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# Many-Polaron States in the Holstein–Hubbard Model

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A variational approach is proposed to study some properties of the adiabatic Holstein–Hubbard model which describes an assembly of fermionic charges interacting with a static atomic lattice. The sum of the electronic energy and the lattice elastic energy is proved to have minima with a many-polaron structure in a certain domain of model parameters. Our analytical work consists in expanding 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.

## 1. INTRODUCTION

The Holstein model involves an electron-phonon coupling in ref. 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[3–5] and high critical temperature superconductivity[6–8]. These studies were based on the rigorous Aubry's proof[2] which has been improved by C. Baesens and R. S. MacKay in ref. 9. In the anti-integrable (AI) limit where the transfer integral of the fermionic charges is zero (see in ref. 10 for a revue about the anti-integrability), the explicit forms

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of some Hamiltonian eigenstates can be found and they are continuously expanded with respect to the charge transfer. The main point of this approach is the strong electron-phonon coupling assumption. In the opposite limit of a weak coupling, the well-known BCS[11] and Gutzwiller[12] ansatzs have been successfully developed in different models for a large class of problem.

With no electron-electron interaction, except the Pauli principle, a many-electron problem is usually reduced to find the eigenstates of a one-particle Hamiltonian in which is introduced a chemical potential to fix the charge carrier density (see refs. 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 materials, the interplay of the electron-electron Coulombian repulsion with the charge screening may yield the onsite Hubbard coupling which breaks the one-particle method. For our purposes, after extending the Holstein model with the Hubbard interaction, it is yet possible to prove that some results of refs. 2, 9 are still valid. To that aim, we develop a variational approach where the energy functional $F_{ad}$ is obtained from the bracketing of the adiabatic Holstein Hubbard Hamiltonian. For a weak charge transfer t, minimizing this functional with respect to the static displacement fields shows that some energy minima have a many-polaron structure. With the $L_\infty$ norm, the atomic displacements of the many-polaron minima are proved to be continuous with respect to the transfer t in the vicinity of the AI limit. As a consequence, the $F_{ad}$ potential has some polaron minima in a finite domain of the model parameters.

## 2. ADIABATIC HOLSTEIN HUBBARD MODEL

The Holstein Hubbard Hamiltonian is written as follows:

$$\mathcal{H} = \sum_i \hbar\omega_0 (a_i^\dagger a_i) + g n_i (a_i^\dagger + a_i) + \upsilon n_{i,\uparrow} n_{i,\downarrow} - \lambda n_i - T \sum_{(i:j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma} \qquad (2.1)$$

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 † 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 $\upsilon > 0$ and the chemical potential is noted $\lambda$. 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:

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

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

$$U = \frac{\upsilon}{E_0} \qquad t = \frac{T}{E_0} \qquad \gamma = \frac{1}{4}\left(\frac{\hbar\omega_0}{2g}\right)^4 \qquad \mu = \frac{\lambda}{E_0} \tag{2.5}$$

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:

$$H_{ad} = \sum_i \left(\frac{1}{2}u_i^2 + \left(\frac{u_i}{2} - \mu\right) n_i + U n_{i\uparrow} n_{i\downarrow}\right) - t \sum_{(i:j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma} \tag{2.6}$$

The displacement operators $\{u_i\}$ are now scalar variables that are noted as a vector $\vec{u} \in \mathscr{S}(N)$ where $\mathscr{S}(N) = \mathscr{R}^N$ 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

$$H_{el} = \sum_i \left(\frac{u_i}{2} - \mu\right) n_i + U n_{i\uparrow} n_{i\downarrow} - t \sum_{(i:j),\sigma} C_{i,\sigma}^\dagger C_{j,\sigma} \tag{2.7}$$

The energy is now written in the variational form:

$$F(\vec{u}, \psi) = \sum_i \tfrac{1}{2}u_i^2 + \langle\psi|\, H_{el}\, |\psi\rangle \tag{2.8}$$

where $|\psi\rangle$ is a normalized electronic wave function for $N_{el}$ fermion charges. It is projected on the usual fermion basis, i.e., $|\psi\rangle = \sum_\nu \psi_\nu\, |e_\nu\rangle$ where $\nu$ is

a $N_{el}$-multiple site-spin index and $|e_\nu\rangle = \Pi_{(i,\sigma_i)\in\nu} C^\dagger_{i,\sigma_i} |\varnothing\rangle$. Differentiating Eq. (2.8) with respect to $u_i$ and $\psi_\nu$, the conditions for the local extrema are:

$$u_i = -\frac{\langle\psi| n_i |\psi\rangle}{2} \tag{2.9}$$

$$H_{el} |\psi\rangle = E |\psi\rangle \tag{2.10}$$

where $E$ is the Lagrange factor due to the $\psi$ normalization. The Schroedinger 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 continuous. The adiabatic potential $F_{ad}$ is also continuous in the $\mathscr{S}(N)$ space but its first derivatives are not necessary continuous as it can be shown in the AI limit.

## 3. 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 $E_i(u_i)$:

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

$$H_i |\pi_i\rangle = E_i(u_i) |\pi_i\rangle \tag{3.2}$$

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 $u_i \in \{-1, -1/2, 0\}$. For 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 denote $\delta_i$ the onsite spectrum gap between the ground state energy and the first excited state energy. This gap is non-zero $\delta_i > 0$ except 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.

## 4. 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 $\mathscr{S}(\mathrm{N})$. The $F_{ad}$ gradient is given by:

$$\phi_i = u_i + \frac{\langle \psi |\, n_i \,| \psi \rangle}{2} \tag{4.1}$$

Let us introduce the following operators:

$$\begin{aligned} P_{1,i} &= n_{i\uparrow} n_{i\downarrow} \\ P_{2,i} &= n_{i\uparrow} (1 - n_{i\downarrow}) \\ P_{3,i} &= n_{i\downarrow} (1 - n_{i\uparrow}) \\ P_{4,i} &= 1 - n_{i\downarrow} - n_{i\uparrow} + n_{i\uparrow} n_{i\downarrow} \end{aligned} \tag{4.2}$$

They verify $\sum_\alpha P_{\alpha,i} |\psi\rangle = |\psi\rangle$ for all $\psi$ state. We choose to write $P_{\alpha,i} |\psi\rangle = x_{\alpha,i} |\psi_{\alpha,i}\rangle$ 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 $x_{g_i} = x_{\alpha = g_i, i}$. 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, $x_{g_i}$ variates with t and it can be proved that (see Lemma 6):

$$(1 - x_{g_i}^2)^{\frac{1}{2}} < \frac{2 n_c n_s^{\frac{1}{2}} t}{\delta - t n_c (n_s - 2)} \tag{4.3}$$

where $n_c$ is the number of the nearest neighbors, $n_s$ is the number of distinct $H_i$ eigenvalues. 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 $u_i$:

$$\phi_i = \frac{\partial F_{ad}}{\partial u_i} = u_i + \sum_{\alpha, \beta} x_{\alpha, i} \cdot x_{\beta, i} \cdot \langle \psi_{\alpha, i} | \frac{n_i}{2} | \psi_{\beta, i} \rangle \tag{4.4}$$

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:

$$\phi_i = u_i + \tfrac{1}{2} \sum_{\alpha} x_{\alpha, i}^2 \langle \psi_{\alpha, i} | \, n_i \, | \psi_{\alpha, i} \rangle \tag{4.5}$$

Let denote $n_{\alpha, i} = \langle \psi_{\alpha, i} | \, n_i \, | \psi_{\alpha, i} \rangle$ 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

$$\phi_i = \rho_i - \frac{n_{g_i}}{2} (1 - x_{g_i}^2) + \frac{1}{2} \sum_{\alpha \neq g_i} x_{\alpha, i}^2 n_{\alpha, i} \tag{4.6}$$

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. (4.6) 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 $\vec{\rho} \cdot \vec{\phi}$ is now detailed:

$$\vec{\rho} \cdot \vec{\phi} = \sum_i \rho_i^2 + \rho_i \cdot \left( -(1 - x_{g_i}^2) \frac{n_{g_i}}{2} + \sum_{\alpha \neq g_i} x_{\alpha, i}^2 \frac{n_{\alpha, i}}{2} \right) \tag{4.7}$$

Focusing on the terms of the right hand side sum, some simple arguments give the following inequalities:

$$\rho_i \cdot (1 - x_{g_i}^2) \frac{n_{g_i}}{2} < \sup_i \, (1 - x_{g_i}^2) \, |\rho_i| \tag{4.8}$$

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

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

$$\rho_i^2 + \rho_i \cdot \left( -(1-x_{g_i}^2)\frac{n_{g_i}}{2} + \sum_{\alpha \neq g_i} x_{\alpha,i}^2 \frac{n_{\alpha,i}}{2} \right) > \rho_i^2 - 2|\rho_i| \cdot \sup_i (1-x_{g_i}^2) \quad (4.10)$$

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:

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

Defining the subset $\mathscr{B}(R)$ such as $\vec{u} \in \mathscr{B}(R)$ if $|u_i(0)-u_i| < R$ for all i index, the boundary of $\mathscr{B}(R)$ is denoted $B(R)$. 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 $\vec{u}_{min}(t) \in \mathscr{B}(R_{AI})$ 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., $\sup_i |u_{min,i}(t)-u_i(0)| < R_{AI}$.

## 5. CONCLUSION

The present proof holds for any displacement field which is a minimum of the adiabatic potential $F_{ad}$ such as the gap $\delta \neq 0$. For nearly all $(\mu, U)$ values, the displacements of the many-polaron minima vary continuously with respect to the fermionic charge 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 $F_{ad}$ continuity with respect to the displacements. Consequently, the adiabatic potential has some minima with a many-polaron structure for a finite domain of the model parameters. Nevertheless, the absolute minimum of $F_{ad}$, i.e., the ground state of the adiabatic Holstein–Hubbard model cannot yet be determined for all the parameters. To that aim, a numerical investigation might be required but no idea emerges to tackle the case of a non zero Hubbard coupling with many charge carriers, except a meanfield theory as proposed in ref. 2 or a small electron number model. The latter possibility is presented in refs. 6 and 7 where the phase diagram is calculated for 2 electrons. For a two-dimensional atomic lattice, a critical point where 3 different types of bipolaron coexist 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 mobility and its binding energy reach $100K$ with realistic input parameters (Eq. (2.5)). This result allowed some

conjectures about the mechanism which yields the high critical temperature superconductivity of cuprates.

The present study can be extended straighforwardly 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[13] might have non trivial anti-integrable limits which makes our arguments much less efficient.

## 6. 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 $|\psi\rangle = \sum_\alpha P_{\alpha,i} |\psi\rangle$ we have $|\psi\rangle = \sum_\alpha x_{\alpha,i} |\psi_{\alpha,i}\rangle$ where the normalized states $\psi_{\alpha,i}$ and $x_{\alpha,i} |\psi_{\alpha,i}\rangle = P_{\alpha,i} |\psi\rangle$ are introduced 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 $H_{\bar{i}} = H_{el} - H_i + t \sum_{i:j,\sigma} C^+_{i,\sigma} C_{j,\sigma} + C^+_{j,\sigma} C_{i,\sigma}$ 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 $H_{\bar{i}}$ and $H_i$ commute with the projectors $P_{\alpha,i}$:

$$K_i = H_{\bar{i}} + H_i \tag{6.1}$$

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 $H_{\bar{i}}$ and $H_i$ are decoupled, the state $\phi_0$ is a product of the $H_{\bar{i}}$ 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

$$\langle \Phi_0 | H_{\bar{i}} = |\Phi_0\rangle = E_0 \tag{6.2}$$

$$\langle \Phi_0 | H_{el} |\Phi_0\rangle = \langle \Phi_0 | K_i |\Phi_0\rangle = E_0 \tag{6.3}$$

$$\langle \psi_{g_i} | K_i |\psi_{g_i}\rangle \geqslant E_0 \tag{6.4}$$

From the identity $P^2_{\alpha,i} = P_{\alpha,i}$, 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 $\langle \psi_{\alpha,i} | K_i |\psi_{\alpha,i}\rangle = \langle \psi_{\alpha,i} | H_{el} |\psi_{\alpha,i}\rangle$. If $\delta_i$ is the first excited state energy of $H_i$:

$$\langle \psi_{\alpha \neq g_i,i} | H_i |\psi_{\alpha \neq g_i,i}\rangle \geqslant \delta_i \tag{6.5}$$

$$\langle \psi_{\alpha \neq g_i,i} | K_i |\psi_{\alpha \neq g_i,i}\rangle = \langle \psi_{\alpha \neq g_i,i} | H_{\bar{i}} |\psi_{\alpha \neq g_i,i}\rangle + \langle \psi_{\alpha \neq g_i,i} | H_i |\psi_{\alpha \neq g_i,i}\rangle \tag{6.6}$$

$$\langle \psi_{\alpha \neq g_i,i} | K_i |\psi_{\alpha \neq g_i,i}\rangle \geqslant \langle \psi_{\alpha \neq g_i,i} | H_{\bar{i}} |\psi_{\alpha \neq g_i,i}\rangle + \delta_i \geqslant E_0 + \delta_i \tag{6.7}$$

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

$$\langle \psi_{\alpha \neq g_i,\, i} |\, K_i \,| \psi_{\alpha \neq g_i,\, i} \rangle \geqslant E_0 + \delta_i \tag{6.8}$$

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

$$H_{el} = K_i + \sum_{\alpha \neq \alpha'} P_{\alpha,\, i} H_{el} P_{\alpha',\, i} \tag{6.9}$$

and bracketing by $\psi$:

$$\langle \psi |\, H_{el} \,| \psi \rangle = \sum_\alpha x_{\alpha,\, i}^2 \langle \psi_{\alpha,\, i} |\, K_i \,| \psi_{\alpha,\, i} \rangle + \sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, H_{el} \,| \psi_{\beta,\, i} \rangle \tag{6.10}$$

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

$$\sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, H_{el} \,| \psi_{\beta,\, i} \rangle = -t \sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, \Delta \,| \psi_{\beta,\, i} \rangle \tag{6.11}$$

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

$$\langle \psi |\, H_{el} \,| \psi \rangle = \sum_\alpha x_{\alpha,\, i}^2 \langle \psi_{\alpha,\, i} |\, K_i \,| \psi_{\alpha,\, i} \rangle - t \sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, \Delta \,| \psi_{\beta,\, i} \rangle \tag{6.12}$$

and combining the inequalities (6.4, 6.8):

$$\langle \psi |\, H_{el} \,| \psi \rangle \geqslant E_0 + \delta_i \sum_{\alpha \neq g_i} x_{\alpha,\, i}^2 - t \sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, \Delta \,| \psi_{\beta,\, i} \rangle \tag{6.13}$$

As we choose to map the atomic lattice on $\mathscr{L}^d$, the number of first neighboring sites is $n_c = 2d$. With Eq. (6.3), one now writes the set of following equations where $E = \langle \psi |\, H_{el} \,| \psi \rangle$:

$$\langle \Phi_0 |\, H_{el} \,| \Phi_0 \rangle \geqslant E$$

$$E_0 \geqslant E \to E_0 \geqslant E \geqslant E_0 + \delta_i \sum_{\alpha \neq g_i} x_{\alpha,\, i}^2 - t \sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, \Delta \,| \psi_{\beta,\, i} \rangle$$

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

$$\delta_i \sum_{\alpha \neq g_i} x_{\alpha,\, i}^2 \leqslant t \sum_{\alpha \neq \beta} x_{\alpha,\, i} x_{\beta,\, i} \langle \psi_{\alpha,\, i} |\, \Delta \,| \psi_{\beta,\, i} \rangle$$

$$\delta_i(1-x_{g_i}^2) \leqslant 2n_c t \sum_{\alpha \neq \beta} x_{\alpha,i} x_{\beta,i}$$

$$(1-x_{g_i}^2)\,\delta_i \leqslant n_c t \left[ \left( \sum_{\alpha} x_{\alpha,i} \right)^2 - \sum_{\alpha} x_{\alpha,i}^2 \right]$$

$$(1-x_{g_i}^2)\,\delta_i \leqslant n_c t \left[ \left( \sum_{\alpha} x_{\alpha,i} \right)^2 - 1 \right]$$

$$(1-x_{g_i}^2)\,\delta_i \leqslant n_c t \left[ \left( \sum_{\alpha \neq g} x_{\alpha,i} + x_{g_i} \right)^2 - 1 \right] \tag{6.14}$$

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

$$\sum_{\alpha \neq g} x_{\alpha,i} \leqslant \sqrt{\sum_{\alpha \neq g_i} 1} \sqrt{\sum_{\alpha \neq g_i} x_{\alpha,i}^2}$$

$$\sum_{\alpha \neq g_i} x_{\alpha,i} \leqslant \sqrt{n_s} \sqrt{1-x_{g_i}^2}$$

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

$$(1-x_{g_i}^2)\,\delta_i \leqslant n_c t[(n_s^{\frac{1}{2}}(1-x_{g_i}^2)^{\frac{1}{2}} + x_{g_i})^2 - 1] \tag{6.15}$$

and it is now easy to obtain:

$$(1-x_{g_i}^2)^{\frac{1}{2}} < \frac{2n_c n^{\frac{1}{2}} t}{\delta_i - n_c t(n_s - 1)} \tag{6.16}$$

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:

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

Let write $x_{g_i}^2 = x_{2,i}^2 + x_{3,i}^2$ such as this inequality is now written:

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

If we now assume 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 sites i:

$$(1-x_{g_i}^2)^{\frac{1}{2}} < \frac{2n_c n_s^{\frac{1}{2}} t}{\delta - n_c t(n_s - 2)} \tag{6.19}$$

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