Many-polaron states in the Holstein-Hubbard model

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Abstract

A variational approach is proposed to determine some properties of the adiabatic Holstein-Hubbard model which describes the interactions between a static atomic lattice and an assembly of fermionic charge carriers. The sum of the electronic energy and the lattice elastic energy is proved to have minima with a polaron structure in a certain domain of the phase diagram. Our analytical work consists in the expansion of these energy minima from the zero electronic transfer limit which remarkably holds for a finite amplitude of the onsite Hubbard repulsion and for an unbounded lattice size.

Key words: polaron; bipolaron; Holstein; Hubbard.

I. INTRODUCTION

The Holstein model involves an electron-phonon coupling [1] which yields a polaron ground-state provided the amplitude of this coupling is large enough compared with the electronic transfer integral. This result was demonstrated by S. Aubry et al. in Ref. [2] by assuming that the lattice modes have a negligible kinetic energy. In this adiabatic regime, the description of phonons is given by the static atomic displacements. During the last decade, the so called small polaron of the adiabatic Holstein model has been of a great interest to investigate some challenging problems such as: charge density wave [3, 4] and
high critical temperature superconductivity \cite{10, 11}. These studies were based on the rigorous Aubry’s proof \cite{2} which has been improved by C. Baesens and R. S. MacKay in Ref. \cite{9}. In the anti-integrable (AI) limit where the transfer integral of the fermionic charges is zero (see \cite{10} for a revue about the anti-integrability), it is possible to find the explicit forms of the Hamiltonian eigenstates and to expand them numerically with respect to the charge transfer.

With no electron-electron interaction, excepted the Pauli principle, a many-electron problem is usually reduced to find the eigenstates of one particle Hamiltonian in which is introduced a chemical potential to fix the charge density (see \cite{2, 5} for the case of the Holstein model). The ground state is thus given by the product of the one particle eigenstates, energies of which are smaller than the Fermi level. In some cases, the interplay of the Coulombian interaction with a charge screening may yield an onsite Hubbard repulsion which breaks this method. After extending the Holstein model with the Hubbard interaction, it is yet possible to develop a variational approach where the energy functional $F_{ad}$ is issued from the bracketing of the adiabatic Holstein Hubbard Hamiltonian. Minimizing this functional with respect to the displacement fields, for a zero charge transfer $t$ shows that some energy minima are the products of onsite polaron, onsite bipolaron and vacuum site. For the weak value of $t$, the study of the first derivatives of $F_{ad}$ with respect to the atomic displacements indicates at least one energy minimum with a displacement field which is similar to a AI polaron structure. In the $L_\infty$ norm meaning, the distance between this minimum and the AI polaron state is bounded by a charge transfer function which goes to zero continuously. As a consequence, in the vicinity of the AI limit, the displacement fields
of the many-polaron minima are proved to evolve continuously with \( t \) which implies that the \( F_{ad} \) potential has some polaron-type minima in a finite domain of the phase diagram.

II. ADIABATIC HOLSTEIN HUBBARD MODEL

The Holstein Hubbard Hamiltonian is written as follows:

\[
\mathcal{H} = \sum_i \hbar \omega_0 (a_i^\dagger a_i) + gn_i (a_i^\dagger + a_i) + \nu n_i \uparrow n_i \downarrow - \nu n_i - T \sum_{(i,j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma}^\dagger \tag{2.1}
\]

where the atomic lattice is mapped on \( \mathbb{Z}^d \), i.e., \( i \in \mathbb{Z}^d \) with \( d = \{1, 2, 3\} \), the anihilation operators at site \( i \in \mathbb{Z}^d \) for both phonons and fermions are \( a_i \) and \( C_i \), respectively. The corresponding creation operators are written with a dag exponent. The \( n_i \) operator is given by \( \sum_{\sigma=(\uparrow, \downarrow)} C_{i,\sigma}^\dagger C_{i,\sigma} \) and the sum \( \sum_{(i,j)} \) is performed over the \( i \) neighboring site indexes. For simplicity, the phonon contribution is only one optical phonon branch with frequency \( \omega_0 \). The electron-phonon coupling amplitude is \( g \), the onsite Hubbard repulsion is scaled by \( \nu > 0 \) and the chemical potential is noted \( \nu \). The displacement and momentum operators at site \( (i) \) are given by:

\[
u_i = \frac{\hbar \omega_0}{4g} (a_i^\dagger + a_i) \tag{2.2}
\]

\[
p_i = i \frac{2g}{\hbar \omega_0} (a_i^\dagger - a_i) \tag{2.3}
\]

Substituting the phonon operators in Eq.(2.1) and dividing this equation by the energy parameter \( E_0 = \frac{8g^2}{\hbar \omega_0} \) give:

\[
H = \sum_i \left( \frac{1}{2} u_i^2 + (\frac{u_i}{2} - \mu) n_i + Un_i \uparrow n_i \downarrow \right) - t \sum_{(i,j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma}^\dagger + \frac{\gamma}{2} \sum_i p_i^2 \tag{2.4}
\]

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where $H$ is an adimensional Hamiltonian with the parameters:

$$
U = \frac{\nu}{E_0} \quad t = \frac{T}{E_0} \quad \gamma = \frac{1}{4} \left( \frac{\hbar \omega_0}{2g} \right)^4 \quad \mu = \frac{\nu}{E_0}
$$

(2.5)

In the adiabatic limit, the coefficient $\gamma$ is neglected which is valid at large electron-phonon coupling, i.e., the amplitude $g$ is large compared with the phonon zero point energy $\hbar \omega_0/2$.

We obtain an adiabatic Hamiltonian:

$$
H_{ad} = \sum_i \left( \frac{1}{2} u_i^2 + \frac{u_i}{2} - \mu \right) n_i + U n_{i\uparrow} n_{i\downarrow} - t \sum_{(i,j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma}
$$

(2.6)

The displacement operators $\{u_i\}$ are now scalar variables that are noted as a vector $\vec{u} \in \mathcal{S}(N)$ where $\mathcal{S}(N) = \mathbb{R}^N$ is a real space, dimension of which is equal to the unbounded number of lattice sites $N$. The adiabatic Hamiltonian is a sum of an electronic Hamiltonian $H_{el}$ and the lattice elastic energy, i.e., $H_{ad} = \sum_i \frac{1}{2} u_i^2 + H_{el}$ where

$$
H_{el} = \sum_i \left( \frac{u_i}{2} - \mu \right) n_i + U n_{i\uparrow} n_{i\downarrow} - t \sum_{(i,j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma}
$$

(2.7)

The energy is now written in the variational form:

$$
F(\vec{u}, \psi) = \sum_i \frac{1}{2} u_i^2 + <\psi|H_{el}|\psi>
$$

(2.8)

where $|\psi>$ is a normalized electronic wave function for $N_{el}$ fermion charges. It is projected on the usual fermion basis, i.e., $|\psi> = \sum_\nu \psi_\nu |e_\nu>$ where $\nu$ is a $N_{el}$-multiple site-spin index and $|e_\nu> = \Pi_{(i,\sigma)\in\nu} C_{i,\sigma}^\dagger |\emptyset>$. Differentiating Eq.(2.8) with respect to $u_i$ and $\psi_\nu$, the conditions for the local extrema are:
where $E$ is the Lagrange factor due to the $\psi$ normalization. The Shroedinger equation Eq.(2.10) implies that $\psi$ is a $H_{el}$ eigenstate with the associated eigenvalue $E$ which is the electronic energy. Assuming that $\psi$ is a $H_{el}$ ground state for a given $\vec{u}$, the total energy is now given by the functional $F_{ad}(\vec{u}) = \sum_i \frac{1}{2}u_i^2 + E(u_i)$ which depends only on the displacement variables. The $\psi$ wave function may be non-unique.

Working with the $L_\infty$ norm in the suitable space, the $F$ functional and its derivatives with respect to $u_i$ and $\psi_\nu$ are continue. The adiabatic potential $F_{ad}$ is also continue in the $S(N)$ space but its first derivatives are not necessary continue as it can be shown in the AI limit.

### III. THE ANTI-INTEGRABLE LIMIT

In the anti-integrable (AI) limit, the fermionic charge transfer is zero, and thus the whole lattice sites are decoupled. The Hamiltonian $H_{el}$ is a sum of onsite Hamiltonian $H_i$ and the $H_{el}$ ground state $\psi$ is a product of onsite eigenstate $\pi_i$ with the energy $E_i(u_i)$:

$$H_i = \left( \frac{u_i}{2} - \mu \right)n_i + Un_{i\uparrow}n_{i\downarrow} \quad \text{(3.1)}$$

$$H_i|\pi_i> = E_i(u_i)|\pi_i> \quad \text{(3.2)}$$
The constants \((\mu, U)\) fix which type of state is the \(H_i\) ground state for a given displacement \(u_i\). Selecting a set of \(N_{el}\) onsite states which have the lowest energy \(E_i\) provides an electronic ground state \(\psi\) for \(H_{el}\). The site \(i\) is occupied either by a bipolaron, i.e., 2 electrons with opposite spin or by a polaron, i.e., only 1 electron with spin up or down or else the site \(i\) is not occupied. Using Eq. 2.9, the optimum displacement field is such that \(u_i = -1\) for a bipolaron, or \(u_i = -1/2\) for a polaron or \(u_i = 0\) if the site \(i\) is unoccupied. In the case of a bipolaron onsite ground state with the optimum displacement \(u_i = -1\), the \(H_i\) eigenvalues are \((U - 2\mu - 1, -\mu - 1/2, 0)\). For a polaron, the \(H_i\) eigenvalues are \((U - 2\mu - 1/2, -\mu - 1/4, 0)\) and for a vacuum site \((U - 2\mu, -\mu, 0)\). In order to determine whether a polaron structure is a local \(F_{ad}\) minimum, it is sufficient to test the \(H_i\) ground state for the different values of the onsite displacement \(u_i \in \{-1, -1/2, 0\}\). As example, for \(\mu = -3/32\) and \(U = 3/8\), the \(H_i\) ground state is a bipolaron for \(u_i = -1\), a polaron for \(u_i = -1/2\), and it is a vacuum for \(u_i = 0\), so any displacement field consisting of an assembly of \(u_i \in \{-1, -1/2, 0\}\) is a \(F_{ad}\) minimum. On the opposite, if \(\mu = -1/8\) and \(U = 1\), the configuration which contains at least a displacement \(u_i = -1\) are not stable because the bipolaron is no longer the \(H_i\) ground state.

Let us note \(\delta_i\) the onsite spectrum gap between the ground state energy and the first excited state energy. This gap is non-zero \(\delta_i > 0\) excepted for some specific values of \((\mu, U)\). As a consequence for nearly all \((\mu, U)\) constants, the onsite ground state is not degenerate excepting the spin degeneracy which occurs for the polaron.
IV. EXPANSION OF POLARON STRUCTURES

As soon as the transfer integral $t$ is non-zero, one may guess that the AI polaron states should still be $F_{ad}$ minima, at least for a certain range of parameter. Here we propose a proof that confirms this guess. Our demonstration is based on the $F_{ad}$ gradient study in the space of the displacement configurations $S(N)$. The $F_{ad}$ gradient is given by:

$$\phi_i = u_i + \frac{\langle \psi | n_i | \psi \rangle}{2}$$ \hspace{1cm} (4.1)

Let us introduce the following operators:

$$P_{1,i} = n_{i\uparrow} n_{i\downarrow}$$
$$P_{2,i} = n_{i\uparrow} (1 - n_{i\downarrow})$$
$$P_{3,i} = n_{i\downarrow} (1 - n_{i\uparrow})$$
$$P_{4,i} = 1 - n_{i\downarrow} - n_{i\uparrow} + n_{i\uparrow} n_{i\downarrow}$$ \hspace{1cm} (4.2)

They verify $\sum_\alpha P_{\alpha,i} | \psi > = | \psi >$ for all $\psi$ state. We choose to note $P_{\alpha,i} | \psi > = x_{\alpha,i} | \psi_{\alpha,i} >$ where the state $\psi_{\alpha,i}$ is normalized and $x_{\alpha,i}$ is a real positive scalar. The gap $\delta_i$ is assumed to have a lower bound $\delta$, i.e., $\delta_i > \delta > 0$ which is valid for nearly all $(\mu, U)$ constants. Then only one $x_{\alpha,i}$ is non-zero at the AI limit and it is equal to one, the corresponding index $\alpha$ is noted $g_i$. If $g_i$ is equal to either 1 or 4 then we note $x_{g_i} = x_{\alpha=g,i}$. If $g_i$ is equal to either 2 or 3, the site $i$ is occupied by a polaron with a spin up or down. In such a case, the onsite ground state is spin-degenerate and we note $x_{g_i} = \sqrt{x_{2,i}^2 + x_{3,i}^2}$. As soon as the electronic transfer is non-zero, $x_{g_i}$ varies with $t$ and it can be proved that (see Lemma [VI]):
\[(1 - x_{g,i}^2)^{\frac{1}{2}} < \frac{2n_c n_s^2 t}{\delta - t n_c (n_s - 2)} \quad (4.3)\]

where \(n_c\) is the number of the nearest neighbors, \(n_s\) is the number of distinct \(H_i\) eigen values.

The inequality Eq. (4.3) implies the continuity of \(x_{g,i}\) with respect to \(t\) in the vicinity of the AI limit.

The potential \(F_{ad}\) is now derived with respect to \(u_i\):

\[
\phi_i = \frac{\partial F_{ad}}{\partial u_i} = u_i + \sum_{\alpha,\beta} x_{\alpha,i} x_{\beta,i} < \psi_\alpha | n_i | \psi_\beta > \quad (4.4)
\]

As \(P_{\alpha,i} P_{\beta,i} = \delta_{\alpha,\beta} P_{\alpha,i}\) where \(\delta_{\alpha,\beta}\) is the Kroeneker symbol and as \(n_i\) commutes with the \(P_{\alpha,i}\) operators:

\[
\phi_i = u_i + \frac{1}{2} \sum_{\alpha} x_{\alpha,i}^2 < \psi_\alpha | n_i | \psi_\alpha > \quad (4.5)
\]

Let note \(n_{\alpha,i} = < \psi_\alpha | n_i | \psi_\alpha >\) and let write \(u_i = u_i(0) + \rho_i\) where \(u_i(0)\) is the onsite displacement at \(t = 0\). The Eq.(4.5) is rewritten as follows

\[
\phi_i = \rho_i - \frac{n_{g,i}}{2} (1 - x_{g,i}^2) + \frac{1}{2} \sum_{\alpha \neq g_i} x_{\alpha,i}^2 n_{\alpha,i} \quad (4.6)
\]

where we used Eq. (2.9) in the AI limit to find \(u_i(0) = -\frac{n_{g,i}}{2}\). The sum in the right hand side of Eq. (1.6) is performed over the indexes \(\alpha \neq g_i\) for \(g_i = \{1, 4\}\) and over the indexes \(\alpha = \{1, 4\}\) for \(g_i = \{2, 3\}\).

The scalar product \(\vec{\rho} . \vec{\phi}\) is now detailed:

\[
\vec{\rho} . \vec{\phi} = \sum_i \rho_i^2 + \rho_i (- (1 - x_{g,i}^2) \frac{n_{g,i}}{2} + \sum_{\alpha \neq g_i} x_{\alpha,i}^2 \frac{n_{\alpha,i}}{2}) \quad (4.7)
\]
Focussing on the terms of the right hand side sum, some simple arguments give the following inequalities:

\[ \rho_i (1 - x_{g_i}^2) \frac{n_{g_i}}{2} < \sup_i (1 - x_{g_i}^2) |\rho_i| \]  
(4.8)

\[ \rho_i \sum_{\alpha \neq g_i} x_{\alpha,i}^2 \frac{n_{\alpha,i}}{2} > -\sup_i (1 - x_{g_i}^2) |\rho_i| \]  
(4.9)

So each term of the sum in the Eq. (4.7) verifies

\[ \rho_i^2 + \rho_i (1 - x_{g_i}^2) \frac{n_{g_i}}{2} + \sum_{\alpha \neq g_i} x_{\alpha,i}^2 \frac{n_{\alpha,i}}{2} > \rho_i^2 - 2|\rho_i| . \sup_i (1 - x_{g_i}^2) \]  
(4.10)

which is positive if \( |\rho_i| > 2\sup_i (1 - x_{g_i}^2) \) and with Eq. (4.3) it is equivalent to \( |\rho_i| > R_{AI} \) with writing:

\[ R_{AI} = \frac{8n_c^2n_s t^2}{(\bar{\delta} - tn_c(n_s - 1))^2} \]  
(4.11)

Defining the subset \( \mathcal{B}(R) \) such as \( \vec{u} \in \mathcal{B}(R) \) if \( |u_i(0) - u_i| < R \) for all i index, the boundary of \( \mathcal{B}(R) \) is noted \( B(R) \). For any \( \vec{u} \in B(R > R_{AI}) \), the product \( (\vec{u}(0) - \vec{u}) \cdot \vec{\phi}(\vec{u}) \) is positive and thus there is at least one displacement configuration \( \vec{u}_{\text{min}}(t) \in \mathcal{B}(R_{AI}) \) which is a local minimum of \( F_{ad} \). As a consequence, The potential \( F_{ad} \) has a minimum in the \( \vec{u}(0) \) vicinity at most at a \( R_{AI} \) distance in the \( L_\infty \) norm meaning, i.e., \( \sup_i |u_{\text{min},i}(t) - u_i(0)| < R_{AI} \).

**V. CONCLUSION**

The present proof holds for any displacement field which is a minimum of the adiabatic potential \( F_{ad} \) in the AI limit and such as the gap \( \delta \neq 0 \). For nearly all \((\mu, U)\) values,
the displacements of the polaronic minima variate continuously with respect to the fermion transfer \( t \) in the vicinity of the AI limit where \( t=0 \). So it is about the total energy of these minima because of the \( F_{\text{ad}} \) continuity with respect to the displacements. Consequently, the adiabatic potential has some minima with a many-polaron structure in a finite region of the phase diagram. Nevertheless, the absolute minimum of \( F_{\text{ad}} \), i.e., the ground state of Holstein-Hubbard model can not yet be determined for all the parameters. To that purpose, a numerical investigation might be required but no idea emerge to tackle the case of a non zero Hubbard coupling with many charge carriers, excepted to compute a meanfield as proposed in Ref. [2] or to study a model with a small electron number. The latter possibility is presented in [3,7] where the phase diagram is calculated for 2 electrons. For a two-dimensional atomic lattice, a critical point where coexist 3 different types of bipolaron was found far from any trivial limit. In this specific region, because of the bipolaron degeneracy, the bipolaron tunneling (or equivalently the inverse of the ground state effective mass) is very sensitive to the quantum fluctuations which are yielded by a non-zero \( \gamma \) (Eq. (2.5)) Ref. [8]. Around the critical point, both the bipolaron ground state mobility and its binding energy reach 100\( K \) with realistic input parameters (Eq. (2.3)). This result allowed some conjectures about the mechanism which yields the high critical temperature superconductivity of cuprates.

The present study can be extended straightforwardly for a non harmonic phonon potential as for an atomic lattice embedded in an external magnetic field. However an extension to a different electron-phonon coupling such as the SSH model [11] might have non trivial anti-integrable limit which makes our arguments much less efficient.
VI. LEMMA

We choose the $H_i$ ground state energy as the energy reference. We shall assume the non-degeneracy of this ground state so only one projector $P_{g,i}$ is such as $H_i P_{g,i} |\psi\rangle = 0$ for all $\psi$. As $|\psi\rangle = \sum_\alpha P_{\alpha,i} |\psi_{\alpha,i}\rangle$ where is introduced the normalized states $\psi_{\alpha,i}$ and $x_{\alpha,i} |\psi_{\alpha,i}\rangle = P_{\alpha,i} |\psi\rangle$ which implies $\sum_\alpha |x_{\alpha,i}|^2 = 1$. It is possible to choose the $\psi_{\alpha,i}$ such as the $x_{\alpha,i}$ are real positive for all $\alpha$. One notes $K_i = \sum_\alpha P_{\alpha,i} H_{el} P_{\alpha,i}$ and $\overline{H}_i = H_{el} - H_i + t \sum_{i:j,\sigma} C_{i,\sigma}^+ C_{j,\sigma} + C_{j,\sigma}^+ C_{i,\sigma}$ where $(i : j)$ are the $i$ neighboring sites. As $P_{\alpha,i} [C_{i,\sigma}^+ C_{j,\sigma} + C_{j,\sigma}^+ C_{i,\sigma}] P_{\alpha,i} = 0$ and as $\overline{H}_i$ and $H_i$ commute with the projectors $P_{\alpha,i}$:

$$K_i = H_{el} + H_i$$ (6.1)

Let $\Phi_0$ be the $K_i$ ground state with energy $E_0$. Using $P_{\alpha,i} P_{\beta,i} = \delta_{\alpha,\beta} P_{\alpha,i}$ where $\delta_{\alpha,\beta}$ is the Kroeneker symbol, then $K_i P_{\alpha,i} |\Phi_0\rangle = P_{\alpha,i} K_i |\Phi_0\rangle = E_0 P_{\alpha,i} |\Phi_0\rangle$.

As $H_{el}$ and $H_i$ are decoupled, the state $\phi_0$ is a product of the $H_{el}$ ground state and the $H_i$ ground state. It follows that $P_{g,i} |\Phi_0\rangle = |\Phi_0\rangle$ and $P_{\alpha \neq g,i} |\Phi_0\rangle = 0$ and it is now easy to establish that

$$<\Phi_0 | H_{el} | \Phi_0 > = E_0$$ (6.2)

$$<\Phi_0 | H_i | \Phi_0 > = <\Phi_0 | K_i | \Phi_0 > = E_0$$ (6.3)

$$<\psi_{g,i} | K_i | \psi_{g,i} > \geq E_0$$ (6.4)

From the identity $P_{\alpha,i}^2 = P_{\alpha,i}$, one deduces that for all $\psi$, $|\psi_{\alpha,i}\rangle = P_{\alpha,i} |\psi\rangle$, $P_{\alpha,i} |\psi_{\alpha,i}\rangle = |\psi_{\alpha,i}\rangle$ and $<\psi_{\alpha,i} | K_i | \psi_{\alpha,i} > = <\psi_{\alpha,i} | H_{el} | \psi_{\alpha,i} >$. If $\delta_i$ is the first excited state energy of $H_i$:

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\[ < \psi_{\alpha \neq g_i} | H_i | \psi_{\alpha \neq g_i} > \geq \delta_i \]  
(6.5)

\[ < \psi_{\alpha \neq g_i} | K_i | \psi_{\alpha \neq g_i} > = < \psi_{\alpha \neq g_i} | H_i | \psi_{\alpha \neq g_i} > + < \psi_{\alpha \neq g_i} | H_i | \psi_{\alpha \neq g_i} > \]  
(6.6)

\[ < \psi_{\alpha \neq g_i} | K_i | \psi_{\alpha \neq g_i} > \geq < \psi_{\alpha \neq g_i} | H_i | \psi_{\alpha \neq g_i} > + \delta_i \geq E_0 + \delta_i \]  
(6.7)

The previous results Eq. (6.7) is necessary valid if \( \psi \) is the \( H_{el} \) ground state:

\[ < \psi_{\alpha \neq g_i} | K_i | \psi_{\alpha \neq g_i} > \geq E_0 + \delta_i \]  
(6.8)

Multiplying \( H_{el} \) by the identity (\( \sum P_{\alpha,i} = Id \)) gives:

\[ H_{el} = K_i + \sum_{\alpha \neq \alpha'} P_{\alpha,i} H_{el} P_{\alpha',i} \]  
(6.9)

and bracketing by \( \psi \):

\[ < \psi | H_{el} | \psi > = \sum_{\alpha} x_{\alpha,i}^2 < \psi_{\alpha,i} | H_{el} | \psi_{\alpha,i} > + \sum_{\alpha \neq \beta} x_{\alpha,i} x_{\beta,i} < \psi_{\alpha,i} | H_{el} | \psi_{\beta,i} > \]  
(6.10)

As \( n_{i,\sigma} \) and \( n_{j,\sigma'} \) commute with each other for all suffix \( i, j \), \( \sigma \) and \( \sigma' \), and as \( P_{\alpha,i} P_{\beta \neq \alpha,i} = 0 \):

\[ \sum_{\alpha \neq \beta} x_{\alpha,i} x_{\beta,i} < \psi_{\alpha,i} | H_{el} | \psi_{\beta,i} > = -t \sum_{\alpha \neq \beta} x_{\alpha,i} x_{\beta,i} < \psi_{\alpha,i} | \Delta | \psi_{\beta,i} > \]  
(6.11)

One deduces a simplification of the Eq. (6.10):

\[ < \psi | H_{el} | \psi > = \sum_{\alpha} x_{\alpha,i}^2 < \psi_{\alpha,i} | K_i | \psi_{\alpha,i} > - t \sum_{\alpha \neq \beta} x_{\alpha,i} x_{\beta,i} < \psi_{\alpha,i} | \Delta | \psi_{\beta,i} > \]  
(6.12)

and combining the inequalities (6.4, 6.8):

\[ < \psi | H_{el} | \psi > \geq E_0 + \delta_i \sum_{\alpha \neq g_i} x_{\alpha,i}^2 - t \sum_{\alpha \neq \beta} x_{\alpha,i} x_{\beta,i} < \psi_{\alpha,i} | \Delta | \psi_{\beta,i} > \]  
(6.13)
As we choose to map the atomic lattice on $\mathbb{Z}^d$, the number of first neighboring sites is $n_c = 2d$. With Eq. (6.3), one now writes the set of following equations where $E = \langle \psi | H_{el} | \psi \rangle$:

$$
\langle \Phi_0 | H_{el} | \Phi_0 \rangle \geq E
$$

$$
E_0 \geq E \rightarrow E_0 \geq E_0 + \delta_i \sum_{\alpha \neq g_i} x_{\alpha,i}^2 - t \sum_{\alpha \neq \beta} x_{\alpha,i}x_{\alpha,i} < \psi_{\alpha,i} | \Delta | \psi_{\beta,i} >
$$

$$
\langle \psi_{\alpha,i} | \Delta | \psi_{\beta,i} > = \langle \psi_{\alpha,i} | \sum_{i, j, \sigma} C_+^{i, \sigma} C_j^{i, \sigma} + C_+^{i, \sigma} C_j^{i, \sigma} | \psi_{\beta,i} \rangle \leq 2n_c
$$

$$
\begin{align*}
\delta_i \sum_{\alpha \neq g_i} x_{\alpha,i}^2 & \leq t \sum_{\alpha \neq \beta} x_{\alpha,i}x_{\alpha,i} < \psi_{\alpha,i} | \Delta | \psi_{\beta,i} > \\
\delta_i (1 - x_{g_i}^2) & \leq 2n_c t \sum_{\alpha \neq \beta} x_{\alpha,i}x_{\beta,i} \\
(1 - x_{g_i}^2) \delta_i & \leq n_c t [(\sum_{\alpha} x_{\alpha,i})^2 - 1] \\
(1 - x_{g_i}^2) \delta_i & \leq n_c t [(\sum_{\alpha} x_{\alpha,i} + x_{g_i})^2 - 1] 
\end{align*}
$$

(6.14)

The Cauchy-Schwartz inequality applied to the sum $\sum_{\alpha \neq g} x_{\alpha,i}$ gives:

$$
\begin{align*}
\sum_{\alpha \neq g} x_{\alpha,i} & \leq \sqrt{\sum_{\alpha \neq g_i} 1} \sqrt{\sum_{\alpha \neq g_i} x_{\alpha,i}^2} \\
\sum_{\alpha \neq g_i} x_{\alpha,i} & \leq \sqrt{n_s} \sqrt{1 - x_{g_i}^2}
\end{align*}
$$

where $n_s = 3$ is the maximum number of distinct $H_i$ eigenvalues. With Eq. (6.14), it follows that

$$
(1 - x_{g_i}^2) \delta_i \leq n_c t [(n_s^2 (1 - x_{g_i}^2) + x_{g_i})^2 - 1]
$$

(6.15)
and it is now easy to obtain:

\[ (1 - x_{g,i}^2)^{\frac{1}{2}} < \frac{2n_c \frac{1}{2} t}{\delta_i - n_c t (n_s - 1)} \] (6.16)

The latest result holds for the case of a non-degenerate \( H_i \) ground state. Regarding the case of a polaron at site i, the atomic orbital is occupied by 1 electron with either spin up or spin down. The onsite ground state is spin-degenerate but the same arguments as for the non-degenerate case can be used to establish the following inequality:

\[ (1 - x_{2,i}^2 - x_{3,i}^2)^{\frac{1}{2}} < \frac{2n_c (n_s - 1)^{\frac{1}{2}} t}{\delta_i - n_c t (n_s - 2)} \] (6.17)

Let write \( x_{g,i}^2 = x_{2,i}^2 + x_{3,i}^2 \) such as this inequality is now written:

\[ (1 - x_{g,i}^2)^{\frac{1}{2}} < \frac{2n_c (n_s - 1)^{\frac{1}{2}} t}{\delta_i - n_c t (n_s - 2)} \] (6.18)

If we now assum that there is a lower bound \( \delta \) for the onsite gap \( \delta_i > \delta > 0 \), then the combination of the Eqs. (6.16, 6.18) gives for all site i :

\[ (1 - x_{g,i}^2)^{\frac{1}{2}} < \frac{2n_c \frac{1}{2} t}{\delta - n_c t (n_s - 2)} \] (6.19)
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