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LETTER TO THE EDITOR

Unitary transformation scheme for polaron and bipolaron correlation models

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Abstract. On the basis of the modified Lang–Firsov-transformed Holstein–Hubbard model, effective polaron and bipolaron models are derived within the unified framework of Schrieffer–Wolff-type transformations in the strong correlation limit. The resulting polaronic t–J and bipolaronic local pairing models obtained for large positive and negative on-site interactions, respectively, exhibit different renormalizations of the hopping and interaction terms in the moderately heavy and light polaron and bipolaron cases.

There is growing experimental evidence that lattice polarons and bipolarons may play an important role in explaining many characteristics of high-T_c cuprates [1] and the hopping transport in nickelates [2]. In their own right, the properties of small and large polarons and bipolarons have attracted renewed interest. Understanding the formation of polarons and bipolarons at finite densities on the basis of microscopic models is one of the basic problems in this field. Along those lines, Das *et al* [3] have investigated the Holstein t–J model by means of the Gutzwiller approximation. In our previous slave-boson work [4] we have studied polaron formation by applying a modified variational Lang–Firsov transformation (MVLF) to the Holstein–Hubbard model. Aleksandrov *et al* [5] have derived an effective bipolaron model by a unitary transformation procedure, where the bipolaron parameters are expressed in terms of dynamical multiphonon correlation functions.

The aim of this paper is to derive effective polaron and bipolaron models from the Holstein–Hubbard model in the large-positive and large-negative interaction limits within a systematic and unified scheme of Schrieffer–Wolff-type transformations [6]. By this operator-algebraic approach, which differs from the procedure described by Aleksandrov *et al* [5], we obtain, in the moderately heavy- and light-polaron cases, two effective polaronic t–J and bipolaron models. Methodically, the underlying approximations are detailed in all limiting cases.

We consider a system of correlated electrons locally coupled to a dispersionless phonon mode with frequency ω_0, described by the Holstein–Hubbard model

$$\mathcal{H} = -t \sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sqrt{\varepsilon_p \hbar\omega_0} \sum_i (b_i^{\dagger} + b_i)\, n_i + \mathcal{H}_{\mathrm{ph}} \qquad (1)$$

where $\mathcal{H}_{\mathrm{ph}} = \hbar\omega_0 \sum_i (b_i^{\dagger} b_i + \frac{1}{2})$ and $n_i = \sum_\sigma n_{i\sigma}$. Treating polaron formation at finite densities in the non-dimerized paraphase by the variational approach outlined in [4], we perform the MVLF:

$$\mathcal{H}_p = \mathcal{U}^{\dagger} \mathcal{H} \mathcal{U} \qquad \mathcal{U}(\gamma) = \exp\left\{ -\sqrt{\varepsilon_p/\hbar\omega_0} \sum_i (b_i - b_i^{\dagger})[n + \gamma(n_i - n)] \right\} \qquad (2)$$

where n is the mean polaron density. Here the variational parameter γ ($0 \leqslant \gamma \leqslant 1$) measures the strength of the polaron effect. The polaron Hamiltonian is given by

$$\mathcal{H}_{\mathrm{p}} = \mathcal{H}_0 + \mathcal{H}_t + \mathcal{H}_\gamma + \mathcal{H}_{\mathrm{ph}} \tag{3}$$

$$\mathcal{H}_0 = -\tilde{\varepsilon}_{\mathrm{p}} \sum_i n_i + \tilde{U} \sum_i n_{i\uparrow} n_{i\downarrow} \tag{4}$$

$$\mathcal{H}_t = -t \sum_{\langle i,j\rangle\sigma} \Phi_{ij} c_{i\sigma}^\dagger c_{j\sigma} \tag{5}$$

$$\mathcal{H}_\gamma = (\gamma - 1)\sqrt{\varepsilon_{\mathrm{p}} \hbar\omega_0} \sum_i (b_i^\dagger + b_i)(n_i - n) + (\gamma - 1)^2 n^2 \varepsilon_{\mathrm{p}} N \tag{6}$$

where

$$\tilde{\varepsilon}_{\mathrm{p}} = \varepsilon_{\mathrm{p}}\,[\gamma(2-\gamma) + 2n(1-\gamma)^2] \tag{7}$$

$$\tilde{U} = U - 2\varepsilon_{\mathrm{p}}\gamma(2-\gamma) \tag{8}$$

$$\Phi_{ij} = \exp\left\{\gamma\sqrt{\varepsilon_{\mathrm{p}}/\hbar\omega_0}(b_i - b_i^\dagger + b_j^\dagger - b_j)\right\}. \tag{9}$$

For $\gamma \equiv 1$, $\mathcal{H}_{\mathrm{p}}$ is the well known small-polaron Hamiltonian [7].

Taking the average $\overline{(\ldots)}$ of $\mathcal{H}_{\mathrm{p}}$ over the transformed phonon ground state an effective polaron model may be obtained. In this approach the residual polaron–multiphonon interaction, proportional to $\Phi_{ij} - \overline{\Phi_{ij}}$, is neglected. As shown by recent exact cluster diagonalizations for the Holstein–Hubbard model [8], this is a good approximation in the light-polaron case $\rho = \overline{\Phi_{ij}} \lesssim 1$ (realized for $\varepsilon_{\mathrm{p}}, \hbar\omega_0 \ll t$ with $\gamma \ll 1$ or for $\hbar\omega_0 \gg t, |\tilde{U}|$ with $\gamma \lesssim 1$ [4]). On the other hand, as was pointed out by Aleksandrov *et al* [9], the adiabatic Holstein heavy polaron (realized for $\hbar\omega_0 < t$ and $\varepsilon_{\mathrm{p}} > zt$, where z is the coordination number) cannot be obtained by the phonon-averaging procedure. Taking into account the anharmonic lattice fluctuations, which become important at finite polaron densities and in the intermediate coupling regime, we perform the average of $\mathcal{H}_{\mathrm{p}}$ over the squeezed phonon state [10]:

$$|\tilde{\Psi}_{\mathrm{ph}}\rangle = \exp\left\{\alpha \sum_i (b_i^\dagger b_i^\dagger - b_i b_i)\right\}|0\rangle. \tag{10}$$

This yields the effective polaron model [4]

$$\overline{\mathcal{H}}_{\mathrm{p}} = \mathcal{H}_0 + \overline{\mathcal{H}}_t + \left[\tfrac{1}{4}\hbar\omega_0(\tau^2 + \tau^{-2}) + (\gamma - 1)^2 n^2 \varepsilon_{\mathrm{p}}\right] N \tag{11}$$

where $\overline{\mathcal{H}}_t$ is given by (5) with Φ_{ij} replaced by the polaron band narrowing

$$\rho = \exp\{-\varepsilon_{\mathrm{p}}\gamma^2\tau^2/\hbar\omega_0\}. \tag{12}$$

The second variational parameter $\tau^2 = \exp\{-4\alpha\}$ ($\alpha > 0$) describes squeezing effects [10]. Next, we derive effective polaron and bipolaron models in the strong correlation limit (large $|\tilde{U}|$) for non-adiabatic moderately heavy Lang–Firsov polarons ($t < \hbar\omega_0$, $0.3 \lesssim \rho < 1$; $\gamma \lesssim 1$) and for light polarons.

Let us first consider the *moderately heavy-polaron case*, where multiphonon fluctuations become important [8]. We separate $\mathcal{H}_t$ into contributions from polaron transitions without and with changes in the number of doubly occupied sites:

$$\mathcal{H}_t = \mathcal{T}_0 + \mathcal{V} \qquad \mathcal{V} = \mathcal{T}_1 + \mathcal{T}_{-1} \tag{13}$$

$$\mathcal{T}_0 = -t \sum_{\langle i,j\rangle\sigma} \Phi_{ij}(c_{i\sigma}^\dagger(1-n_{i\bar\sigma})c_{j\sigma}(1-n_{j\bar\sigma}) + c_{i\sigma}^\dagger n_{i\bar\sigma}c_{j\sigma}n_{j\bar\sigma}) \tag{14}$$

$$\mathcal{T}_1 = -t \sum_{\langle i,j\rangle\sigma} \Phi_{ij}c_{i\sigma}^\dagger n_{i\bar\sigma}c_{j\sigma}(1-n_{j\bar\sigma}) \qquad \mathcal{T}_{-1} = \mathcal{T}_1^\dagger. \tag{15}$$

Note that

$$[\mathcal{H}_0, \mathcal{T}_m] = m\tilde{U}\mathcal{T}_m \qquad m = 0, \pm 1. \tag{16}$$

In the processes described by (13) the on-site energy changes by $m\tilde{U}$, where multiphonon emissions and absorptions take place. For large $|\tilde{U}|$, the transitions with $m = \pm 1$ are energetically unfavourable.

Now we apply the recursive scheme of Schrieffer–Wolff-type transformations developed by MacDonald *et al* [11] for the Hubbard model to the polaron Hamiltonian (3). Eliminating transitions between states with differing numbers of doubly occupied sites up to $\mathrm{O}(\tilde{U}^{-1})$, we perform the unitary transformation

$$\mathcal{H}_{\mathrm{p}}' = \mathrm{e}^{\mathcal{S}}\mathcal{H}_{\mathrm{p}}\mathrm{e}^{-\mathcal{S}} \qquad \mathcal{S} = \mathcal{S}^{(1)} + \mathcal{S}^{(2)} \tag{17}$$

$$\mathcal{S}^{(1)} = \frac{1}{\tilde{U}}(\mathcal{T}_1 - \mathcal{T}_{-1}) \qquad \mathcal{S}^{(2)} = \frac{1}{\tilde{U}^2}([\mathcal{T}_1, \mathcal{T}_0] - [\mathcal{T}_0, \mathcal{T}_{-1}]). \tag{18}$$

The generators $\mathcal{S}^{(1)}$ and $\mathcal{S}^{(2)}$ are chosen such that

$$[\mathcal{S}^{(1)}, \mathcal{H}_0] = -\mathcal{V} \qquad [\mathcal{S}^{(2)}, \mathcal{H}_0] = -[\mathcal{S}^{(1)}, \mathcal{T}_0]. \tag{19}$$

Thus we get

$$\mathcal{H}_{\mathrm{p}}' = \mathcal{H}_0 + \mathcal{T}_0 + \mathcal{H}_\gamma + \mathcal{H}_{\mathrm{ph}} + \tfrac{1}{2}[\mathcal{S}^{(1)}, \mathcal{V}] + [\mathcal{S}^{(1)}, \mathcal{H}_\gamma] + [\mathcal{S}^{(1)}, \mathcal{H}_{\mathrm{ph}}] + \mathrm{O}(\tilde{U}^{-2}). \tag{20}$$

After lengthy but straightforward calculations we obtain

$$\frac{1}{2}[\mathcal{S}^{(1)}, \mathcal{V}] = \frac{2zt^2}{\tilde{U}}\sum_i n_{i\uparrow}n_{i\downarrow} + \frac{2t^2}{\tilde{U}}\sum_{\langle i,j\rangle}\Phi_{ij}^2 C_i^\dagger C_j + \frac{2t^2}{\tilde{U}}\sum_{\langle i,j\rangle}(S_iS_j - \tfrac{1}{4}n_in_j) + \mathcal{H}_3. \tag{21}$$

$\mathcal{H}_3$ denotes the three-site contributions, and $C_i^\dagger = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$ is the pair-creation operator.

Considering the large-positive-$\tilde{U}$ limit, we project $\mathcal{H}_{\mathrm{p}}'$ onto the subspace with no double occupancy and thereafter take the average over the phonon state (10). Obviously, we have $\langle\tilde\Psi_{\mathrm{ph}}|\mathcal{H}_\gamma|\tilde\Psi_{\mathrm{ph}}\rangle = 0$. Moreover, we get $\langle\tilde\Psi_{\mathrm{ph}}|[\mathcal{S}^{(1)}, \mathcal{H}_{\mathrm{ph}}]|\tilde\Psi_{\mathrm{ph}}\rangle = 0$. The term $\langle\tilde\Psi_{\mathrm{ph}}|[\mathcal{S}^{(1)}, \mathcal{H}_\gamma]|\tilde\Psi_{\mathrm{ph}}\rangle = 2\varepsilon_{\mathrm{p}}\gamma(\gamma-1)(\overline{\mathcal{T}}_1 + \overline{\mathcal{T}}_{-1})/\tilde{U}$ will be neglected due to the small prefactor $\gamma - 1$. As a result, we obtain the effective polaronic t–J model

$$\mathcal{H}_{\mathrm{p}}^{t-J} = -\tilde\varepsilon_{\mathrm{p}}\sum_i \tilde n_i - t_{\mathrm{p}}\sum_{\langle i,j\rangle\sigma}\tilde c_{i\sigma}^\dagger \tilde c_{j\sigma} + J\sum_{\langle i,j\rangle}(S_iS_j - \tfrac{1}{4}\tilde n_i\tilde n_j)$$
$$- t_{\mathrm{p},3}\sum_{\langle ijk\rangle\sigma}((\tilde c_{i\sigma}^\dagger \tilde c_{j\bar\sigma}^\dagger \tilde c_{j\bar\sigma}\tilde c_{k\sigma} + \tilde c_{i\bar\sigma}^\dagger \tilde c_{j\bar\sigma}\tilde c_{j\sigma}^\dagger \tilde c_{k\sigma}) + \mathrm{HC}) + \frac{\hbar\omega_0}{4}(\tau^2 + \tau^{-2}) \tag{22}$$

where

$$t_{\rm p} = \rho t \qquad t_{\rm p,3} = \rho t^2/\tilde{U} \qquad J = 2t^2/\tilde{U}. \tag{23}$$

$\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i\bar{\sigma}})$, and the summation $\langle ijk \rangle$ extends over all nearest-neighbours pairs $\langle ij \rangle$ and $\langle jk \rangle$. Note that the superexchange is not influenced by the polaron formation, whereas the restricted hopping and three-site terms are renormalized by the polaron band narrowing. This is in accordance with the results obtained for a modified Holstein t–J model, where the phonon mode couples to the empty sites [3].

In the large-negative-$\tilde{U}$ limit, the formation of on-site bipolarons takes place. Since in this case there are no real polarons, we project $\mathcal{H}'_{\rm p}$ onto the subspace of empty and doubly occupied sites. After averaging over the phonon state (10) we get the effective bipolaron model:

$$\mathcal{H}_{\rm b} = -\varepsilon_{\rm b} \sum_i N_i - t_{\rm b} \sum_{\langle i,j \rangle} C_i^\dagger C_j + V \sum_{\langle i,j \rangle} N_i N_j + \frac{\hbar\omega_0}{4}(\tau^2 + \tau^{-2})N \tag{24}$$

where the projection of n_i yields $2N_i$ with $N_i = C_i^\dagger C_i$. $t_{\rm b}$ and V denote the effective bipolaron transfer integral and the intersite repulsion, respectively, given by

$$t_{\rm b} = 2\rho^4 t^2/|\tilde{U}| \qquad V = 2t^2/|\tilde{U}|. \tag{25}$$

Besides a renormalization of the bipolaron binding energy $\varepsilon_{\rm b} - 2\varepsilon_{\rm p} = |\tilde{U}| + 2zt^2/|\tilde{U}|$, the polaron–multiphonon interaction gives rise to a heavy-bipolaron mass $\propto \rho^{-4}$ which is due to virtual transitions to unpaired polarons accompanied by multiphonon emissions. The results (25) are in agreement with those derived by Aleksandrov *et al* [5] in the limit $\hbar\omega_0 \ll |\tilde{U}|$.

In the *light-polaron case*, we derive effective polaron and bipolaron models in the strong correlation limit starting from the model $\overline{\mathcal{H}}_{\rm p}$ (equation (11)). Following the same steps as in the derivation of (22) and (24), one easily sees that all parameters of $O(t^2)$ are equally renormalized by ρ^2. Since the term $\langle \tilde{\Psi}_{\rm ph} | [\mathcal{S}^{(1)}, \mathcal{H}_\gamma] | \tilde{\Psi}_{\rm ph} \rangle$ is proportional to $\gamma(\gamma - 1)$, it can be dropped again.

Therefore, in the large-positive-$\tilde{U}$ limit we get $\overline{\mathcal{H}}_{\rm p}^{t-J}$ given by (22), where

$$\bar{t}_{\rm p} = t_{\rm p} \qquad \bar{t}_{\rm p,3} = \rho t_{\rm p,3} \qquad \bar{J} = \rho^2 J. \tag{26}$$

Compared with the polaronic t–J model (22) and (23), in the light-polaron case the superexchange (26) is slightly reduced. Obviously, for $\varepsilon_{\rm p} = \hbar\omega_0 = 0$, equation (22) reduces to the standard t–J model.

Correspondingly, in the large-negative-$\tilde{U}$ limit we obtain the effective bipolaron model $\overline{\mathcal{H}}_{\rm b}$, where $\bar{\varepsilon}_{\rm b} = 2\varepsilon_{\rm p} + |\tilde{U}| + 2z(\rho t)^2/|\tilde{U}|$ and

$$\bar{t}_{\rm b} = t_{\rm b}/\rho^2 \qquad \bar{V} = \rho^2 V. \tag{27}$$

Compared with the heavy-bipolaron parameters (25), the mass is proportional to ρ^{-2}, and the bipolaron repulsion is weakened. In this case the bipolaron motion does not involve virtual phonon processes. This is in accord with the result by Aleksandrov *et al* [5] in the anti-adiabatic limit $\hbar\omega_0 \gg |\tilde{U}|$. Let us point out that the application of the phenomenological large-negative-U Hubbard model to the bipolaron problem is justified only for rather weak mass renormalization. Different versions of the negative-U Hubbard model and the resulting pairing models [12, 13] were extensively studied in the literature (see [14] and references therein), where models of the structure (24) are isomorphous to the quantum anisotropic pseudospin Heisenberg model [15].

In the t–J model, polaron formation may change the ratio of the interaction to the hopping terms from $J/t < 1$ (holding for high-T_c cuprates) to $J/t_p \propto \rho^{-1} > 1$. Note that for $J > t$ the two-dimensional t–J model shows phase separation, whereas for $J \ll t$ it does not [16]. Equally, in the heavy-bipolaronic pairing model, the ratio $V/t_b \propto \rho^{-4}$ is appreciably enhanced compared with the pairing models studied in the context of the large-negative-U Hubbard model [15]. Altogether, the polaron and bipolaron effects provide a microscopic foundation for a realistic extension of the t–J and pairing model parameter regions.

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