NONADIABATIC EFFECTS IN A GENERALIZED JAHN-TELLER LATTICE MODEL: HEAVY AND LIGHT POLARONS, PAIRING AND METAL-INSULATOR TRANSITION

Eva Majerníková†‡∗, J. Riedel† and S. Shpyrko†‡**
† Department of Theoretical Physics, Palacký University, Tř. 17. listopadu 50, CZ-77207 Olomouc, Czech Republic
‡ Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta, SK-84 228 Bratislava, Slovak Republic

The selfconsistent ground state polaron potential of one-dimensional lattice of two-level molecules with spinless electrons and two dispersionless phonon modes with linear coupling and quantum phonon-assisted (nonadiabatic) transitions between the levels is found anharmonic in phonon displacements. As a function of these, the potential shows a crossover from two nonequivalent broad minima to a single narrow minimum which correspond to the positions of the levels in the ground state. Generalized variational approach respecting the mixing of levels (reflection) via a variational parameter implies prominent nonadiabatic effects: (i) In the limit of the symmetric EJT Jahn-Teller situation they cause transition between the regime of the predominantly one-level "heavy" polaron and a "light" polaron oscillating between the levels due to phonon assistance with almost vanishing polaron displacement. Vanishing polaron selflocalization implies enhancement of the electron transfer due to decrease of the "heavy" polaron mass (undressing) at the point of the transition. There can occur pairing of "light" polarons due to exchange of virtual phonons. Continuous transition to new energy ground state close to the transition from "heavy" polaron phase to "light" (bi)polaron phase occurs. In the "heavy" phase, we have found anomalous (anharmonic) enhancements of quantum fluctuations of the phonon coordinate, conjugated momentum and their product in the ground state as functions of the effective coupling which reach their maxima at EJT JT symmetry. They decrease rapidly to their harmonic values as soon as the "light" phase is stabilized. (ii) Nonadiabatic dependence of the polaron mass (Debye-Waller screening) on the optical phonon frequency appears. (iii) The contribution of Rabi oscillations to the transfer enhances significantly quantum shift of the insulator-metal transition line to higher values of the critical effective electron-phonon coupling supporting so the metallic phase. In the EJT case, insulator-metal transition can coincide with the transition between the "heavy" and the "light" (bi)polaron phase only at certain (strong) effective electron-phonon interaction.

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I. INTRODUCTION

Recently an interest in electron-phonon models was renewed owing to high-Tc superconducting layered cuprates and fullerene compounds which exhibit structure instability due to strong Jahn-Teller effect accompanied by an evident isotope effect. Here, nonadiabatic (quantum) fluctuations were found to be important since the majority of the superconducting structures exhibited low values of the Fermi energy, comparable to the phonon energy and large isotope effect. Nonadiabatic fluctuations also appeared relevant in manganese-based perovskites at Jahn-Teller distortion assisted by formation of JT polaron and causing oxygen isotope effect and a colossal magnetoresistance. The mechanism of nonadiabatic pairing was proposed by several authors: Manini et al., Zheng et al., Kresin et al., Pietronero et al. for C60 compounds and recently also for the challenging new superconductor MgB2. Theories of pairing mechanism based on polarons (bipolarons), including also electron-electron interactions evoked great interest as well.

Nonadiabatic fluctuations affect the charge transport because they reduce the polaron band narrowing (i.e. polaron renormalization of the electron mass). Fluctuations increase near the phase transitions destroying the phase coherence for weak interactions and shifting the critical couplings to higher values. However, numerical simulations of different lattice models (Fradkin and Hirsch, Borghi et al., McKenzie et al.) prove a general statement that the resulting quantum fluctuations are much more pronounced than those obtained by variational approaches, e.g. by Zheng et al., Feinberg et al., L., and Chen et al. Namely, the quantum shift of critical values of the electron-phonon coupling from numerical simulations to higher values (preferring so the metallic phase) was shown to exceed considerably their variational values. Moreover, the numerical simulations of two-level lattice electron-phonon systems in one dimension by Feinberg et al. and by Borghi et al. evidence anomalous increase of quantum fluctuations of the phonon coordinate and of the conjugated momentum as well as anomalous increase of their product referring to enhancement of anharmonic effects. The
simulations manifest a dramatic increase of phonon fluctuations and of their product far beyond the standard uncertainty principle. The inadequacy of the variational approaches was ascribed to insufficiency of the squeezed coherent phonons (harmonic oscillators) to comprise anharmonic behavior of the phonons in two-level (band) models.

Since the early beginning, the Jahn-Teller model was investigated mainly in chemistry as a prototype model of electron-phonon interaction for localized centers in solids. It was used to study the instability of the orbitally degenerate electronic states of highly symmetric ionic configuration against ionic distortions in localized molecular centers in crystals. The effect was explained by Jahn-Teller theorem about lifting the degeneracy of an orbitally degenerate electronic state by symmetry lowering distortions of nuclear configurations. This effect is also involved, e.g., in physics of structural phase transitions in solids doped with Jahn-Teller active ions for mechanisms based on tunneling between two electronic levels coupled to phonon modes in optical and paramagnetic ion spectra.

Though JT effect was considered as the most representative nonadiabatic system, Born-Oppenheimer approximation has been extensively used although it is valid only in the limit of large local distortions. Inconsistency of the adiabatic approach for small distortions was analyzed by Wagner.

Importance of JT effect in physics was increased due to above-mentioned discovery of JT effect based structural transitions in some high-$T_c$ superconductors and in manganese-based perovskites. Therefore, the consideration is now focused on lattice versions of the JT model.

In this paper we will investigate an extended lattice of JT molecules: site molecules with doubly degenerate electron level coupled to two internal phonon modes with different symmetries and different coupling constants. The antisymmetric mode splits the levels, the symmetric one couples the levels via phonon assisted on-site and intersite electron transitions (Rabi oscillations). As we show, these transitions are especially important if the difference of the effective potential minima as a function of the phonon displacement is of the order of the phonon energy (symmetric Jahn-Teller molecules). We shall use a generalized variational approach which will account more aspects of nonadiabaticity: Instead of simple squeezed coherent phonons, as a more appropriate variational ansatz for phonons we take two-center squeezed coherent wave function which accounts for possibility of the phonon-mediated coupling of levels. The variational wave function of the two-level electron-phonon systems with reflection symmetry (antisymmetry) of the coherent phonon states related to both the levels $\phi_+$ and $\phi_-$ was first introduced by Shore and Sander as linear combinations $\phi_+ + \eta \phi_-$ and $\phi_- + \eta \phi_+$, $\eta$ being new (reflection) variational parameter. The approach has been widely exploited and further developed by Wagner et al. for exciton ((211)), dimer ((221) and (222)) systems (with the tunneling between the levels in contrast to the phonon-assisted electron transitions of our model); here the notation $(xyz)$ is used for $x$ as number of the levels, $y$ as the number of the sites, and $z$ as number of the electrons in a cell). The detailed comparison of the ground state energies (GSE) of different variational phonon wave functions for an exciton-phonon or dimer-phonon model confirmed the two-peak variational choice as the most suitable one, i.e., giving the best fitting of the exact solution in the medium and strong coupling regime.

Similar structure of the wave function was proposed for the phonon wave function coupled to two electronic states of a double-well potential by Kresin et al. in their model of the nonadiabatic origin of the isotope effect in high-$T_c$ superconductors.

In the Section II, we formulate variational approach for our model. We find effective ground state potential as a function of all (four) phonon variational parameters (displacements of two phonon modes, squeezing and reflection (mixing)).

In the Section III, we compare variational results for the ground state energy of the two-center squeezed coherent phonon wave function with the adiabatic ground state energy and identify the region of importance of the reflection ($\eta$) and nonsymmetry ($\chi = \beta/\alpha$) parameters to be the region close to $\chi = 1$ (E$\infty$ JT symmetry). Special importance of the symmetric (Jahn-Teller) lattice molecules occurs as a specific condition for which the reflection parameter is the most effective. At this symmetry, there takes place a nonadiabatic transition between the polaron dominantly selflocalized within one level, "heavy" polaron of a broad minimum and the almost delocalized, "light" polaron of a narrow minimum (with vanishing displacement) oscillating between close levels via both onsite and intersite phonon assisted tunneling: Namely, the coherent phonons 2 are accompanied by Rabi oscillations of the electron between the levels due to the phonon mode 1. The latter virtual phonons mediate the coupling of polarons which may occupy the levels.

We compare ground state characteristics of the "heavy" and "light" region as functions of pairs of competing classical (effective coupling) and quantum (phonon frequency, tunnelling) parameters. The self-trapping due to electron-phonon coupling competes with the lattice transfer of electrons (band width) which itself is being renormalized by the Debye-Waller factor. The characteristics of the related insulator-metal transition, the value of the gap and consequently the critical coupling are determined by the complex interplay of the transfer supporting the metallic phase and of the electron-phonon coupling supporting the insulating phase. The shift of the critical line to higher values of the critical couplings due to quantum effects is discussed in the Section IV.

In the Section V, we investigate anomalous behavior of the squeezed ground state quantum fluctuations of the canonically conjugated phonon coordinates and their product on the effective coupling ($\mu$) and effective po-
tential asymmetry (χ) parameters, namely the strong anharmonic fluctuations which reach their maximum values again at χ = 1. They decrease to the harmonic oscillator values for χ > 1. A related model is a lattice of two-level dimers with one spin electron at each site ((222) lattice model) studied by exact numerical methods by Borghi et al. The present model differs from that one, but concerning the quantum fluctuations of the phonon coordinate and momenta qualitatively the same results as for their model are expected.

We remark that variational methods are widely used for electron-phonon lattice models.

Fully analytic nonvariational approach with nonconservation of the number of phonons was performed for a local (D = 0) dimer by Weber-Milbrodt. Unfortunately, in the extended (D=1) lattice model this method acquires extreme mathematical complexity. It was used as a basis for numerical study of the above mentioned lattice model.

II. EXTENDED (LATTICE) GENERALIZED JAHN-TELLER MODEL

We investigate 1D lattice of spinless double degenerated electron states linearly coupled to two intramolecular phonon modes described by Hamiltonian

$$H = \Omega \sum_{n,i=1,2} (b_{in}^\dagger b_{in} + 1/2) + \sum_{n} \left( \alpha (b_{in}^\dagger + b_{in}) \sigma_{zn} - \beta (b_{2n}^\dagger + b_{2n}) \sigma_{xn} \right) - \frac{T}{2} \sum_{n,j=1,2} (R_{i,j} + R_{-i,j}) I_n.$$  

where $b_{i,n}, i = 1, 2$ are phonon annihilation operators, and the Pauli matrices $\sigma_{zn}$ represent two-level electron system. They satisfy identities $[\sigma_{zn}, \sigma_{jn}] = i \sigma_{kn}$, $l = x, y, z,$ representing $1/2$-pseudo-spins related to the electron densities in a usual way, i.e. $\sigma_{xn} = \frac{1}{2} (c_{1,n}^\dagger c_{2,n} + c_{2,n}^\dagger c_{1,n})$, $\sigma_{yn} = \frac{1}{2} (c_{1,n}^\dagger c_{1,n} - c_{2,n}^\dagger c_{2,n})$, $\sigma_{zn} = \frac{1}{2} (c_{1,n}^\dagger c_{2,n} - c_{2,n}^\dagger c_{1,n})$, $I_n = \frac{1}{2} (c_{1,n}^\dagger c_{1,n} + c_{2,n}^\dagger c_{2,n})$ is a unit matrix, and $c_{i,n}$ are electron annihilation operators. The operator $R_{\pm i,j} = e^{\pm ipa}$ of the displacement by a lattice constant $\pm a$ acts in both the electron and phonon space, $R_{\pm i,j} f_n = f_{n\pm 1} R_{\pm i,j}$.

In terms of the creation-annihilation electron and phonon operators the Hamiltonian can be cast as follows:

$$H = \sum_n \Omega \sum_{i=1,2} (b_{in}^\dagger b_{in} + 1/2) + \frac{\alpha}{2} (n_{1n} - n_{2n})(b_{1n}^\dagger + b_{1n}) - \frac{\beta}{2} (c_{1n}^\dagger c_{2n} + c_{2n}^\dagger c_{1n})(b_{2n}^\dagger + b_{2n})$$

$$- \frac{T}{2} \sum_{j=1,2} (c_{j,n}^\dagger c_{j,n+1} + H.c.).$$

For $\beta = -\alpha$, the interaction part of (2)

$$\alpha \left( b_{1n}^\dagger + b_{1n}, b_{2n}^\dagger + b_{2n}, - (b_{1n}^\dagger + b_{1n}) \right)$$  

yields the rotationally symmetric $E \otimes e$ form, with a pair (an antisymmetric and a symmetric under reflection) of double degenerated vibrations. This is, e.g., the case of $Cu^{+ +}$ ions with $d^0$ configurations in high-$T_c$ cuprates [32, 33].

Taking $\alpha \neq \beta$ removes the degeneration of the vibronic states breaking the rotational symmetry of the electron-phonon interaction model still staying within the class of JT models [34, 35].

The dispersionless optical phonon mode $b_1$ splits the degenerated unperturbed electron level ($j = 1/2$) while the mode $b_2$ mediates the electron transitions between the levels. This latter term represents phonon-assisted tunneling, a mechanism of the nonclassical (nonadiabatic) nature as well as the pure tunneling in related exciton and dimer models.

Evidently, Hamiltonian (1) ($\alpha \neq \beta$) is reflection-symmetric, $G^{(el)} G^{(ph)} H = H$.

$$|2\rangle = G^{(el)} |1\rangle, \quad (G^{(el)})^2 = 1,$n

$$G^{(ph)} (b_{1n}^\dagger \pm b_{1n}) = -(b_{1n}^\dagger \pm b_{1n}) G^{(ph)} , \quad (G^{(ph)})^2 = 1, \quad (4)$$

where $G^{(ph)} = \exp(i\pi b_{1n}^\dagger b_{1n})$ is the phonon reflection operator. While the phonon 1 is antisymmetric under the reflection, phonon 2 remains symmetric.

In addition, the transfer part of (2) exhibits $SU(2)$ symmetry of the left- and right-moving electrons (holes).

Let us note that the quantum phonon assistance of the electron tunneling ($\beta$-term in (2) and (1)) constitutes the difference of the model from the related dimer and exciton quantum models where instead of $\beta \sum_n (b_{2n}^\dagger + b_{2n}) \sigma_{xn}$ of (2) there stands $\Delta \sigma_{zn}$, where $\Delta$ is the distance between the levels [29, 30].

The local part of (4) can be diagonalized in electron subspace by the Fulton-Gouterman unitary operator $U_n \equiv U_{2n} U_{1n}$, where

$$U_{i,n} = \frac{1}{\sqrt{2}} \left( 1, G_{i,n} \right), \quad G_{i,n} = \exp(i\pi b_{in}^\dagger b_{in}) \equiv G^{(ph)}_{i,n},$$

as follows:

$$\tilde{H}_L = \sum_n U_n H_0 U_n^{-1} = \Omega \sum_{n,i=1,2} \left( b_{in}^\dagger b_{in} + \frac{1}{2} \right)$$

$$+ \frac{1}{2} \sum_n [\alpha (b_{1n}^\dagger + b_{1n}) - \beta (b_{2n}^\dagger + b_{2n}) G_{1n}] I_n.$$  

On the other hand, in the transfer term

$$\tilde{H}_T = -\frac{T}{2} \sum_n (V_{n,1} R_1 + V_{n,-1} R_{-1})$$

there appears a nondiagonality
\( \Phi_{1,2} \equiv \phi_1 \psi_1 \pm \phi_2 \psi_2 \)

\[
\Phi_{1,2} = \frac{1}{\sqrt{C}} [(\phi_+ + \eta \phi_-) \psi_1 \pm (\phi_- + \eta \phi_+) \psi_2] \\
= \frac{1}{\sqrt{C}} [\phi_+(\psi_1 \pm \eta \psi_2) \pm \phi_-(\psi_2 \pm \eta \psi_1)],
\]

where \( \phi_+ \) and \( \phi_- \) are symmetric components related to both the levels. Each of these components was chosen in a form which accounted for mixing with the reflected state via new variational parameter. This choice was stated to be the best variational wave function, i.e., yielding the lowest ground state energy.

The method was further developed by Wagner et al. for dimers and excitons. We shall adopt this approach in what follows by taking

\[
\Phi_{1,2} = \frac{1}{\sqrt{C}} [(\phi_+ + \eta \phi_-) \psi_1 \pm (\phi_- + \eta \phi_+) \psi_2]
\]

with upper sign for the ground state \( \Phi_1 \) and lower sign for the excited state \( \Phi_2 \).

In \( \Phi_{1,2} \), \( \phi_1 = \phi_+ + \eta \phi_- \) and \( \phi_2 = \phi_- + \eta \phi_+ \) are phonon wave functions related to two levels with mixing of the bare \( \phi_+ \) (\( \phi_- \)) and reflected \( \phi_- \) (\( \phi_+ \)) parts mediated by the variational parameter \( \eta \).

Further, \( \psi_1 \) and \( \psi_2 \) are components of the electron state vector related to the upper and lower level, respectively,

\[
\psi_1(n) = \epsilon_{1n}^\dagger |0_e\rangle, \quad \psi_2(n) = \epsilon_{2n}^\dagger |0_e\rangle,
\]

where \( [0_e] \) is the electron vacuum. Note that the last line of \( \Phi_{1,2} \) allows us to interpret alternatively the parameter \( \eta \) as reflection parameter of the electron states as well.

The squeezed coherent phonon wave functions

\[
\phi_\pm |\gamma_1m(n), \gamma_2m(n), r_m(n)\rangle = D_{1,\pm} |\gamma_1m(n)\rangle D_2 |\gamma_2m(n)\rangle S_1 |r_m(n)\rangle |0_{ph}\rangle,
\]

are related to lower (\( \phi_+ \)) and higher (\( \phi_- \)) level; \( |0_{ph}\rangle \) is the phonon vacuum.

The generators of the coherent phonons are functionals of related displacements

\[
D_{1,\pm} |\gamma_1m(n)\rangle = \exp \sum_n \pm |\gamma_1m(n)b_1^\dagger - \gamma^*_1m(n)b_1m\rangle, \quad D_2 |\gamma_2m(n)\rangle = \exp \sum_n |\gamma_2m(n)b_2^\dagger - \gamma^*_2m(n)b_2m\rangle,
\]

as well as the generator of squeezing

\[
S_1 |r_m(n)\rangle = \exp \sum_r r_m(n)(b_1^2 - b_1^\dagger b_1m). \tag{14}
\]

Respective generator of the mode 2, \( S_2 |r_2m(n)\rangle = 1 \), because Hamiltonian \( H \) is linear in \( b_2, b_2^\dagger \) and \( r_2m(n) = 0 \).

The normalization condition then reads

\[
\frac{1}{N^2} \sum_{m,n} C_{1m}(n) = C, \tag{15}
\]

where

\[
C_{1m}(n) = 1 + \eta^2 + 2\eta \exp(-2|\gamma_1m(n)|^2), \tag{16}
\]

and

\[
\tilde{\gamma}_1m(n) \equiv \gamma_1m(n) \exp(-2r_m(n)). \tag{17}
\]

Generally, \( \gamma_{jm}(n) \) is a nonlocal quantity which represents the displacement of the mode \( j \) at the site \( m \) due to an electron at the site \( n \), \( \gamma_{jm}(n) = \frac{1}{\sqrt{N}} \sum_{m,n} \gamma_{jn}(n) \exp(-i q n a) \). We take

\[
\gamma_{jn}(n) = \frac{\gamma_j}{\sqrt{N}} \exp(i q n a) \rightarrow \gamma_{jm}(n) = \gamma_j \delta_{m,n}. \tag{18}
\]

where \( \gamma_j \) are independent of \( n \). Eq. \( \Phi_{1,2} \) indicates that the phonon displacement accompanies the electron at the site \( n \). The same is valid for the squeezing, \( r_m(n) = r_\delta_{m,n} \).

Full Bloch solution to the transformed lattice Hamiltonian \( H = H_L + H_T \), \( H \) is chosen as a generalized Fulton-Gouterman variational ansatz \( \PsiFG(k) \) in the vector form (Eq. \( \Phi_{1,2} \))

\[
\Psi_{FG}(k) = \frac{1}{\sqrt{C}} \sum_n \exp(i k n a) \left( \phi_1(n) \psi_1(n) \phi_2(n) \psi_2(n) \right), \tag{19}
\]

where the electron parts \( \psi_1 \) are defined by \( \psi \) and the phonon parts \( \phi \) by \( \Phi_{1,2} \) and \( \tilde{\gamma}_{jm}(n) \) of \( \tilde{\gamma} \).
We have investigated the model (3) in a former paper with respect to the stability of a soliton ground state against quantum fluctuations. However, the variational wave function we used did not account for the two-center nature of the wave function here respected by the reflection parameter $\eta$ (18).

In what follows the ground state energy as function of optimized variational parameters $\eta$, $\gamma_1, \gamma_2, r$ will be determined.

### III. THE GROUND STATE

When considering the ground state of $\tilde{H} = \tilde{H}_L + \tilde{H}_T$, (6) and (7), we omit the electron and phonon dynamic terms by setting $k = 0, q = 0$.

By averaging $\tilde{H} = \tilde{H}_L + \tilde{H}_T$ (6) and (7) over the phonon wave functions (19) with (8) and (11) one obtains for the site Hamiltonian (8) (Appendix B)

$$\langle \tilde{H}_L \rangle / N \equiv H_{ph} + H_{int},$$

where

$$H_{ph} = \frac{\Omega}{2} (\cosh 4r + 1) I$$

$$+ \Omega \frac{1 + \eta^2 - 2\eta e^{-8r_1} \exp(-2|\gamma_1|^2)}{1 + \eta^2 + 2\eta \exp(-2|\gamma_1|^2)} |\gamma_1|^2 I + \Omega |\gamma_2|^2 I,$$

$$H_{int} \equiv H_\alpha + H_\beta = \frac{\alpha (1 - \eta^2)}{1 + \eta^2 + 2\eta \exp(-2|\gamma_1|^2)} |\gamma_1|^2 \sigma_z - \frac{\beta (1 + \eta^2) \exp(-2|\gamma_1|^2) + 2\eta}{1 + \eta^2 + 2\eta \exp(-2|\gamma_1|^2)} |\gamma_2|^2 I,$$

where $H_\alpha$ and $H_\beta$ are $\alpha$- and $\beta$-dependent parts of the interaction $H_{int}$ (23). From the transfer Hamiltonian $H_T$ (9) there remains

$$\langle \tilde{H}_T \rangle N = -T \exp(-W) M$$

$$\equiv 2 (H_{T1} I + H_{T2} i\sigma_y + H_{T3} \sigma_z + H_{T4} \sigma_x).$$

The Debye-Waller factor $\exp(-W) M$ in (24) is given in the Appendix B. The differential part of the Debye-Waller factor $W$ in the ground state is zero. For $M$ it holds

$$M = [(1 + E_1^2) I + (1 - E_1^2) E_2 \sigma x_n]$$

$$\times [(1 + E_2^2) I + (1 - E_2^2) \sigma x],$$

where $E_i$ are given by (Appendix B)

$$E_1 \equiv \exp(-2|\gamma_1|^2), \quad E_2 \equiv \exp(-2|\gamma_2|^2).$$

Expressions $E_1$ and $E_2$ in the ground state are independent of $q$ and $n$ because of the form of $\gamma_{iq}(n) = \gamma_i \exp(-iqn)$.
The "heavy" polaron is dominant at \( \chi < 1 \) where the broad minimum \( \gamma_1 < 0 \) is dominating. (ii) Close to \( \chi = 1 \), the energies of two minima go very close together (their difference is of the order of the phonon energy \( \Omega \)). They drop to one narrow minimum which represents a new ground state. Close to \( \chi = 1 \), continuous transition to a new ground state occurs. It stabilizes at \( \chi > 1 \), where (optimized) \( \gamma_1 \) value is close to 0 and \( \gamma_2 > 0 \). This region is referred to as a "light" polaron region because, owing to the abrupt decrease of \( \gamma_1 \approx 0 \) at \( \chi > 1 \), the effective mass of the intralevel polaron drops to almost its free-electron value, i.e., the polaron selflocalization vanishes in the "light" region. Because of this "undressing", the transport characteristics of the excited electron would increase. Moreover, due to the tiny distance between the levels, their coupling takes place by the exchange of virtual phonons. At suitable conditions, in the excited state, when both levels are occupied by electrons of opposite spins, the mechanism of virtual phonon exchange implies the pairing of electrons, i.e. formation of "light" bipolarons.

The ground state energy, especially its behavior dependent on pairs of parameters \( \chi, \Omega \) and \( \chi, \mu \) is illustrated in details in Fig. 2. While being weakly \( \Omega \)-dependent, the energy strongly decreases with \( \chi \) inside the "light" phase (Fig. 2a). The position of the phase line is slightly shifted from \( \chi = 1 \) at \( \Omega = 0 \) to higher values of \( \chi \) with increasing \( \Omega \). This is consistent with the fact that the phonon fluctuations are most effective when the difference of the energies of the phases is of the order of the phonon energy.

The ground state energy in the "heavy" region (\( \chi < 1 \)) is independent of \( \chi \), its decrease inside the "light" region (\( \chi > 1 \)) is dependent on the effective coupling \( \mu \) (Fig. 2b). The energy decrease due to \( \mu \) is stronger in the "light" phase (depending on \( \chi \)) than in the "heavy" phase.

The region of importance of reflection measure \( \eta \) and \( r \) is illustrated in the Fig. 3. There we show the difference between the ground state energy with \( r \) and \( \eta \) omitted and ground state with four variational parameters calculated numerically. However, contribution due to \( r E_G(\eta, r = 0) \) is small except of the region of fluctuations visualized in Fig. 4. One can see, that the selflocalization due to phonons 2 in the "heavy" region \( \sim -\gamma_2 \) clearly implies the "cave" in the ground state energy due to the reflection measure \( \eta \) (anharmonicity) of the ground state (Fig. 3). (ii) "light" polaron (\( \gamma_1 \) small, \( E_1 \approx 1, H_{T_2}, H_{T_3} \approx 0 \)):

\[
\gamma_1 \approx \frac{-\alpha e^{4r}}{2 TE_1^2 \left( 1 + \frac{2^2}{2^2} + \frac{\Omega e^{4r}}{TE_1^2} \right)},
\]

\( \gamma_2 \) is small except of the region of fluctuations visualized in Fig. 4. One can see, that the selflocalization due to phonons 2 in the "heavy" region \( \sim -\gamma_2 \) clearly implies the "cave" in the ground state energy due to the reflection measure \( \eta \) (anharmonicity) of the ground state (Fig. 3). (ii) "light" polaron (\( \gamma_1 \) small, \( E_1 \approx 1, H_{T_2}, H_{T_3} \approx 0 \)):

\[
\gamma_1 \approx \frac{-\alpha e^{4r}}{2 TE_1^2 \left( 1 + \frac{2^2}{2^2} + \frac{\Omega e^{4r}}{TE_1^2} \right)} \approx 10^{-8},
\]

\[
\gamma_2 \approx \frac{\beta}{2 TE_2^2 (2 + \frac{\Omega}{TE_1^2})}.
\]

In the "light" region the fluctuations of \( \gamma_1 \) are missing as well as the fluctuations of the energy. This is consistent with the above result of the resistance of the narrow minimum against \( \eta \).

For both "heavy" and "light" polaron a dependence of \( \gamma_1 \) on the nonadiabaticity parameter \( \Omega/T \) appears. It implies the dependence of the Debye-Waller factor and consequently of the polaron mass on the phonon frequency \( \Omega \). This can be thought of as an analogy of the isotope effect at zero temperature.

In the "heavy" phase, electron transitions mediated by phonons 2 to the upper level enhance fluctuations \( \sim \gamma_2 \) which mix phonons 2 with phonons 1 and contribute to the fluctuations of the ground state energy of the heavy region. This is the reason for the similarity of the results in Figs. 3 and 4.

**IV. METAL-INSULATOR TRANSITION**

To illustrate the effect of various interactions let us consider first a simple two level case \( (T = 0) \). The ground state will be obtained by the numerical minimalization of energy

\[
E^0 = H_{ph} + H_{\alpha} + H_{\beta},
\]

where \( H_{\alpha} \) and \( H_{\beta} \) are \( \alpha \) and \( \beta \) dependent components of the interaction term \( H_{int} \). The result is of the form

\[
E^0_G = \frac{\Omega}{2} (\cosh 4r^0 + 1) - H_{P\alpha} - H_{P\beta},
\]

where the label 0 specifies the optimized variational values. In \( (34) \), \( H_{P\alpha} \) and \( H_{P\beta} \) are contributions of the selflocalization energies of two coupled polarons proportional to \( \alpha^2/2\Omega \) and \( \beta^2/2\Omega \), respectively. The splitting of the levels is implied to be

\[
\Delta^0 = 2|E^0_G|.
\]

Respectively a lattice of JT molecules \( (T \neq 0) \) shows either metallic or insulating phase behavior depending
on whether the splitted bands overlap or not. Usually the resulting situation depends strongly on the phonon renormalization of the gap and of the electron band including phonon fluctuations.

Our aim here is to investigate the metal-insulator transition due to the competition of the polaron localization and the delocalization due to the transfer including the phonon assisted electron transfer effects. Namely, the transport terms $H_{T_i}$ compete the level splitting because of the complex interplay of the diagonal and off-diagonal contributions to the band width. In order to find the value of the gap as an order parameter of the metallic-insulator phase transition it is necessary to perform usual renormalization: $SU(2)$ symmetry of the right- and left-moving electrons and holes of the transfer part of Hamiltonian (1) makes it possible to split electron operators onto an electron and a hole part,

$$c_i = c_{i,+} + c_{i,-}, \quad i = 1, 2,$$

(36)

the signs ± indicating directions of the electron motion. In view of the reflection symmetry of the two-level local part of Hamiltonian (1) against the level $E = 0$ in the middle between the levels electron operators (36) can be rewritten in a renormalized form

$$c_1 = c_{1,+}^{(d)} + c_{1,+}^{(h)}, \quad c_2 = c_{2,-}^{(h)} + c_{2,-}^{(d)}.$$  

(37)

This renormalization implies the change of the sign of $T$ ($H_{T_i}$) for holes $(E < 0)$.

There are two pairs of electrons and holes, $c_{1,+}^{(e)}, c_{1,+}^{(h)}$ and $c_{2,-}^{(e)}, c_{2,-}^{(h)}$; i.e., two state vectors $(f_+^e g_-^h)$ and $(-g_- f_+^e)$ which satisfy equations

$$H_m \begin{pmatrix} f_+^e \\ g_-^h \end{pmatrix} + \begin{pmatrix} -\Delta/2 & 0 \\ 0 & \Delta/2 \end{pmatrix} \begin{pmatrix} -g_-^e \\ f_+^h \end{pmatrix} = 0,$$

(38)

$$H_m \begin{pmatrix} -g_-^e \\ f_+^h \end{pmatrix} + \begin{pmatrix} \Delta/2 & 0 \\ 0 & -\Delta/2 \end{pmatrix} \begin{pmatrix} f_+^e \\ g_-^h \end{pmatrix} = 0,$$

(39)

where $H_m$ results from the minimalization of (20) with respect to the variational parameters, (23),

$$H_m = \begin{pmatrix} -E_G & 0 \\ 0 & E_G \end{pmatrix},$$

(40)

and $E_G$ given by (24).

The solution for the gap $\Delta$ reads finally (see Figs. 2b-4b)

$$\Delta = 2|E_G(T \rightarrow -T)|$$

(41)

and implies a condition for the stability of either the insulating phase, if $E_G(T \rightarrow -T) > 0$, or the metallic phase in the opposite case, where $\Delta \equiv 0$.

Fig. 5. depicts both I-M and "heavy"-"light" transitions. In the "heavy" phase, at small $\Omega$ the I-M transition line is determined by the critical coupling $\mu_H(\Omega)$ independent of $\chi$ up to $\chi = 1$. In the "light" phase, the critical coupling $\mu_L(\Omega, \chi) < \mu_L(\Omega)$ decreases with increasing $\chi$. The point $(\chi = 1, \mu_H(\Omega))$ is the only point of coincidence of the "heavy"-"light" transition and the I-M transition. At small $\mu$ the fluctuations support the metallic phase in the "light" region (Fig. 5a), while at small $\chi$ (and sufficiently large $\mu$ that the insulating phase could be stable) they support the metallic phase in the heavy region (Figs. 5a, b).

The I-M transition can appear in the "heavy" region at large $\mu$ (40) and small $\Omega$ (Fig. 2a). From Fig. 3 (medium values of $\mu$) one can locate the region of relevant reflection $\eta$ into the metallic phase, where the bands overlap. The "light" region ($\chi > 1$) is resistant against $\eta$: no similar effect as that shown in Fig. 3 there exists. Therefore, in the "heavy" region the metallic phase is strongly supported due to the fluctuations at weak couplings $\mu$.

"Heavy" phase is therefore metallic in the broad range of parameters except of strong couplings (Fig. 2b). At certain (large) $\mu$ the I-M transition drops close to the line $\chi = 1$, so that the transition coincides with the "heavy" to "light" polaron transition. With decreasing $\mu$ the I-M transition line moves to larger $\chi$ (Fig. 5b): the M-I transition moves away from the "heavy"-"light" transition into the "light" region. In the "light" region the I-M transition line moves to smaller $\mu$ when compared with the heavy region (Fig. 6).

As one can also see from Figs. 6 and 8, the I-M transition line in the phase diagram $\mu, \Omega$ is strongly $\Omega$-dependent. The phase line in the plane $(\mu, \Omega)$ between the phases shows the broadening of the metallic phase with growing $\Omega$, i.e. the metallic phase is supported by the quantum fluctuations. Respective ground state energy slightly increases with $\Omega$.

To make effects of different contributions $H_{T_i}$ more transparent, we can first calculate analytically effect of the diagonal terms $H_{T_1}$ and $H_{T_3}$. (Let us note that neglecting the off-diagonal transfer, i.e. $H_{T_2}$, $i = 2, 4$ in (27), means neglecting the additional splitting of the bands. More precisely, it means neglecting the off-diagonal terms in Eq. (8).)

Minimization of the energy (28) with $H_{T_2} = H_{T_4} = 0$

$$E^1 = H_{ph} + H_\alpha + H_\beta + H_{T_1} + H_{T_3}$$

(42)

implies the ground state of a similar structure as that one of (34),

$$E_G = \frac{\Omega}{2} (\cosh 4r^1 + 1) - H_{T_1}^1 - H_{T_3}^1,$$

(43)

where the label 1 specifies the optimized variational values. Respective splitting yields

$$\Delta^1 = 2|E_G^1 - 2(H_{T_1}^1 + H_{T_3}^1)|$$

$$= 2|H_{T_1}^1 - H_{T_3}^1 - 2(H_{T_1}^1 - H_{T_3}^1)|.$$  

(44)
VI. CONCLUSIONS

The selfconsistent polaron potential provided by the Holstein intralevel and interlevel electron-phonon couplings in our two-level lattice model is highly nonlinear function of phonon displacements (Fig. 1). As a consequence, there occurs a competition between the regime of two nonequivalent broad minima at $\pm \gamma_1$ and $\gamma_2$ close to 0 related to two electron levels and the regime of one narrow minimum at $\gamma_2 > 0$ and $\gamma_1$ close to 0 when both broad minima collapse to a single one, so that both levels drop to that minimum. The broad minima dominate at $\chi < 1$, the narrow one at $\chi > 1$. At E$\otimes$e Jahn-Teller symmetry ($\chi = 1$) energies of the broad and narrow minima coincide and the phonon-assisted tunneling due to the nonadiabatic fluctuations reaches its maximum close to this limit. When $\chi$ is approaching to 1, there occurs pairing of the levels due to the interlevel onsite and intersite polaron tunneling mediated by the exchange of virtual phonons. The narrow minimum is suppressed if the electron transfer energy $T$ decreases.

Hence, we have identified two regions of stability: (i) the region of the dominating "heavy" polaron ($\chi < 1$) related to the broad minimum at negative $\gamma_1$ (the absolute minimum) and $\gamma_2 \approx 0$ and (ii) the region of the dominating "light" polaron ($\chi > 1$) related to the narrow minimum at $\gamma_1 \approx 0$ (Fig. 1). The almost vanishing polaron selflocalization in the "light region" ("undressing") means enhancement of the polaron transfer due to respective decrease of the polaron effective mass. Even in the "heavy" phase the effect can be present due to fluctuations of the "light" phase (Figs. 3 and 4).

Close to the transition from "heavy" to "light" polaron at $\chi = 1$, a continuous transition to new ground state that is stable at $\chi > 1$ occurs (Fig. 2). In this ground state the formation of "light" bipolarons is possible which are characterized by the enhancement of the effective transfer due to the vanishing selflocalization. The pairing of the polarons is caused by virtual exchange of phonons 1 mediated by phonons 2 between the electrons in both levels at suitable configuration. This effect might be of interest from the point of view of bipolaron mechanisms of the superconductivity. The I-M transition and "heavy"-"light" phase coincide in the crossing point of the lines $\chi = 1$ and $\mu_H(\Omega)$ (critical line of I-M transition in the "heavy" phase, Fig. 5a).

The Debye-Waller factor (25) shows nonadiabatic dependence on the phonon frequency $\Omega$ through $\gamma_1$, (32), (27). Then, the effective transfer parameter of electrons is respectively increased and the electron effective mass decreased. This effect reminds on the "isotope effect", however, at zero temperature.

The metal-insulator transition occurs in both regions: "heavy" region is the region of dominating metallic phase, where the transition to the insulating phase can occur only at sufficiently large $\mu$ (Fig. 5). On the other hand, in the "light" region the I-M transition can occur
at relatively small $\mu$ (Figs. 5 and 6). For certain $\mu$ the I-M transition can coincide with the "heavy-light" polaron transition at $\chi = 1$ (Fig. 5a). The interlevel and the combined interlevel and intersite electron Rabi oscillations in the ground state, are identified to be the main reason for the shift of the I-M transition line to stronger effective couplings, i.e. in the support of the metallic phase (Figs. 5 and 7). Fig. 5a illustrates the existence of the "light" polaron in both the insulating and metallic phase.

Fluctuations of the phonon conjugated coordinates and their product exhibit peaks (Fig. 9) in the region of parameters where the effect of $\eta$ (Figs. 3, 4) is relevant. Consequently, the effect appears only in the "heavy" region reaching its maximum at $\chi = 1$ and growing with $\Omega$. The peaks evidence for the strongly anharmonic behavior of the "heavy" polaron in the region of relevance of $\eta$. In the "light" region, there occurs a degeneracy over $\eta$ (no effect of $\eta$ on the minimum of the potential), i.e. no analogous effect of the fluctuations, but nearly a harmonic oscillator is observed. This is obviously due to the specific form of the variational ansatz, which is inspired by the shape of the "pure" heavy polaron (i.e. with $\chi < 1$). Therefore the ansatz\(^9\), reflecting the essentials of the "heavy" polaron, is proper for describing the heavy region, but when concerning the "light" region, it presents, in some extent, a heuristic extrapolation. We could have started from another ansatz underlying the essentials of "light" polaron (which could be, for example, inspired for the "pure" case of $\chi >> 1$) in order to investigate the "light" region and gain some extrapolation towards smaller $\chi$. Naturally, also the transition in E\(\otimes\)e Jahn-Teller case ($\chi \approx 1$), needs further considerations.

VII. ACKNOWLEDGEMENTS

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Appendix A.

We shall use following formulas\(^9\):

\[
D(\gamma)S(r) = S(r)D(\tilde{\gamma}), \quad \tilde{\gamma} = \gamma e^{-2r} \tag{A1}
\]

\[
S^{-1}(r)bS(r) = b \cosh 2r + b^\dagger \sinh 2r \tag{A2}
\]

\[
\langle 0\vert S^{-1}(r_m(n))D^{-1}(\gamma_m(n))D_m(n + 1)S(r_m(n + 1)) \vert n\rangle = \exp\left(-\frac{1}{2}\frac{\gamma_m(n + 1) - \gamma(n)}{2}\right), \tag{A3}
\]

where $\gamma = \gamma e^{-2r}$.

For averages with using virtual Fock states $\vert n\rangle$ we use formulas

\[
\langle 0\vert D^{-1}S^{-1}(-1)^{b\dagger S}SD\vert 0\rangle = \gamma \langle -1\vert b^\dagger S\vert \rangle_g = \sum_{n=0}^{\infty} (-1)^n |\langle n\vert \gamma\rangle|^2, \tag{A4}
\]

where $\vert \gamma\rangle = SD\vert 0\rangle = S\vert \gamma\rangle$ and,

\[
\langle n\vert \gamma\rangle_g = \frac{1}{(n!\mu)^{1/2}} \left(\frac{\nu}{2\mu}\right)^{n/2} H_n \left(\frac{\gamma}{2}\left(\frac{\mu}{\nu}\right)^{1/2}\right)
\times \exp\left(-\frac{|\gamma|^2}{2} + \frac{\nu\gamma^2}{2\mu}\right). \tag{A5}
\]

Here, $\mu = \cosh 2r$, $\nu = \sinh 2r$, $\mu^2 - \nu^2 = 1$, here $\nu$ is real.

Appendix B.

The average of the Hamiltonian in\(^9\) referred to one site results in

\[
\frac{\langle H_L \rangle}{N} = H_{ph} + H_{int}, \quad \text{where}
\]

\[
H_{ph} = \frac{1}{2CN^2} \sum_{m,n} C_{1m,n} (\cosh(4r_m(n)) + 1) I_n
\]

\[
+ \frac{1}{CN^2} \sum_{m,n} (1 + \eta^2 - 2e^{-\sigma_m(n)} \eta \exp(-2|\gamma_1m(n)|^2)) |\gamma_1m(n)|^2 I_n
\]

\[
+ \frac{1}{CN^2} \sum_{n,m} C_{1m,n} |\gamma_2m(n)|^2 I_n. \tag{B1}
\]

\[
H_{int} \equiv H_\alpha + H_\beta = \frac{1}{CN^2} \sum_{n,m} \left\{ \alpha (1 - \eta^2)^2 |\gamma_1m\sigma_z n \right\}
\]

\[-\frac{1}{2} \left[ (1 + \eta^2) \exp(-2|\gamma_1m|^2) + 2\eta |\gamma_2mI_n \right] + H.c., \tag{B2}\]

and

\[
H_T = -\frac{T}{CN^2} \sum_{n,m} C_{1m,n} \exp(-W_m(n)) M_m(n)
\]

\[
\equiv 2(HT_1 I + HT_2 I \sigma_y + HT_3 I \sigma_z + HT_4 I \sigma_x). \tag{B3}
\]
In the continuum limit (B5) yields

\[ E \exp\left(\langle E \rangle\right) \]

With the help of (A4) and (A5) one obtains for \( E_m(n) \) in (B3)

\[ W(n) = \frac{1}{2N} \sum_m \left( \left| \frac{d\gamma_{1m}(n)}{dn} \right|^2 + \left| \frac{d\gamma_{2m}(n)}{dn} \right|^2 \right). \]  

(B4)

In the continuum limit (B5) yields \( E_m(n) \rightarrow \exp(-2|\gamma_m(n)|^2). \)

* Electronic address: majere@prfnw.upol.cz

** on leave of absence from the Institute of Nuclear Research UAN, Pr. Nauki 47, Kiev, Ukraine.

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VIII. FIGURE CAPTIONS

Fig. 1. Potential \( [21] \) for \( \chi = \beta/\alpha = 0.5, \mu = 2 \) and \( \Omega = 0.05 \).

Fig. 2. The ground state energy \( [29] \) in the \( \chi-\Omega \) plane at \( \mu = 2.5 \) (a) and (b) in the \( \chi-\mu \) plane at \( \Omega = 0.5 \). The "light" polaron is evidently much more sensitive to effects of \( \chi \) and \( \mu \) than the "heavy" polaron.

Fig. 3. The range of relevance of the reflection parameter \( \eta \): Difference \( \Delta E_G = E_G(\eta = 0, r = 0) - E_G \), for \( \chi = 1, E_G \) is the exact ground state \( [29] \). For \( \chi < 1 \), the difference increases with \( \chi \) reaching its maximum at \( \chi = 1 \). At \( \chi > 1 \) it drops to zero, i.e. the narrow minimum "light" phase is resistant against \( \eta \).

Fig. 4. Displacement of phonons 2 in the "heavy" region \( \gamma_2^2 \); it evidently causes the "cave" due to reflection \( \eta \) of the ground state energy in the "heavy" region (Fig. 3).

Fig. 5. (a) The gap in the plane of \( \mu \) and \( \chi \) for \( \Omega = 0.5 \). While the critical coupling \( \mu_H(\Omega) \) for I-M transition in the "heavy" phase is very slightly dependent of \( \chi \), \( \mu_L(\Omega, \chi) \) in the "light" phase is \( \chi \) dependent. (b) The shift of the metal-insulator transition in the "heavy" region due to quantum fluctuations at strong coupling (\( \mu > \mu_H(\Omega) \)).

Fig. 6. The gap in the "light" region as function of \( \Omega \) and \( \mu \) for \( \chi = 1.5 \). The fluctuations increase with \( \Omega \).

Fig. 7. The competition of the level splitting and band width \( T \) terms \( [24] \). \( \Delta_0 \) is splitting of the levels \( [25] \), \( \Delta_1 \) neglects the off-diagonal terms \( H_{T_2}, H_{T_4} \), \( [34] \). \( \Delta \) is the exact gap given by \( [11] \).

Fig. 8. Comparison of the phase diagram of the exact model \( [1] \) (solid line) with that one neglecting off-diagonal transfer (dashed line). The metallic phase occurs on the left and the insulator on the right of the respective line.

Fig. 9. Quantum fluctuations of (a) the coordinate \( \Delta^2 Q_1 \), (b) momentum \( \Delta^2 P_1 \) and (c) their product \( \Delta^2 Q_1 \Delta^2 P_1 \). (d) Detail of Fig. 3 underlying the region of parameters of Figs. (a)-(c).
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