the two particles is of the order of the maximum allowed separation. In this case the behavior of the effective potential is enlightening. At the lowest order [$\phi(\vec{R}_m)=\delta_{m,0}$], $V_{eff}(\vec{R}_m)=U\delta_{m,0}+2\omega_0\Sigma_{\vec{q}}[h_{\vec{q}}^2(\vec{R}_m)-2gh_{\vec{q}}(\vec{R}_m)/\sqrt{N}](1+\cos\vec{q}\cdot\vec{R}_m)$. At t'

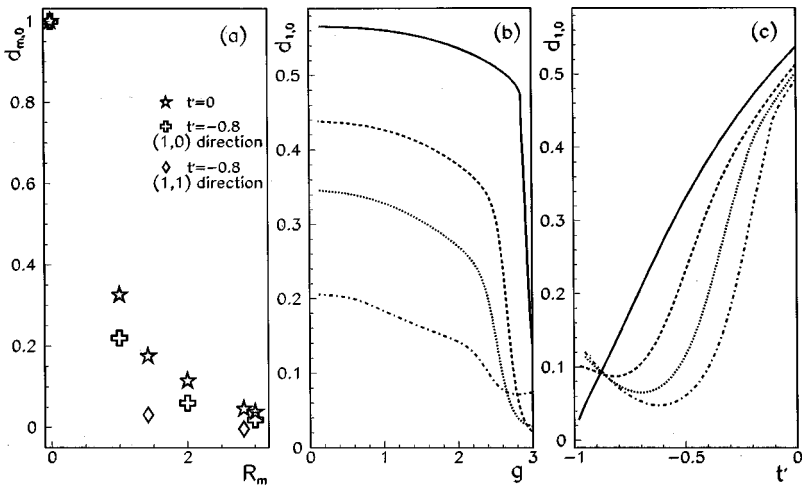

FIG. 3. (a) $d_{m,0}=S(|\vec{R}_m|)/S(|\vec{R}_m|=0)$ ($|\vec{R}_m|$ indicates the modulus of the vector $\vec{R}_m$ in units of the lattice parameter a) is reported at $t/\omega_0=2$ and $g=2$ for two different values of t'; (b) $d_{1,0}=S(1,1)/S(1,0)$ is reported at $t/\omega_0=2$ for different values of t': $t'/\omega_0=0$ (solid line), $t'/\omega_0=-0.4$ (dashed line), $t'/\omega_0=-0.6$ (dotted line), $t'/\omega_0=-0.8$ (dashed-dotted line); (c) $d_{1,0}=S(1,1)/S(1,0)$ is reported at $t/\omega_0=2$ for different values of g: $g=2$ (solid line), $g=2.5$ (dashed line), $g=2.65$ (dotted line), $g=2.75$ (dashed-dotted line). The data refer to two-dimensional lattice in the thermodynamic limit ($N\rightarrow\infty$).

$=0$, the superposition of the polarization clouds produces an isotropic attractive force between the two charge carriers; decreasing t', the effective potential is more attractive along the (1,0) direction and less attractive along (1,1) direction due to the anisotropy in the lattice distortions generated by each polaron, as it results from Fig. 4(c).

Finally we discuss the possible consequences of our results for the formation of striped charge distributions in the Hubbard-Holstein model. First of all, since t' favors the formation of NN intersite bipolaron, we expect that the NNN electron hopping may support, for realistic values of the doping, the formation of striped structures arranged along characteristic directions of the crystal. Furthermore we stress the existence of an intermediate phase where small and large polaron properties coexist. This property of the single polaron, as discussed in previous papers,[24] can support, in a many body problem, a first-order phase transition with coexistence of charged striped domains characterized by different densities and lattice deformations. The possibility of striped structures, fluctuating and short-range ordered, and the eventuality of coexistence of two types of charge carriers forming striped domains have been suggested as possible scenarios for cuprates.[25,8,26] There are also strong experimental evidences from EXAFS,[8,26] neutron scattering,[27] and x-ray scattering[28] in favor of the existence of charged striped structures. In both cases the interplay of t', el-ph, and el-el interactions may significantly affect the physics of the system. Finally we want to stress that the Hamiltonian (1) represents one of the simplest models to take into account the el-el and *e*-ph interactions and that in the case of the cuprates one needs to consider more realistic models of electron-phonon interaction, for example, models where the Cu–O hoppings are modified by the ion displacements.[10] However, the Holstein-Hubbard model is expected to provide useful informations on the physics of these systems, at least on a qualitative level, and it can be an interesting starting point for studying their characteristic features.

In conclusion, we have investigated within a variational approach the influence of next-nearest-neighbor transfer integral on the polaron and bipolaron formation in the two-dimensional Hubbard-Holstein model. It has been shown that a negative value of t' induces a relevant anisotropy in the lattice displacements associated to the polaron formation and favors the mobile intersite bipolaron presence along the (1,0) and (0,1) directions. Finally, we have discussed the relevance of these results for the formation of striped structures arranged along characteristic direction of the crystal and for the coexistence of charged domains characterized by different densities and lattice deformations.

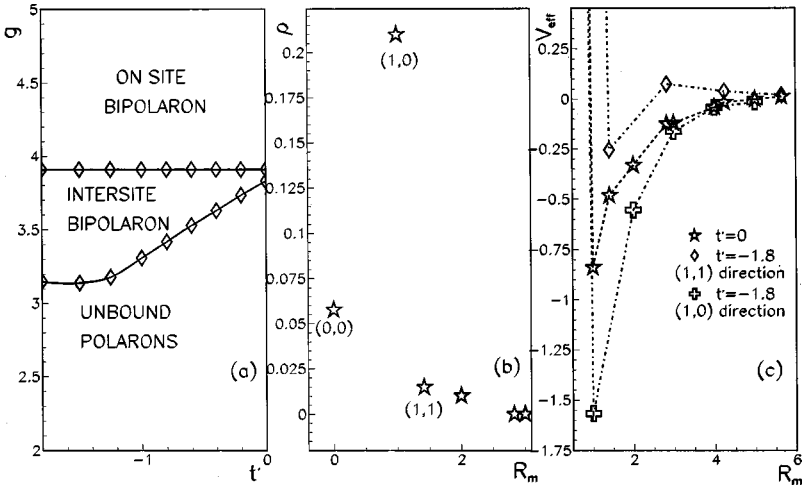

FIG. 4. (a) the phase diagram for $t/\omega_0=4$ and $U/\omega_0=30$ on a square lattice 10×10 with periodic boundary conditions; (b) the density-density correlation function $\rho(|\vec{R}_m|)$ is plotted at $t/\omega_0=4$, $U/\omega_0=30$ for $g=3.5$, and $t'/\omega_0=-1$; (c) $V_{eff}(|\vec{R}_m|)$, measured by twice the one-particle potential energy, is reported at $t/\omega_0=4$, $U/\omega_0=30$, $g=2.8$ for two different values of t'.

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