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Lang-Firsov Transformation in the Generalized Tight-binding Method

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Abstract. The effects of strong electron-phonon interaction in a realistic model of a system with strong Coulomb correlations are analyzed using the Lang and Firsov transformation. It is shown that polaronic and bipolaronic transformations, widely discussed in the literature and associated with a smooth or sharp transitions in the properties of charge carriers when the strength of the electron-phonon coupling changes, determine the switching of the system between the regimes of correlated carriers, polarons or bipolarons. These transitions are controlled by the local electron-phonon interaction of the Holstein type. At the same time, the non local electron-lattice contribution associated with the modulation of the hopping integral plays a major role in the crossover of the polaron and bipolaron regimes in the limit of strong electron correlations.

Keywords: Lang–Firsov transformation, polaron and bipolaron crossover, pd-model.

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1. Lang-Firsov transformation

Let us consider the classical canonical transformation for systems with the strong electron-phonon coupling of the Holstein type. It was proposed by Lang and Firsov [1] for systematic consideration of the perturbation theory of the mobility of small-radius polarons. They managed to record a significant part of the short-ranged electron-phonon interaction in such a way that, during the transformation of the Hamiltonian, they could collect infinite series for the transformed operators. The authors [1] simplified the Hamiltonian of the system by limiting the contribution of the electron-phonon interaction to the local electron variables:

$$H = \sum_m \varepsilon a_m^\dagger a_m + \sum_{m,\mathbf{q}} T_g a_{m+g}^\dagger a_m + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{1}{2} \right) + \sum_{m,\mathbf{q}} \hbar\omega_{\mathbf{q}} a_m^\dagger a_m \left(U_{m,\mathbf{q}} b_{\mathbf{q}}^\dagger + U_{m,\mathbf{q}}^* b_{\mathbf{q}} \right), \quad (1)$$

where $a_m^\dagger\,(a_m)$ are operators of creation (annihilation) of an electron at a site m, $b_{\mathbf{q}}^\dagger\,(b_{\mathbf{q}})$ are operators of creation (annihilation) of a phonon with quasi momentum $\mathbf{q}$; ε is the ground state

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electron energy; the parameter T_g characterizes the hopping energy from site g to m and vice versa; $U_{m,\mathbf{q}}$ is the electron-phonon interaction (EPI) parameter and $\omega_{\mathbf{q}}$ is the phonon mode frequency.

According to the original paper, the canonical transformation $\tilde{H} = e^S H e^{-S}$ of the Hamiltonian (1) with the unitary operator S in the form:

$$S = \sum_{m,\mathbf{q}} a_m^\dagger a_m \left(b_{\mathbf{q}}^\dagger U_{m,\mathbf{q}} - b_{\mathbf{q}} U_{m,\mathbf{q}}^* \right),$$

leads to a new Hamiltonian:

$$\tilde{H} = \sum_m a_m^\dagger a_m \left(\varepsilon - \Delta\right) + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \frac{1}{2} \right) + \sum_{m,g} T_g \hat{\Phi}_{m,g} a_{m+g}^\dagger a_m,$$

which describes the energy of polarons, lattice oscillators, and their residual interaction. Here $\Delta = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left|U_{m,\mathbf{q}}\right|^2$ is the polaron shift of the atomic energy of the ground states of charge carriers and $\hat{\Phi}_{m,g} = \exp\left[\sum_{\mathbf{q}} \left(b_{\mathbf{q}}^\dagger \Delta_{m,m+g,\mathbf{q}} - b_{\mathbf{q}} \Delta_{m,m+g,\mathbf{q}}^* \right) \right]$ is the renormalization of the hopping integral, it depends on the strength of the electron-phonon coupling: $\Delta_{m,m+g,\mathbf{q}} = U_{m,\mathbf{q}} - U_{m+g,\mathbf{q}}$. In the transformed Hamiltonian, the contribution characterizing the interaction of electrons at different sites through the exchange of virtual phonons is discarded, since it is less than the Coulomb correlations of electrons not taken into account in the original model.

The modified Lang and Firsov transformation, which includes the nonlocal electron-phonon interaction, is also found in the literature. In the general case, analysis of the obtained renormalizations is complicated, however, there are some results that generalize the Holstein theory of polarons. For example, within the framework of the Holstein–Peierls model, the authors of [2, 3] obtain an expression describing the temperature narrowing of the polaron bandwidth and demonstrate that nonlocal electron-phonon coupling plays an important role in organic molecular crystals.

2. Extended pd-model

Realistic models of systems with strong electron-phonon interaction contain more numbers of contributions compared to the Hamiltonian (1). In addition to the nonlocal electron-lattice interaction, these can be multiband effects, Coulomb correlations, and much more. Let us consider an extended pd-model combining contributions essential for describing the nature of high-temperature superconductors based on copper oxides. The Hamiltonian of the model has the form:

$$H = H_{pd} + H_{e-ph} + H_{ph}, \tag{2}$$

here H_{pd} is a well-known pd model describing the hole carriers in the orbitals of oxygen p and copper$d$; it takes into account both the Coulomb interaction of holes in the same and different orbitals and the strong overlap of the orbitals [4].

The term H_{e-ph} describes the interaction of electrons with lattice vibrations. We consider only one optical fully symmetric mode, the dispersion of which can be neglected. Deviations of atoms from their equilibrium positions when bonds are stretching lead to modulations of the single-site energy of charge carriers in copper orbitals (local Holstein-type EPI) and of the hopping integral between the copper and oxygen orbitals (non-local Peierls-type EPI). The H_{ph} part corresponds to the energy of free phonons.

Let us show the complete form for each part of the Hamiltonian (2):

$$H_{pd} = \sum_{\mathbf{g},l,\sigma,\alpha} \left(\varepsilon_\alpha n^\alpha_{\mathbf{g}_\alpha,\sigma} + \frac{1}{2} U_\alpha n^\alpha_{\mathbf{g}_\alpha,\sigma} n^\alpha_{\mathbf{g}_\alpha,\bar{\sigma}} \right) + \sum_{\mathbf{g}\mathbf{g}',ll',\sigma} P_{pp} t_{pp} \left(p^\dagger_{\mathbf{g}_l,\sigma} p_{\mathbf{g}'_{l'},\sigma} + \text{H.c.} \right) + \\ + \sum_{\mathbf{g},l,\sigma} P_{pd} t_{pd} \left(d^\dagger_{\mathbf{g},\sigma} p_{\mathbf{g}_l,\sigma} + \text{H.c.} \right) + \sum_{\mathbf{g},l,\sigma\sigma'} V_{pd} n^p_{\mathbf{g}_l,\sigma} n^d_{\mathbf{g},\sigma'}. \quad (3)$$

Here $d^\dagger_{\mathbf{g},\sigma}$ ($d_{\mathbf{g},\sigma}$) and $p^\dagger_{\mathbf{g}_l,\sigma}$ ($p_{\mathbf{g}_l,\sigma}$) are operators of creation (annihilation) of a hole with spin σ on copper and oxygen orbitals in positions specified by vectors $\mathbf{g}$ and $\mathbf{g}_l$ respectively. The index l enumerates oxygen atoms in the unit cell at the site $\mathbf{g}$; $n^\alpha_{\mathbf{g}_\alpha,\sigma}$ is the hole number operator, where $\mathbf{g}_\alpha = \mathbf{g}$ for $\alpha = d$, and $\mathbf{g}_\alpha = \mathbf{g}_l$ for $\alpha = p$; ε_α is the local energy of a hole in the p or d orbital; t_{pp} and t_{pd} are hopping integrals, U_α, V_{pd} are Coulomb repulsion parameters. The factors P_{pp} and P_{pd} are equal to 1 (-1) if in the region of orbital overlap their phase signs coincide (differ). In the general case, the Hamiltonian (3) describes compounds of transition metal with an incompletely filled d orbitals.

The energy of free phonons in the Hamiltonian (2) has the form:

$$H_{ph} = \sum_{\mathbf{q}} \hbar\omega_0 \left(f^\dagger_{\mathbf{q}} f_{\mathbf{q}} + \frac{1}{2} \right) = \sum_{\mathbf{g}} \hbar\omega_0 \left(f^\dagger_{\mathbf{g}} f_{\mathbf{g}} + \frac{1}{2} \right), \quad (4)$$

where $f^\dagger_{\mathbf{q}}$ is the phonon creates operator with a quasi momentum $\mathbf{q}$ and $f^\dagger_{\mathbf{g}}$ is its Fourier image, ω_0 is the frequency of lattice oscillations.

A significant short-ranged part of the electron-phonon interaction can be written as [6]:

$$H_{e-ph} = \sum_{\mathbf{g},\sigma} M_d \left(f^\dagger_{\mathbf{g}} + f_{\mathbf{g}} \right) d^\dagger_{\mathbf{g},\sigma} d_{\mathbf{g}} + \sum_{\mathbf{g},l,\sigma} M_{pd} P_{pd} \left(f^\dagger_{\mathbf{g}} + f_{\mathbf{g}} \right) \left(d^\dagger_{\mathbf{g},\sigma} p_{\mathbf{g}_l,\sigma} + \text{H.c.} \right), \quad (5)$$

where M_d and M_{pd} are the electron-phonon interaction parameters for Holstein and Peierls type contributions, respectively.

3. Lang-Firsov transformation for intercluster part

Assuming that the strong coupling approximation is valid for the system (2) in the limit of strong electron correlations, we analyze the effects of electron-phonon interaction using the Lang and Firsov transformation. Following the ideology of the generalized tight-binding method, we divide the system into clusters and represent the Hamiltonian (2) as the sum of the intracluster contribution H_c and the intercluster interaction H_{cc}:

$$H = H_c + H_{cc}. \quad (6)$$

Such splitting is possible if we go from the operators $p^\dagger_{\mathbf{g}_l,\sigma}$ ($p_{\mathbf{g}_l,\sigma}$) to the new ones, $b^\dagger_{\mathbf{g},\sigma}$ ($b_{\mathbf{g},\sigma}$), centered on copper orbitals and orthogonal in the nearest cells. A similar transformation for the displacement operators [5] translates the operators $f^\dagger_{\mathbf{g}}$ ($f_{\mathbf{g}}$) into the new $A^\dagger_{\mathbf{g}}$ ($A_{\mathbf{g}}$) [6]. As a result, the intracluster part of the Hamiltonian (2) is given by:

$$H_c = \sum_{\mathbf{g},\sigma,\beta} \left(\varepsilon_\beta n^\beta_{\mathbf{g},\sigma} + \frac{1}{2} U_\beta n^\beta_{\mathbf{g},\sigma} n^\beta_{\mathbf{g},\bar{\sigma}} \right) + \sum_{\mathbf{g},\sigma} \left(t^{bd}_{00} \left(d^\dagger_{\mathbf{g},\sigma} b_{\mathbf{g},\sigma} + H.c. \right) + \sum_{\sigma'} V_{bd} n^d_{\mathbf{g},\sigma} n^b_{\mathbf{g},\sigma'} \right) + \\ + \sum_{\mathbf{g},\sigma} \left(M^d_{00} \varphi^A_{\mathbf{g}} n^d_{\mathbf{g},\sigma} + M^{bd}_{000} \varphi^A_g \left[d^\dagger_{\mathbf{g},\sigma} b_{\mathbf{g},\sigma} + \text{H.c.} \right] \right) + \sum_{\mathbf{g}} \hbar\omega_0 \left(A^\dagger_{\mathbf{g}} A_{\mathbf{g}} + \frac{1}{2} \right). \quad (7)$$

where $\beta = d, b$ is the orbital index in the new representation. Changes in the parameters of the original Hamiltonian (2) are result from the transition to the basis of Wannier functions.

Omitting the insignificant details of the polaronic version of the generalized tight-binding method [6], we only indicate that $M_{00}^{d} = M_{d}\mu_{00}$, $M_{000}^{bd} = -2M_{pd}\mu_{00}^{2}$ and the coefficient $\mu_{00} \approx 0.96$.

Let us carry out the canonical transformation of the Hamiltonian H_c, limiting ourselves to local contributions of the Holstein type EPI, that is, we put $M_{pd} = 0$. Then unitary operator is:

$$S = \sum_{\mathbf{g},\sigma} \frac{M_{00}^{d}}{\hbar\omega_0} \left(A_{\mathbf{g}}^{\dagger} - A_{\mathbf{g}}\right) n_{\mathbf{g},\sigma}^{d},$$

and the Hamiltonian (7) takes the form:

$$H_c = \sum_{\mathbf{g},\sigma} \left[\left(\varepsilon_d - \Delta\right) n_{\mathbf{g},\sigma}^{d} + \varepsilon_b n_{\mathbf{g},\sigma}^{b}\right] + \sum_{\mathbf{g},\frac{1}{2}\sigma} \left[\left(U_d - 2\frac{\left(M_{00}^{d}\right)^2}{\hbar\omega_0}\right) n_{\mathbf{g},\sigma}^{d} n_{\mathbf{g},\bar{\sigma}}^{d} + U_b n_{\mathbf{g},\sigma}^{b} n_{\mathbf{g},\bar{\sigma}}^{b}\right] +$$

$$+ \sum_{\mathbf{g},\sigma\sigma'} V_{bd} n_{\mathbf{g},\sigma}^{d} n_{\mathbf{g},\sigma'}^{b} + \sum_{\mathbf{g},\sigma} t_{00}^{bd} \left(\tilde{d}_{\mathbf{g},\sigma}^{\dagger} b_{\mathbf{g},\sigma} + \text{H.c.}\right) + \sum_{\mathbf{g}} \hbar\omega_0 \left(A_{\mathbf{g}}^{\dagger} A_{\mathbf{g}} + \frac{1}{2}\right). \qquad (8)$$

The residual polaron-lattice interaction results from the renormalization of the orbital overlap integral, associated with the transformation $\tilde{d}_{\mathbf{g},\sigma}^{\dagger} = d_{\mathbf{g},\sigma}^{\dagger} \exp\left[\frac{M_{00}^{d}}{\hbar\omega_0}\left(A_{\mathbf{g}}^{\dagger} - A_{\mathbf{g}}\right)\right]$. In the polaron shift of the atomic level $\Delta = \frac{\left(M_{00}^{d}\right)^2}{\hbar\omega_0} \langle n_{\mathbf{g},\sigma}^{d}\rangle$ we have explicitly preserved the mean of the particle number operator. We assume that $\langle n_{\mathbf{g},\sigma}^{d}\rangle$ is not necessarily close to 1 even at small doping of the system due to the redistribution of charges carries between the orbitals b and d.

The equation (8) correlates with the well-known paper [7] of A. Aleksandrov and co-authors. The differences are associated with the formulation of the Hamiltonian (2), which takes into account, in addition to Coulomb correlations, multiband effects, and the structure of the unit cell. In addition, for the estimates below we use the realistic parameters of the Hamiltonian (2), determined from *ab initio* calculations, and compare the results with the conclusions obtained [8, 9] by the exact diagonalization of the cluster H_c.

Carrying out a similar procedure, we consider the renormalizations of the Hamiltonian H_c due to the contribution of the Peierls-type EPI; so, we set $M_d = 0$. Then we define the unitary operator in a form which is similar to the nonlocal contribution of the EPI, and, using the Baker-Campbell-Hausdorff formula, we find a new representation of the Hamiltonian operators. Avoiding cumbersome expressions, we note that the transformation of a pair of hole creation (annihilation) operators in the orbitals of copper and oxygen, $d_{\mathbf{g},\sigma}^{\dagger}$ ($d_{\mathbf{g},\sigma}$) and $b_{\mathbf{g},\sigma}^{\dagger}$ ($b_{\mathbf{g},\sigma}$), formally is a rotation in two-dimensional Minkowski space with angle $\theta = \frac{M_{000}^{bd}}{\hbar\omega_0}\left(A_{\mathbf{g}}^{\dagger} + A_{\mathbf{g}}\right)$. Changes to phonon operators have the form:

$$\tilde{A}_{\mathbf{g}} = A_{\mathbf{g}} - \sum_{\sigma\prime} \frac{M_{000}^{bd}}{\hbar\omega_0} \left(d_{\mathbf{g},\sigma\prime}^{\dagger} b_{\mathbf{g},\sigma\prime} + \text{H.c.}\right). \qquad (9)$$

In the transformed Hamiltonian, equation (9) gives renormalizations proportional to the value $\frac{M_{000}^{bd\ 2}}{\hbar\omega_0}$ and describing (i) the change in the interorbital Coulomb interaction, (ii) spin fluctuations in the b and d orbitals without charge transfer, as well as (iii) effective interorbital electron-phonon interaction associated with charge transfer without spin-flip and (iv) effective interorbital spin-phonon interaction, corresponding to charge transfer with a change of spin. These processes are caused by the exchange of virtual phonons between carriers in different orbitals. Note also that process (i) contributes both ε_d and ε_b energies to the polaron shift.

4. Analysis of the effects of local and non-local EPI

We introduce dimensionless electron-phonon coupling constants $\lambda_d = \frac{(M_d)^2}{\hbar\omega_0 W}$ and $\lambda_{bd} = \frac{(M_{bd})^2}{\hbar\omega_0 W}$, characterizing contributions of Holstein (local) and Peierls (non-local) types. Here, W is the width of the bare bond, which is not renormalized by EPI and Coulomb effects. For ease of comparison, all electronic structures parameters of the pd-model (3) have been chosen in accordance with the paper [9], in which the effects of EPI were investigated for the cell H_c and the total 2 Hamiltonians in the framework of polaronic version of the generalized tight binding method: $\varepsilon_d = 0,\ \varepsilon_p = 1.5,\ t_{pp} = 0.86,\ t_{pd} = 1.36,\ U_d = 9,\ U_p = 4,\ V_{pd} = 1.5,\ W = 2.15$, all in eV.

The first case is $\lambda_{bd} = 0$. Let us consider the single-particle states, the atomic energy ε_d of which decreases under strong local electron-phonon interaction by the value $\Delta = \frac{\left(M^d_{00}\right)^2}{\hbar\omega_0}\langle n^d_{\mathbf{g},\sigma}\rangle$. If the polaron shift Δ is larger than the width of the charge carrier band W, then the formation of an energetically more favorable band of polaron states begins near the Fermi level of the system. The critical EPI strength is $\lambda^{c1}_d = \frac{1}{\mu^2_{00}\langle n^d_{\mathbf{g},\sigma}\rangle}$ For given parameters, this occurs for the electron-phonon coupling strength $\lambda^{c1}_d \geqslant 1.1$ if $\langle n^d_{\mathbf{g},\sigma}\rangle \approx 1$; at lower values of $\langle n^d_{\mathbf{g},\sigma}\rangle$, due to the strong hybridization of the orbitals p and d, the value of λ^{c1}_d increases. In the electronic structure of the extended pd-model (2), a narrow polaron band appears [8] in certain directions of the Brillouin zone.

Now let us consider two-particle states and estimate the value of the second critical parameter of the local EPI, at which the Coulomb interaction at the copper sites effectively vanishes or becomes negative. The equation (8) gives the value of $\lambda^{c2}_d = \frac{U_d}{2\mu^2_{00}W}$. So, for $U_d = 9$ we obtain $\lambda^{c2}_d \approx 2.2$. The screening of the Coulomb potential by electron-phonon interaction forms a tendency to the formation of bipolarons (here, local bipolarons). The process is accompanied by a significant transfer of charge carries from the p to the d orbital at $\lambda_d \geqslant \lambda^{c2}_d$ [8].

In the limit of strong electron correation we get that $\lambda^{c1}_d < \lambda^{c2}_d$. Obviously, a decrease in the Coulomb interaction U_d leads to a decrease in λ^{c2}_d. In the Holstein model, $(\lambda_{bd} = 0)$ the crossover of the critical values marking the polaronic λ^{c1}_d and bipolaronic λ^{c2}_d regimes take place at $U_d < \frac{1}{\langle n^d_{\mathbf{g},\sigma}\rangle} 2W$. It corresponds to the case of weak or intermediate Coulomb correlations. However, in a more realistic approach that takes into account the contribution of nonlocal EPI, such a crossover occurs in the limit of strong electron correlations for $(\lambda_{bd} \neq 0)$ [9]. The replacement of the polaron and bipolaron regimes is accompanied by changes in the electronic structure associated with the redistribution of the density of charge carriers in favor of the p orbital and with the 'relocation" of the chemical potential into the band of the two-particle states for hole doped system. This proves the essential role of the nonlocal EPI in the formation of bipolarons in a correlated system and emphasizes the need to take its effects into account in such problems as, for example, the search for light bipolarons.

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Преобразование Ланга-Фирсова в обобщенном методе сильной связи

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Аннотация. В настоящей работе с помощью преобразования Ланга и Фирсова анализируются эффекты сильного электрон-фононного взаимодействия в реалистичной модели системы с сильными кулоновскими корреляциями. Показано, что широко обсуждаемые в литературе поляронные и биполяронные трансформации, связанные с плавным или резким изменением свойств носителей заряда при изменении силы электрон-фононной связи, определяют переключение системы между режимами коррелированных носителей, поляронов или биполяронов. При этом существенную роль в кроссовере поляронного и биполяронного режимов в пределе сильных электронных корреляций играет нелокальный электрон-фононный вклад, связанный с модуляцией интеграла перескока между различными орбиталями.

Ключевые слова: преобразование Ланга и Фирсова, кроссовер поляронов и биполяронов, pd-модель.