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THE SOLITON GROUND STATE OF AN ELECTRON OR EXCITON IN THE EXTENDED JAHN-TELLER SYSTEM IN ONE DIMENSION

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In this paper a variational method for the intermediate ground state of a quasiparticle (exciton, electron or hole) interacting with dispersionless optical vibrations in a one-dimensional chain of the E-e Jahn-Teller systems is investigated. The intermediate and strong nonadiabatic range constitutes a kind of "critical" region, where the electron-phonon coupling constant g and the nonadiabatic parameter γ are approximately equal to one. We have investigated the conditions for the existence and for the stability of a soliton ground state of the extended one-dimensional Jahn-Teller system in one dimension which is affected by quantum fluctuations of optical phonons. The soliton was found to be stable for a sufficiently strong electron-phonon coupling strength. Although the nonadiabatic parameter γ is chosen sufficiently large, comparable to one, the presented model for the one-dimensional chain of the E-β Jahn-Teller systems leads to substantially lower ground state energies, in contrast with one which is presented in previous studies. Our soliton ground state energies, for the one-dimensional chain of the E-β Jahn-Teller systems, are in good agreement with those which are presented for the one-dimensional chain of one-level molecules in previous studies.

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1 Introduction

The interaction of an electron, a hole or an exciton with vibrations of a crystal lattice leads to some peculiar phenomena, one of which is an autolocalization or self-trapping of the quasiparticle. This phenomena is interesting in one-dimensional systems in connection with the soliton regime of charge and energy transport. In the last time various analytical and numerical investigations of Davydov's soliton [1–3] were carried out because the attempts to study the problem of the ground state of an electron using a translationally invariant ground state wave functions have not led to satisfying results. Electron-phonon bound states are relevant for understanding various physical effects. Nonadiabatic effects become important if the scales of phonon and electron energies are comparable, i.e., the ratios $\hbar\omega/T$ (ω is the phonon frequency, T is the intersite electron transfer parameter) are not too small.

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In contrast to the lattice of Jahn-Teller molecules, the quantum effects in the E-e Jahn-Teller system are quite well understood [4–6]. We investigate the ground state of an electron (exciton)-phonon system in the extended Jahn-Teller system in one dimension, and estimate the conditions necessary for the realization of a spontaneously localized state in the case of the interaction with a dispersionless optical mode.

In the tight-binding approximation the Hamiltonian of the extended Jahn-Teller system in one dimension has the form

$$\begin{aligned} H = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \Bigg\{ \hbar\omega \sum_{k=1}^{2} \left(b_{n,k}^{+} b_{n,k} + \frac{1}{2} \right) + \alpha_0 \left(c_{n,2}^{+} c_{n,2} - c_{n,1}^{+} c_{n,1} \right) X_{n,1} \\ - \beta_0 \left(c_{n,2}^{+} c_{n,1} + c_{n,1}^{+} c_{n,2} \right) X_{n,2} - T \sum_{j=1}^{2} \left(c_{n,j}^{+} c_{n+1,j} + c_{n+1,j}^{+} c_{n,j} \right) \Bigg\} , \end{aligned} \tag{1}$$

where N is the number of sites, $X_{n,k} = (b_{n,k}^{+} + b_{n,k})/\sqrt{2}$ for $k = 1, 2$ and $b_{n,k}^{+}$ and $b_{n,k}$ are the creation and the annihilation boson operators for site n of mode k (frequency ω), respectively, α_0 and β_0 are the electron-phonon coupling constants, $c_{n,j}^{+}, c_{n,j}$ are the electron creation and annihilation operators for site n related to two degenerate levels, $j = 1, 2$, respectively, and T is the intersite electron transfer parameter. The first interaction term causes the splitting of the degenerate level, and the second one represents phonon-assisted transitions between the levels. Transitions between the levels 1 and 2 of the two neighbour sites are not allowed.

2 The approximation of the intermediate ground state

The calculation of the expectation value of H consists of the next five steps:

Step 1

By means of the unitary transformation

$$U = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} U_n , \quad U_n = U_{n,2} U_{n,1} ,$$

where

$$U_{n,k} = \frac{1}{\sqrt{2}} \left[\left(1_B + (-1)^k G_k(n) \right) \left(\frac{1_n}{2} - \mathrm{i}_0 \sigma_{ny} \right) + \left(1_B + (-1)^{k+1} G_k(n) \right) \left(\sigma_{nx} + \sigma_{nz} \right) \right],$$

$$G_k(n) = \exp\left(\mathrm{i}_0 \pi b_{n,k}^{+} b_{n,k} \right) \quad \text{for } k = 1, 2,$$

$$\sigma_{nx} = (1/2) \left(|n,1\rangle\langle n,2| + |n,2\rangle\langle n,1| \right) ,$$

$$\sigma_{ny} = -\mathrm{i}_0 \,(1/2)\,(|n,2\rangle\langle n,1| - |n,1\rangle\langle n,2|)\ ,$$
$$\sigma_{nz} = (1/2)\,(|n,2\rangle\langle n,2| - |n,1\rangle\langle n,1|)\,,$$
$$1_n = |n,1\rangle\langle n,1| + |n,2\rangle\langle n,2|,$$
$$|n,j\rangle = c^+_{n,j}|0\rangle_e \qquad \text{for } j = 1 \text{ and } 2,$$

$|0\rangle_e$ is the electron vacuum state, $|n,i\rangle\langle n,j|$ are the projection operators from the linear space generated by the vector $|n,j\rangle$ on the linear space generated by the vector $|n,i\rangle$ $(i,j = 1,2)$, $\mathrm{i}_0 = \sqrt{-1}$, and 1_B is the unit operator on the space of boson functions, the unitary transformed Hamiltonian is obtained from (1)

$$U\frac{H}{\hbar\omega}U^+ = \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \left\{ \sum_{k=1}^{2} \left(b^+_{n,k} b_{n,k} + \frac{1}{2} \right) 1_n + \left(\frac{\alpha_0}{\hbar\omega} X_{n,1} - \frac{\beta_0}{\hbar\omega} G_1(n)\, X_{n,2} \right) 1_n \right.$$
$$-\frac{T}{\hbar\omega}\Big\{ \left[1_B + G_1(n)\,G_1(n+1)\right]\left[1_B + G_2(n)\,G_2(n+1)\right] (|n,1\rangle\langle n+1,1| + |n,2\rangle\langle n+1,2|)$$
$$+ \left[1_B - G_1(n)\,G_1(n+1)\right]\left[G_2(n) + G_2(n+1)\right] (|n,1\rangle\langle n+1,1| - |n,2\rangle\langle n+1,2|) \Big\}$$
$$-\frac{T}{\hbar\omega}\Big\{ \left[1_B + G_1(n)\,G_1(n+1)\right]\left[1_B - G_2(n)\,G_2(n+1)\right) (|n,2\rangle\langle n+1,1| + |n,1\rangle\langle n+1,2|)$$
$$+ \left[1_B - G_1(n)\,G_1(n+1)\right]\left[G_2(n) - G_2(n+1)\right] (|n,1\rangle\langle n+1,2| - |n,2\rangle\langle n+1,1|) \Big\}$$
$$\left. + \text{h.c.} \right\}. \tag{2}$$

Step 2

The choice of a suitable trial ground state wave function for the Hamiltonian (2) is the central problem for the ground state energy approximation. We choose the following form of the ground state wave function:

$$\Psi_K = \sum_{j=1}^{2} \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \beta_j(m)\, e^{\mathrm{i}_0 K m} |m,j\rangle D(m)\, |0\rangle_{ph}\,, \tag{3}$$

where

$$|0\rangle_{ph} = \prod_{m=(-\frac{N}{2}+1)}^{\frac{N}{2}} \prod_{k=1}^{2} |0\rangle_{ph,m,k}$$

and $|0\rangle_{ph,m,k}$ is the vacuum state of mode k for site m, K is the wave vector,

$$D(m) = \exp\left[(1/\sqrt{N}) \sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{k=1}^{2} \zeta_{n,k}(m) \left(b_{n,k}^{+} - b_{n,k}\right)\right]$$

and $\zeta_{n.k}(m)$ and $\beta_j(m)$ are the real variational parameters. $D(m)\,|0\rangle_{ph}$ is nothing else than the lattice state associated to the polaron centered on site m, and it describes a superposition of coherent states,

$$\exp\left[(1/\sqrt{N})\zeta_{n,k}(m)\left(b_{n,k}^{+} - b_{n,k}\right)\right].$$

This choice is the generalization of the ground state wave function given in [7] for a quasi-particle interacting with dispersionless optical vibrations in a one-dimensional one-level chain of molecules.

The expectation value of $U\,(H/\hbar\omega)\,U^{+}$ in the trial ground state (3) has the form

$$\begin{aligned}
&\langle \Psi_K, U\frac{H}{\hbar\omega}U^{+}\Psi_K\rangle = \\
&\sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \Bigg\{ \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{j=1,2} \beta_j^2(n) \sum_{k=1}^{2} \frac{\zeta_{m,k}^2(n)}{N} + \frac{\alpha_0}{\hbar\omega}\sqrt{2}\frac{\zeta_{n,1}(n)}{\sqrt{N}} \sum_{j=1}^{2} \beta_j^2(n) \\
&-\frac{\beta_0}{\hbar\omega}\sqrt{2}\frac{\zeta_{n,2}(n)}{\sqrt{N}} \exp\left(-2\frac{\zeta_{n,1}^2(n)}{N}\right) \sum_{j=1}^{2} \beta_j^2(n) - \frac{T}{4\hbar\omega}\cos(K) \sum_{i,j,\Delta} \lambda_{i,j,\Delta} \qquad (4)\\
&\times\left\{\beta_i(n)\,\beta_j(n+1)\exp\left[-W_\Delta(n,n+1)\right] + \beta_i(n)\,\beta_j(n-1)\exp\left[-W_\Delta(n,n-1)\right]\right\}\Bigg\},
\end{aligned}$$

where

$$\begin{aligned}
&W_\Delta(n, n\pm 1) = \sum_{k=1}^{2} W_k^{\pm}(n) \\
&+\sum_{k=1}^{2}\left(\left[1-(-1)^{\delta_k^n}\right] \frac{\zeta_{n,k}(n\pm 1)}{\sqrt{N}} \frac{\zeta_{n,k}(n)}{\sqrt{N}} + \left[1-(-1)^{\delta_k^{n\pm 1}}\right] \frac{\zeta_{n\pm 1,k}(n\pm 1)}{\sqrt{N}} \frac{\zeta_{n\pm 1,k}(n)}{\sqrt{N}}\right)
\end{aligned}$$

with

$$W_k^{\pm}(n) = \frac{1}{2N} \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} \left|\zeta_{m,k}(n\pm 1) - \zeta_{m,k}(n)\right|^2,$$

$$\Delta = (\delta_1^n, \delta_1^{n\pm 1}, \delta_2^n, \delta_2^{n\pm 1}),$$

where $\delta_k^n, \delta_k^{n\pm 1}$ are equal to 0 or 1 for every $n = -\frac{N}{2}+1, \ldots, \frac{N}{2}$ and for $k = 1$ and 2, and the values $\lambda_{i,j,\Delta}$ for $i, j = 1$ and 2 are equal to $+1, -1$, or 0, respectively. The definition of the values $\lambda_{i,j,\Delta}$ is clear from the shape of the Hamiltonian (2), and it can be illustrated as

$$\lambda_{1,2,(1,1,0,0)} = +1, \quad \lambda_{2,1,(1,1,1,1)} = -1, \quad \lambda_{1,1,(1,0,0,0)} = 0, \quad \lambda_{1,1,(0,0,0,0)} = +1.$$

From the shape of the Hamiltonian (2), we come to the next equalities:

$$(\delta_1^n, \delta_1^{n+1}, \delta_2^n, \delta_2^{n+1}) = (\delta_1^n, \delta_1^{n-1}, \delta_2^n, \delta_2^{n-1}) = (\delta_1^0, \delta_1^{0-1}, \delta_2^0, \delta_2^{0-1}) = (\delta_1^0, \delta_1^{0+1}, \delta_2^0, \delta_2^{0+1})$$

for every $n = -\frac{N}{2} + 1, ..., \frac{N}{2}$.

Step 3

We choose the method of the Lagrange multipliers to find the minimum of the expectation value (4).

In our model the Lagrangian of the form

$$\Lambda = \langle \Psi_K, U \frac{H}{\hbar\omega} U^+ \Psi_K \rangle - E\Big(\sum_{n,j} \beta_j^2(n) - 1\Big) \tag{5}$$

is considered, where E is the Lagrange multiplier.

The method of Lagrange multipliers then leads to

$$\frac{\partial \Lambda}{\partial \beta_j(n)} = E\beta_j(n), \tag{6}$$

$$\frac{\partial \Lambda}{\partial \zeta_{q,k}^*(n)} = 0, \tag{7}$$

with $j = 1$ and 2,

$$\zeta_{q,k}^*(n) = \left(1/\sqrt{N}\right) \sum_{m=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-\mathrm{i}_0 qm} \zeta_{m,k}(n),$$

$$n = -N/2 + 1, ..., N/2,$$

and

$$q = (2\pi/N)\, m \text{ for } m = -N/2 + 1, ..., N/2.$$

It is evident that the equations (6) can be rewritten as

$$\begin{aligned} E\beta_j(n) &= \beta_j(n) \sum_m \sum_k \frac{\zeta_{m,k}^2(n)}{N} + \sqrt{2}\frac{\alpha_0}{\hbar\omega} \frac{\zeta_{n,1}(n)}{\sqrt{N}} \beta_j(n) \\ &- \sqrt{2}\frac{\beta_0}{\hbar\omega} \frac{\zeta_{n,2}(n)}{\sqrt{N}} \exp\left(-2\frac{\zeta_{n,1}^2(n)}{N}\right) \beta_j(n) - \frac{T}{4\hbar\omega} \cos(K) \\ &\times \sum_{j'=1}^{2} \sum_{\Delta} \lambda_{j,j',\Delta} \left[\beta_{j'}(n+1) \exp(-W_\Delta(n, n+1)) + \beta_{j'}(n-1) \exp(-W_\Delta(n, n-1))\right], \end{aligned} \tag{8}$$

where j, n, m and Δ are defined above.

Step 4

Because the expectation value $\langle \Psi_K, U\left(H/\hbar\omega\right) U^{+}\Psi_K \rangle$ contains $2N^2+2N$ variable parameters, equations (6) and (7) are not soluble for the large N in the general case, and therefore it is necessary to use a suitable approximate method for their solution.

In this paper the following variational method for the solution of the equations (6) and (7) is used:

The solution $\beta_j\left(n\right)$ of equations (8) for $j = 1, 2$ is considered in the form

$$\beta_j\left(n\right) = \kappa_j \psi_0\left(n\right), \tag{9}$$

where κ_j is a real variational parameter which is independent on n, and $\psi_0\left(n\right)$ is a probability density function fulfilling the condition

$$\sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \psi_0^2\left(n\right) = 1. \tag{10}$$

As $\langle \Psi_K, \Psi_K \rangle = 1$, the next equation is valid:

$$\sum_{n=-\frac{N}{2}+1}^{\frac{N}{2}} \sum_{j=1}^{2} \beta_j^2\left(n\right) = 1. \tag{11}$$

The equations (9), (10), and (11) lead to the next condition for variational parameters κ_j:

$$\sum_{j=1}^{2} \kappa_j^2 = 1. \tag{12}$$

Further, we assume that values

$$\frac{\zeta_{n,k}\left(n\right)}{\sqrt{N}}, \quad \frac{\zeta_{n+1,k}\left(n+1\right)}{\sqrt{N}}, \quad \frac{\zeta_{n-1,k}\left(n-1\right)}{\sqrt{N}}, \tag{13}$$

$$\frac{\zeta_{n,k}\left(n+1\right)}{\sqrt{N}}, \quad \frac{\zeta_{n,k}\left(n-1\right)}{\sqrt{N}}, \quad \frac{\zeta_{n+1,k}\left(n\right)}{\sqrt{N}}, \quad \frac{\zeta_{n-1,k}\left(n\right)}{\sqrt{N}}, \tag{14}$$

and $W_k^{\pm}\left(n\right)$ for each n are well approximated by the real variational parameters $\zeta_k\left(0\right), \zeta_k\left(1\right)$ and W_k for $k = 1, 2$, respectively, which are all independent of n. This assumption is considered in [8], too. Because the values $W_k^{\pm}\left(n\right)$ for $k = 1$ and 2, are non-negative, the values W_k are also considered to be non-negative.

In the Appendix B the expressions which define the values $\zeta_k(0)$ and $\zeta_k(1)$ for $k = 1, 2$ are given.

Another approximation which is used in our model is the so-called continuum approximation of the parameter n (i.e., $n = y/a$, where y is a real number and a is the lattice constant) [7–8].

By means of the approximations which are considered in Step 4, the equations (8) can be rewritten into the next approximate form:

$$
\begin{aligned}
E\kappa_j\psi_0(n) &= \kappa_j\psi_0(n)\frac{1}{N}\sum_{q,k}\left|\zeta_{q,k}(n)\right|^2+\sqrt{2}\frac{\alpha_0}{\hbar\omega}\zeta_1(0)\,\kappa_j\psi_0(n)\\
&-\sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2(0)\exp\left(-2\left(\zeta_1(0)\right)^2\right)\kappa_j\psi_0(n)-\frac{T}{2\hbar\omega}\cos(K)\sum_{j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'} \qquad (15)\\
&\times\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right)\right)\psi_0(n)\\
&-\frac{T}{4\hbar\omega}\cos(K)\sum_{j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\\
&\times\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right)\right)\frac{\mathrm{d}^2}{\mathrm{d}n^2}\psi_0(n)\ ,
\end{aligned}
$$

for $j=1,2$.

By means of the condition (12), we can transform the equations (15) into

$$
E\psi_0(n)=\left(-\mu\frac{\mathrm{d}^2}{\mathrm{d}n^2}+U(n)-2\mu\right)\psi_0(n)\,, \qquad (16)
$$

where

$$
\begin{aligned}
\mu &= \frac{T}{4\hbar\omega}\cos(K)\sum_{j,j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\kappa_j\\
&\quad\times\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right)\right),\\
U(n) &= \frac{1}{N}\sum_{q,k}\left|\zeta_{q,k}(n)\right|^2+\sqrt{2}\frac{\alpha_0}{\hbar\omega}\zeta_1(0)-\sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2(0)\exp\left(-2\left(\zeta_1(0)\right)^2\right).
\end{aligned}
$$

The equation (16) is the nonlinear Schrödinger equation and it can be very easily proved that the value μ is positive in the case that $\cos(K)>0$ (see Appendix C). To investigate the energy E in the equation (16) at an arbitrary value of the electron-phonon interaction, and to compare our results with those given in [7–8], we shall use a direct variational method and choose the trial function of the ground state of the electron in a chain in the form

$$
\psi_0(n)=\sqrt{\frac{\kappa}{2}}\frac{1}{\cosh(\kappa n)}, \qquad (17)
$$

where κ is a real variational parameter.

By means of the method which is presented in Appendix A, we can transform the system of equations (7) into

$$
\left(\hat{\lambda}+\varepsilon\hat{U}\right)\vec{c}_k(q)=\left(\hat{\gamma}^{(k)}+\mu_k\hat{U}\right)\vec{\nu}^{(1)}(q) \qquad (18)
$$

for $k = 1$ and 2. Here, $\hat{\lambda}$ and $\hat{U}$ are infinite matrices with elements

$$\lambda_{ij} = \left(-1 - \mu\left[\kappa^2 + (2\pi/N)^2\, i^2\right]\right)\delta_{ij}\,,$$
$$U_{ij} = \int_{-\infty}^{+\infty} \Phi_i^*\,(m)\left(1/\cosh^2(\kappa m)\right)\Phi_j\,(m)\mathrm{d}m\,,$$

i and j are equal to $0, \pm 1, \pm 2, ...$ and δ_{ij} is Kronecker's symbol, $\Phi_j\,(m) = \left(1/\sqrt{N}\right)$ $\times \exp\left(j\mathrm{i}_0\,(2\pi/N)\,m\right)$, $\Phi_i^*\,(m)$ is the number conjugate of $\Phi_i\,(m)$,$\varepsilon = 2\mu\kappa^2$, $\vec{c}_k\,(q)$ is the infinite vector with elements $c_{j,k}\,(q)$ fulfilling the equation

$$\psi_0\,(n)\,\zeta_{q,k}\,(n) = \sum_{j=-\infty}^{+\infty} c_{j,k}\,(q)\Phi_j^*\,(n)\,, \tag{19}$$

for $k = 1$ and 2 and $\vec{\nu}^{(1)}\,(q)$ is the infinite vector with elements $\nu_p^{(1)}\,(q) = \int_{-\infty}^{+\infty} e^{\mathrm{i}_0 qm}\psi_0\,(m)$ $\times\Phi_p\,(m)\,\mathrm{d}m$, for $p = 0, \pm 1, \pm 2, \ldots,$

$$\mu_{k'} = -\frac{T}{2\hbar\omega}\cos\left(K\right)\sum_{j,j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\kappa_j\left[1-(-1)^{\delta^0_{k'}}\right]$$
$$\times\ \exp\left(-\sum_{k=1}^{2}\left(W_k + \left(\left[1-(-1)^{\delta^0_k}\right] + \left[1-(-1)^{\delta^{0\pm1}_k}\right]\right)\zeta_k\,(0)\,\zeta_k\,(1)\right)\right)\zeta_{k'}\,(1)\,\kappa^2$$

for $k' = 1$ and 2, $\hat{\gamma}^{(k)}$ is the infinite matrix of elements $\gamma_{ps}^{(1)} = \delta_{ps}\{A_1 + B_1\cos\left[(2\pi/N)\,p\right]\}$ for $k = 1, 2$ and $\gamma_{ps}^{(2)} = \delta_{ps}\{A_2 + B_2\cos\left[(2\pi/N)\,p\right]\}$ for $k = 1, 2$, respectively, and p and s are equal to $0, \pm 1, \pm 2, \ldots,$ and δ_{ps} is Kronecker's symbol.

Further,

$$A_1 = \sqrt{2}\frac{\alpha_0}{\hbar\omega} + 4\sqrt{2}\frac{\beta_0}{\hbar\omega}\exp\left(-2\zeta_1^2\,(0)\right)\zeta_2\,(0)\,\zeta_1\,(0) + \zeta_1\,(1)\,\frac{T}{2\hbar\omega}\cos(K)\left(1+\frac{1}{2}\kappa^2\right)$$
$$\times\ \sum_{j,j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\kappa_j\left[1-(-1)^{\delta^0_1}\right]$$
$$\times\exp\left(-\sum_{k=1}^{2}\left(W_k + \left(\left[1-(-1)^{\delta^0_k}\right] + \left[1-(-1)^{\delta^{0\pm1}_k}\right]\right)\zeta_k\,(0)\,\zeta_k\,(1)\right)\right) \tag{20}$$

$$B_1 = \zeta_1\,(0)\,\frac{T}{2\hbar\omega}\cos(K)\sum_{j,j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\kappa_j\left[1-(-1)^{\delta^{0\pm1}_1}\right]$$
$$\times\ \exp\left(-\sum_{k=1}^{2}\left(W_k + \left(\left[1-(-1)^{\delta^0_k}\right] + \left[1-(-1)^{\delta^{0\pm1}_k}\right]\right)\zeta_k\,(0)\,\zeta_k\,(1)\right)\right)\,, \tag{21}$$

$$A_2 = -\sqrt{2}\frac{\beta_0}{\hbar\omega}\exp\left(-2\zeta_1^2\left(0\right)\right) + \zeta_2\left(1\right)\frac{T}{2\hbar\omega}\cos(K)\left(1+\frac{1}{2}\kappa^2\right)$$
$$\times \sum_{j,j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\kappa_j\left[1-(-1)^{\delta_2^0}\right]$$
$$\times\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k\left(0\right)\zeta_k\left(1\right)\right)\right)\,, \tag{22}$$

$$B_2 = \zeta_2\left(0\right)\frac{T}{2\hbar\omega}\cos(K)\sum_{j,j',\Delta}\lambda_{j,j',\Delta}\kappa_{j'}\kappa_j\left[1-(-1)^{\delta_2^{0\pm1}}\right]$$
$$\times\;\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k\left(0\right)\zeta_k\left(1\right)\right)\right)\,. \tag{23}$$

Step 5

After multiplying (16) by $\psi_0\left(n\right)$, and performing the integration $\int\limits_{-\infty}^{+\infty}()\mathrm{d}n$, we obtain the next energy functional:

$$E = \frac{1}{3}\kappa^2\mu + \sum_{k=1}^{2}\Bigg\{\left(A_k+\frac{2}{3}\Theta_k a\right)\frac{1}{4}A_k\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}$$
$$+\;\left(A_k+a\Theta_k\right)\Theta_k\frac{1}{2}\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}\left(1+\sqrt{\kappa^2+\frac{1}{\mu}}\right)\exp\left(-\sqrt{\kappa^2+\frac{1}{\mu}}\right)$$
$$+\,B_k^2\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}\frac{1}{8}\left[1+\left(1+2\sqrt{\kappa^2+\frac{1}{\mu}}\right)\exp\left(-2\sqrt{\kappa^2+\frac{1}{\mu}}\right)\right]$$
$$+\,b\Theta_k^2\frac{1}{4}\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}\Bigg\}$$
$$+\,\sqrt{2}\frac{\alpha_0}{\hbar\omega}\zeta_1\left(0\right)-\sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2\left(0\right)\exp\left(-2\zeta_1^2\left(0\right)\right)-2\mu\,, \tag{24}$$

where a, $\zeta_k(0)$ and Θ_k are defined in Appendix B for $k=1$ and 2, A_k and B_k for $k=1$ and 2 are defined in (20–23) and κ and μ are defined in Step 4, and

$$b = \frac{1}{(\lambda\delta)^2}\left\{\frac{1}{(\lambda\delta)^2}\left[\frac{1}{2}\frac{(\lambda\delta)^2}{(1-\lambda\delta)}+\frac{1}{2}\left(\frac{\lambda\delta}{1-\lambda\delta}\right)^{3/2}\arctan\left(\frac{\lambda\delta}{1-\lambda\delta}\right)^{1/2}\right]\right.$$
$$\left.-\frac{2}{\lambda\delta}\sqrt{\frac{\lambda\delta}{1-\lambda\delta}}\arctan\sqrt{\frac{\lambda\delta}{1-\lambda\delta}}+1\right\},$$

where λ and δ are defined in Appendix B.

In the case that $\zeta_1(0) \neq 0$, it can be easily proved that the next inequalities are valid:

$$\begin{aligned}&4\zeta_2^2(0) \leq (\beta_0/\alpha_0)^2\, 4\zeta_1^2(0)\exp\left(-4\zeta_1^2(0)\right)\left[1+4\zeta_2^2(0)+C\right]^2 \leq \\ &\qquad \leq (\beta_0/\alpha_0)^2\, e^{-1}\left[1+4\zeta_2^2(0)+C\right]^2,\end{aligned} \tag{25}$$

where

$$C=\sqrt{T/(\hbar\omega)}\left(2+0.5\kappa^2\right)\left(1+\sqrt{T/(\hbar\omega)}\,\delta\kappa^2\left(1-\sqrt{T/(\hbar\omega)}\delta\kappa^2\right)^{-1}\right).$$

From the inequalities (25), we come to the conclusion that for $\beta_0=0$ is $\zeta_2(0)=0$. Thus, the condition $\beta_0=0$ leads to the next expressions:

$A_1=\sqrt{2}\alpha_0/(\hbar\omega)$, $B_1=0$ (see Appendix C), $A_2=0$, $B_2=0$,

$$\zeta_1(0)=-\sqrt{2}\alpha_0/\left(\hbar\omega 2\mu\kappa\sqrt{C_0}\right)-\delta a\sqrt{2}\alpha_0\sqrt{\mu}\kappa^2/\left(\hbar\omega 2\mu\kappa\sqrt{C_0}\sqrt{\mu\kappa^2+1}\right),$$

where C_0 is defined in Appendix B, $\Theta_1=\delta\sqrt{2}\alpha_0\sqrt{\mu}\kappa^2/\left(\hbar\omega\sqrt{\mu\kappa^2+1}\right)$, $\Theta_2=0$, and $\mu=\cos(K)\exp(-W_1)\,T/(\hbar\omega)$.

After inserting these expressions into the energy functional (24), the next one is obtained:

$$\begin{aligned}E=\;&\frac{1}{3}\kappa^2\mu+\left(2\sqrt{g/\gamma}+a\frac{2}{3}\frac{\sqrt{\mu}\kappa^2}{\sqrt{\mu\kappa^2+1}}\delta 2\sqrt{g/\gamma}\right)\frac{1}{2}\sqrt{g/\gamma}\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}\\
&+\left(2\sqrt{g/\gamma}+a\frac{\sqrt{\mu}\kappa^2}{\sqrt{\mu\kappa^2+1}}\delta 2\sqrt{g/\gamma}\right)\frac{\sqrt{\mu}\kappa^2}{\sqrt{\mu\kappa^2+1}}\delta 2\sqrt{g/\gamma}\\
&\times\frac{1}{2}\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}\left(1+\sqrt{\kappa^2+\frac{1}{\mu}}\right)\exp\left(-\sqrt{\kappa^2+\frac{1}{\mu}}\right)\\
&+b\left(\frac{\sqrt{\mu}\kappa^2}{\sqrt{\mu\kappa^2+1}}\delta 2\sqrt{g/\gamma}\right)^2\frac{1}{4}\frac{1}{\left(1+\mu\kappa^2\right)^{3/2}}\frac{1}{\mu^{1/2}}+2\sqrt{g/\gamma}\zeta_1(0)-2\mu\,,\end{aligned} \tag{26}$$

where we have used

$$\alpha_0/(\hbar\omega)=\sqrt{2g/\gamma},\ g=\alpha_0^2/(2T\hbar\omega),\ \gamma=\hbar\omega/T, \text{ and } \mu\equiv\cos(K)\exp(-W_1)/\gamma\,.$$

The expression (26) together with the condition

$$\zeta_1(0)=-\sqrt{g/\gamma}/\left(\mu\kappa\sqrt{C_0}\right)-\delta a\sqrt{g/\gamma}\sqrt{\mu}\kappa^2/\left(\mu\kappa\sqrt{C_0}\sqrt{\mu\kappa^2+1}\right) \tag{26a}$$

determine the energy dependence on the variational parameters W_1, κ, and δ to be found from the extremum condition for E. This functional dependence, as follows from (26) and (26a), is determined by the numerical values of two parameters, namely, by the nonadiabatic parameter γ and the dimensionless coupling constant g. If the optimal values of W_1, κ, and δ, i.e., W_{1m}, κ_m,

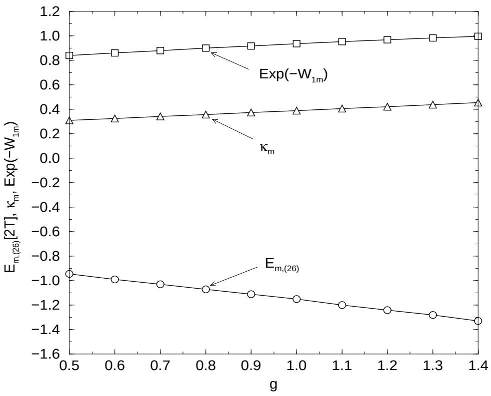

Fig. 1.The minimal values of the energy functional in units of $2T$ and the optimal values of the variational parameters W_1 and κ as a function of g obtained from (26) with respect to (26a), for the case of $\gamma = 0.2$.

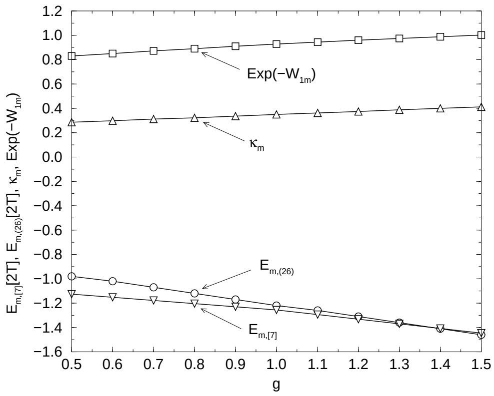

Fig. 2. The minimal values of the energy functional in units of $2T$ and the optimal values of the variational parameters W_1 and κ as a function of g obtained from (26) with respect to (26a), in the case that $\gamma = 0.3$. Because of the comparison with ground state energies of a quasiparticle (exciton, electron and hole) interacting with dispersionless optical vibrations in a one-dimensional one-level chain of molecules, the values $E_{m,[7]}$ obtained from Ref. [7] are presented.

and δ_m are determined, that is for $W_1 = W_{1m}, \kappa = \kappa_m,$ and $\delta = \delta_m$, the value of E arrives to its stable minimum E_m. We have used the penalty method to determine the optimal values of the variational parameters. The optimal values of the variational parameters W_1 and κ, i.e.,W_{1m} and κ_m are presented in Figs. 1, 2, in the case of $\gamma = 0.2$, $\gamma = 0.3$, respectively. The numerical calculations which were performed for various values K lead to the conclusion that the minimal value of the energy functional with respect to the condition (26a) is obtained for $K = 0$. Therefore, the results of the numerical analysis are presented for $K = 0$.

3 Conclusions

In our model we have studied the intermediate coupling and strong nonadiabatic regime for one-dimensional chain of the E-β Jahn-Teller systems, i.e., the range, where the electron-phonon interaction coupling constant g and the nonadiabatic parameter γ are approximately equal to 1. The results of the numerical analysis of Eqs. (26) and (26a) for $\gamma = 0.2$ and 0.3 are shown in Figures 1 and 2, respectively, and in Table 1. These Figures show only those values of $\exp(-W_{1m})$ for which W_{1m} is non-negative. The range where κ_m is increasing as a function of g and W_{1m} is non-negative can be called as an autolocalized one. The following conclusions can be made from the data of the presented ground state energy model:

g	$E_{m,(26)}[2T]$	κ_m	$\exp(-W_{1m})$	δ_m	$\zeta_{1m}(0)$
0.5	-0.98	0.290	0.820	0.981	-0.754
0.6	-1.02	0.301	0.836	0.975	-0.815
0.7	-1.07	0.315	0.854	0.970	-0.867
0.8	-1.12	0.330	0.873	0.964	-0.913
0.9	-1.17	0.343	0.890	0.958	-0.954
1.0	-1.22	0.354	0.910	0.952	-0.990
1.1	-1.26	0.364	0.926	0.945	-1.023
1.2	-1.31	0.376	0.943	0.940	-1.053
1.3	-1.36	0.391	0.962	0.933	-1.080
1.4	-1.41	0.405	0.981	0.928	-1.105
1.5	-1.46	0.420	0.997	0.922	-1.127

Tab. 1. The minimal values of the energy functional in units of $2T$ and the optimal values of the variational parameters $\kappa, W_1, \delta, \zeta_1(0)$ as a function of g obtained from (26) with respect to (26a) in the case that $\gamma = 0.3$.

1. a) if $\alpha_0 = 0$ and $\beta_0 \neq 0$, i.e., if $\zeta_1(0) = 0$ and $\zeta_2(0) \neq 0$, then we obtain from the expressions (C5) and (C11) (see Appendix C),

   $$\Delta E = \left[2T/(\hbar\omega) - T\kappa^2/(3\hbar\omega)\right] \exp\Big(-\sum_{k=1}^{2} W_k\Big) \Big[1 - \exp\big(-4\zeta_2(0)\,\zeta_2(1)\big)\Big] > 0,$$

   and $\kappa_1^2 - \kappa_2^2 = 0$, i.e., $\kappa_1^2 = 1/2$ and $\kappa_2^2 = 1/2$.

   These two relations lead to the conclusion that if the phonons of mode 1 are not present, the electron performs oscillations between the energy levels E_1 and E_2,

   b) if $|\zeta_1(0)| >> 1$, i.e., if $\alpha_0/\hbar\omega >> 1$, then the expression (25) implies that $\zeta_2(0)$ is approximately equal to zero, and (C11) leads to the expression $\kappa_1^2 - \kappa_2^2 \approx 1$, i.e., $\kappa_1^2 \approx 1$ and $\kappa_2^2 \approx 0$,

   c) if $\zeta_1(0) \neq 0$, then $1 > \kappa_1^2 - \kappa_2^2 > 0$, i.e., $1 > \kappa_1^2 > 1/2$ and $1/2 > \kappa_2^2 > 0$.

   The conclusions a), b), and c) which are presented above, lead to the next one: the phonons of mode 1 "settle" the electron on the lower energy level E_1 and the phonons of mode 2 cause the electron oscillations between the energy levels E_1 and E_2, because κ_j^2 is nothing else than the occupation probability of the energy level E_j. The expression (C5) leads to the conclusion that the gap is opened by the interaction of the electron with phonons of mode 1 and 2 during its transfer in the lattice.

2. The excitation energy is reduced by the self-trapping effect. The largest reduction is for the smallest value of the interaction constant g.

3. The numerical calculations which were performed for various values $g \approx 1$ and $\gamma \approx 1$ lead to the next conclusions:

   a) we obtain the value of g_γ for every $\gamma \leq 0.4$, which has the following property: the soliton ground state can be considered as an approximative one for sufficiently large g, $g \leq g_\gamma$. Here, g_γ is that value of g, for which $\exp(-W_{1m}) = 1$ (as a function of g).

b) g_γ is increasing with increasing γ, but slower than γ. We can conclude from Figs. 1 and 2, that the spontaneously localized (autolocalized) state exists in some interval of the coupling constant g although the nonadiabatic parameter γ is chosen rather large, close to one.

4. Fig. 2 shows a good agreement between the ground state energies obtained from Ref. [7] and from (26) with respect to (26a) in the intermediate coupling and strong nonadiabatic regime.

5. The optimal value κ_m as a function of g is not so rapidly increasing as it is presented in [8]. This reality follows from the fact that all roots of κ^2 are considered in our model, what is reflected in parameters a and b, in contrast to the model presented in [8], where not more than the first root of κ^2 is considered in the energy functional.

6. The mathematical model which is presented in [8] considers the ground state energy variational ansatz which has not the norm equal to 1. Futher, the ground state energies which are obtained from Ref. [8] are very different from those in [7], and therefore the results which are presented in [8] cannot represent the ground state energies for an extended Jahn-Teller system in one dimension.

In the next paper the cases with small values g will be solved. This work is under way.

Appendix A

In the case that $k = 1$, the equations (7) can be rewritten into the next form:

$$
\begin{aligned}
&\sum_{j=1}^{2} \beta_j^2(n) \frac{1}{N} \zeta_{q,1}(n) + \sqrt{2} \frac{\alpha_0}{\hbar\omega} \sum_{j=1}^{2} \beta_j^2(n) \frac{1}{N} e^{\mathrm{i}_0 qn} \\
&+ 4\sqrt{2} \frac{\beta_0}{\hbar\omega} \frac{\zeta_{n,2}(n)}{\sqrt{N}} \exp\left(-2 \frac{\zeta_{n,1}^2(n)}{N}\right) \frac{\zeta_{n,1}(n)}{\sqrt{N}} \frac{1}{N} e^{\mathrm{i}_0 qn} \sum_{j=1}^{2} \beta_j^2(n) + \frac{T}{4\hbar\omega} \cos(K) \\
&\times \sum_{i,j,\Delta} \lambda_{i,j,\Delta} \Bigg(\beta_i(n) \beta_j(n+1) \exp\left(-W_\Delta(n, n+1)\right) \left\{ \frac{1}{N} \left(\zeta_{q,1}(n) - \zeta_{q,1}(n+1)\right) \right. \\
&\left. + \left[1 - (-1)^{\delta_1^0}\right] \frac{\zeta_{n,1}(n+1)}{\sqrt{N}} \frac{1}{N} e^{\mathrm{i}_0 qn} + \left[1 - (-1)^{\delta_1^{0 \pm 1}}\right] \frac{\zeta_{n+1,1}(n+1)}{\sqrt{N}} \frac{1}{N} e^{\mathrm{i}_0 q(n+1)} \right\} \\
&+ \beta_i(n) \beta_j(n-1) \exp\left(-W_\Delta(n, n-1)\right) (-1) \left\{ \frac{1}{N} \left(\zeta_{q,1}(n) - \zeta_{q,1}(n-1)\right) \right. \\
&\left. + \left[1 - (-1)^{\delta_1^0}\right] \frac{\zeta_{n,1}(n-1)}{\sqrt{N}} \frac{1}{N} e^{\mathrm{i}_0 qn} + \left[1 - (-1)^{\delta_1^{0 \pm 1}}\right] \frac{\zeta_{n-1,1}(n-1)}{\sqrt{N}} \frac{1}{N} e^{\mathrm{i}_0 q(n-1)} \right\} \Bigg) = 0\,.
\end{aligned}
\tag{A1}
$$

When using the variational parameters $\zeta_k(0), \zeta_k(1)$ and W_k (see Step 4) as approximations of the values defined by Eqs. (13) and (14) and of $W_k^{\pm}(n)$, we obtain from Eqs. (A1)

$$\begin{aligned}
&\sum_{j=1}^{2}\beta_j^2(n)\frac{1}{N}\zeta_{q,1}(n)+\sqrt{2}\frac{\alpha_0}{\hbar\omega}\sum_{j=1}^{2}\beta_j^2(n)\frac{1}{N}e^{\mathrm{i}_0 qn} \qquad \text{(A2)}\\
&+4\sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2(0)\exp\left(-2\zeta_1^2(0)\right)\zeta_1(0)\frac{1}{N}e^{\mathrm{i}_0 qn}\sum_{j=1}^{2}\beta_j^2(n)+\frac{T}{4\hbar\omega}\cos(K)\sum_{i,j,\Delta}\lambda_{i,j,\Delta}\\
&\times\Bigg(\beta_i(n)\beta_j(n+1)\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\zeta_k(1)\right)\right)\\
&\times\left\{\frac{1}{N}\left(\zeta_{q,1}(n)-\zeta_{q,1}(n+1)\right)+\left[1-(-1)^{\delta_1^0}\right]\zeta_1(1)\frac{e^{\mathrm{i}_0 qn}}{N}+\left[1-(-1)^{\delta_1^{0\pm1}}\right]\zeta_1(0)\frac{e^{\mathrm{i}_0 q(n+1)}}{N}\right\}\\
&+\beta_i(n)\beta_j(n-1)\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\zeta_k(1)\right)\right)\\
&\times\left\{\frac{1}{N}\left(\zeta_{q,1}(n)-\zeta_{q,1}(n-1)\right)+\left[1-(-1)^{\delta_1^0}\right]\zeta_1(1)\frac{e^{\mathrm{i}_0 qn}}{N}+\left[1-(-1)^{\delta_1^{0\pm1}}\right]\zeta_1(0)\frac{e^{\mathrm{i}_0 q(n-1)}}{N}\right\}\Bigg)\\
&=0\,.
\end{aligned}$$

Further, when we use approximation (9), expression (12), and the continuum approximation of the parameter n, we obtain

$$\begin{aligned}
&-\psi_0(n)\zeta_{q,1}(n)-\mu\left[\zeta_{q,1}(n)\frac{\mathrm{d}^2}{\mathrm{d}n^2}\psi_0(n)-\frac{\mathrm{d}^2}{\mathrm{d}n^2}\left(\zeta_{q,1}(n)\psi_0(n)\right)\right]\\
&=\sqrt{2}\frac{\alpha_0}{\hbar\omega}\psi_0(n)e^{\mathrm{i}_0 qn}+4\sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2(0)\exp\left(-2\zeta_1^2(0)\right)\zeta_1(0)\psi_0(n)e^{\mathrm{i}_0 qn}+\frac{T}{4\hbar\omega}\cos(K)\\
&\times\sum_{i,j,\Delta}\lambda_{i,j,\Delta}\kappa_i\kappa_j\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\zeta_k(1)\right)\right)\\
&\times\left\{\left[1-(-1)^{\delta_1^0}\right]\zeta_1(1)e^{\mathrm{i}_0 qn}\left(\frac{\mathrm{d}^2}{\mathrm{d}n^2}\psi_0(n)+2\psi_0(n)\right)\right.\\
&\left.+\left[1-(-1)^{\delta_1^{0\pm1}}\right]\zeta_1(0)\sum_{p=-\infty}^{+\infty}2\cos\left(\frac{2\pi}{N}p\right)\nu_p^{(1)}(q)\Phi_p^*(n)\right\}. \qquad \text{(A3)}
\end{aligned}$$

When inserting $\frac{\mathrm{d}^2}{\mathrm{d}n^2}\psi_0\left(n\right)=\frac{1}{\mu}\left(U\left(n\right)-2\mu-E\right)\psi_0\left(n\right)$ (see equation (16)) into the equations (A3), we obtain

$$
\begin{aligned}
&-\sum_j c_{j,1}\left(q\right)\Phi_j^*\left(n\right)-\mu\Bigg[\zeta_{q,1}\left(n\right)\frac{1}{\mu}\left(U\left(n\right)-2\mu-E\right)\psi_0\left(n\right)+\sum_j c_{j,1}\left(q\right)\left(\frac{2\pi}{N}j\right)^2\Phi_j^*\left(n\right)\Bigg]\\
&=\Bigg(\sqrt{2}\frac{\alpha_0}{\hbar\omega}+4\sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2\left(0\right)\exp\left(-2\zeta_1^2\left(0\right)\right)\zeta_1\left(0\right)+\frac{T}{2\hbar\omega}\cos\left(K\right)\\
&\times\sum_{i,j,\Delta}\lambda_{i,j,\Delta}\kappa_i\kappa_j\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k\left(0\right)\zeta_k\left(1\right)\right)\right)\\
&\times\left[1-(-1)^{\delta_1^0}\right]\zeta_1\left(1\right)\Bigg)\sum_{p=-\infty}^{+\infty}\nu_p^{(1)}\left(q\right)\Phi_p^*\left(n\right)+\frac{T}{4\hbar\omega}\cos\left(K\right)\\
&\times\sum_{i,j,\Delta}\lambda_{i,j,\Delta}\kappa_i\kappa_j\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k\left(0\right)\zeta_k\left(1\right)\right)\right)\\
&\times\left[1-(-1)^{\delta_1^0}\right]\zeta_1\left(1\right)\frac{1}{\mu}\left(U\left(n\right)-2\mu-E\right)\sum_{p=-\infty}^{+\infty}\nu_p^{(1)}\left(q\right)\Phi_p^*\left(n\right)+\frac{T}{2\hbar\omega}\cos\left(K\right)\\
&\times\sum_{i,j,\Delta}\lambda_{i,j,\Delta}\kappa_i\kappa_j\exp\left(-\sum_{k=1}^{2}\left(W_k+\left(\left[1-(-1)^{\delta_k^0}\right]+\left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k\left(0\right)\zeta_k\left(1\right)\right)\right)\\
&\times\left[1-(-1)^{\delta_1^{0\pm1}}\right]\zeta_1\left(0\right)\cos\left(\frac{2\pi}{N}i\right)\sum_{p=-\infty}^{+\infty}\nu_p^{(1)}\left(q\right)\Phi_p^*\left(n\right),
\end{aligned}
\tag{A4}
$$

where we have used expression (19) for $k=1$, and the equality

$$\psi_0\left(n\right)e^{\mathrm{i}_0qn}=\sum_{p=-\infty}^{+\infty}\nu_p^{(1)}\left(q\right)\Phi_p^*\left(n\right).$$

After inserting the identity

$$\zeta_{q,1}\left(n\right)U\left(n\right)\psi_0\left(n\right)=\left(2\mu+\mu\kappa^2+E\right)\sum_j c_{j,1}\left(q\right)\Phi_j^*\left(n\right)-2\mu\kappa^2\sum_j\sum_p c_{j,1}\left(q\right)U_{jp}\Phi_p^*\left(n\right),$$

which is valid provided that $\psi_0\left(n\right)=\sqrt{\left(\kappa/2\right)}\left(1/\cosh\left(\kappa n\right)\right)$,
into the equations (A4), multiplying it by $\Phi_i\left(n\right)$, and performing the integration $\int_{-\infty}^{+\infty}()\mathrm{d}n$, we obtain the i-th linear equation of the next infinite linear system:

$$\left(\hat{\lambda}+\varepsilon\hat{U}\right)\vec{c}_1\left(q\right)=\left(\hat{\gamma}^{(1)}+\mu_1\hat{U}\right)\vec{\nu}^{(1)}\left(q\right). \tag{A5}$$

The terms of the expression (A5) are defined below the equation (18).

In the case that $k=2$, we can derive the formula (18) analogously as it was made in the case that $k=1$.

Appendix B

It can be easily proved that $\left\|\varepsilon\hat{\lambda}^{-1}\hat{U}\right\|_{[l^2,l^2]} \leq \left(\left(\mu\kappa^2\right)/\left(1+\mu\kappa^2\right)\right)^{3/4}(4/3)^{1/2}$, where $\hat{\lambda}^{-1}$is the inverse matrix of $\hat{\lambda}$, and $\left\|\varepsilon\hat{\lambda}^{-1}\hat{U}\right\|_{[l^2,l^2]}$ is the norm of $\varepsilon\hat{\lambda}^{-1}\hat{U}$ in the Banach space $[l^2,l^2]$ [9]. In the case that $\left(\left(\mu\kappa^2\right)/\left(1+\mu\kappa^2\right)\right)^{3/4}(4/3)^{1/2} < 1$, we can derive for the approximate solution of the equations (18) by means of the perturbation theory

$$c_{j,k}\left(q\right) \doteq \frac{\gamma_{jj}^{(k)}}{\lambda_{jj}}\nu_j^{(1)}\left(q\right) + \frac{1}{\lambda_{jj}}\left[\mu_k + \lambda\delta\left(A_k + B_k\right)\right]\sum_{m'=0}^{+\infty}\left(\lambda\delta\right)^{m'}\nu_j^{(2m'+3)}\left(q\right), \tag{B1}$$

where $k = 1$ and 2,

$$\lambda = \left(\sqrt{\mu}\kappa^2\right)/\sqrt{\mu\kappa^2+1},\ \nu_j^{(2m+3)}\left(q\right) = \sqrt{\kappa/2}\int_{-\infty}^{+\infty}\Phi_j\left(n\right)\cosh^{-(2m+3)}\left(\kappa n\right)e^{\mathrm{i}_0 qn}\mathrm{d}n,$$

$j = 0, \pm1, \pm2, \ldots,\ m = -1, 0, 1, 2, \ldots,$ and δ is a real variational parameter approximately equal to 1. The optimal value of this parameter has to be determined in the minimum of the energy functional E. The other terms of the expression (B1) are defined in Step 4.

After inserting expression (B1) into formula (19), we obtain for $\zeta_{q,k}\left(n\right)$

$$\begin{aligned}\zeta_{q,k}\left(n\right) &= \frac{1}{\psi_0\left(n\right)}\sum_{j=-\infty}^{+\infty}c_{j,k}\left(q\right)\Phi_j^*\left(n\right)\\ &\approx \frac{1}{\psi_0\left(n\right)}\sum_j\frac{\gamma_{jj}^{(k)}}{\lambda_{jj}}\nu_j^{(1)}\left(q\right)\Phi_j^*\left(n\right)\\ &\quad+\left[\mu_k+\lambda\delta\left(A_k+B_k\right)\right]\frac{1}{\psi_0\left(n\right)}\sum_{m'=0}^{+\infty}\left(\lambda\delta\right)^{m'}\sum_j\frac{1}{\lambda_{jj}}\nu_j^{(2m'+3)}\left(q\right)\Phi_j^*\left(n\right).\end{aligned} \tag{B2}$$

Then, because $\zeta_{m,k}\left(n\right)/\sqrt{N} = \left(1/N\right)\sum_q e^{-\mathrm{i}_0 qm}\zeta_{q,k}\left(n\right)$ we come to

$$\begin{aligned}\frac{\zeta_{m,k}\left(n\right)}{\sqrt{N}} &\approx -\frac{\left(A_k+B_k\right)}{2\mu\kappa\sqrt{C_0}}\frac{\psi_0\left(m\right)}{\psi_0\left(n\right)}\exp\left(-\kappa\sqrt{C_0}|m-n|\right)\\ &\quad+\frac{1}{\psi_0\left(n\right)}\sqrt{\frac{\kappa}{2}}\left[\mu_k+\lambda\delta\left(A_k+B_k\right)\right]\frac{1}{\cosh^3\left(\kappa m\right)-\lambda\delta\cosh\left(\kappa m\right)}\\ &\quad\times\left(-\frac{1}{2\mu\kappa\sqrt{C_0}}\exp\left(-\kappa\sqrt{C_0}|m-n|\right)\right),\end{aligned} \tag{B3}$$

where $C_0 = 1 + 1/\mu\kappa^2$.

In the case of $m = n$, the expression (B3) can be used for the definition of the values $\zeta_k\left(0\right)$ and $\zeta_k\left(1\right)$ as given below.

When $\zeta_k(0)$ is defined as

$$\zeta_k(0) = \int\limits_{-\infty}^{+\infty} \frac{\zeta_{n,k}(n)}{\sqrt{N}} \psi_0^2(n)\,\mathrm{d}n,$$

we obtain

$$\zeta_k(0) = \int\limits_{-\infty}^{+\infty} \frac{\zeta_{n,k}(n)}{\sqrt{N}} \psi_0^2(n)\,\mathrm{d}n \doteq -\frac{(A_k+B_k)}{2\mu\kappa\sqrt{C_0}} - \frac{\Theta_k}{2\mu\kappa\sqrt{C_0}} \sum_{m=0}^{+\infty} (\lambda\delta)^m \int\limits_0^{+\infty} \frac{\mathrm{d}x}{\cosh^{2m+4}(x)}$$

$$= -\frac{(A_k+B_k)}{2\mu\kappa\sqrt{C_0}} - \frac{\Theta_k}{2\mu\kappa\sqrt{C_0}} \sum_{m=0}^{+\infty} (\lambda\delta)^m \frac{(2m+2)!!}{(2m+3)!!} = -\frac{(A_k+B_k)}{2\mu\kappa\sqrt{C_0}} - \frac{\Theta_k}{2\mu\kappa\sqrt{C_0}}\, a\,,$$

where $\Theta_k = \mu_k + \lambda\delta\,(A_k + B_k)$, for $k = 1$ and 2, and

$$a = -\frac{1}{\lambda\delta} + \frac{1}{(\lambda\delta)^2}\left(\frac{\lambda\delta}{1-\lambda\delta}\right)^{1/2} \arctan\left(\frac{\lambda\delta}{1-\lambda\delta}\right)^{1/2}.$$

Analogously, defining

$$\zeta_k(1) = \int\limits_{-\infty}^{+\infty} \frac{\zeta_{n+1,k}(n)}{\sqrt{N}} \psi_0^2(n)\,\mathrm{d}n,$$

we obtain

$$\zeta_k(1) \approx \zeta_k(0) \exp\left(-\kappa\sqrt{C_0}\right).$$

Appendix C

After multiplying (15) by $\psi_0(n)$, and performing the integration $\int\limits_{-\infty}^{+\infty} ()\mathrm{d}n$, we come to

$$E\kappa_1 = J\kappa_1 + L[\kappa_1(\lambda_1 + \lambda_2 + \nu) + \kappa_2(\lambda_1 - \lambda_2)], \tag{C1a}$$

$$E\kappa_2 = J\kappa_2 + L[\kappa_1(\lambda_1 - \lambda_2) + \kappa_2(\lambda_1 + \lambda_2 - \nu)], \tag{C1b}$$

where

$$\lambda_1 = 1 + \exp\left(-4\zeta_1(0)\zeta_1(1)\right), \lambda_2 = \lambda_1 \exp\left(-4\zeta_2(0)\zeta_2(1)\right),$$
$$\nu = 2\exp\left(-2\zeta_2(0)\zeta_2(1)\right)\left(1 - \exp\left(-4\zeta_1(0)\zeta_1(1)\right)\right),$$
$$J = \frac{1}{N}\sum_{q,k}\int \left|\zeta_{q,k}(n)\right|^2 \psi_0^2(n)\,\mathrm{d}n + \sqrt{2}\frac{\alpha_0}{\hbar\omega}\zeta_1(0) - \sqrt{2}\frac{\beta_0}{\hbar\omega}\zeta_2(0)\exp\left(-2\zeta_1^2(0)\right),$$
$$L = \left[-\frac{T}{2\hbar\omega} + \frac{T}{4\hbar\omega}\frac{1}{3}\kappa^2\right]\exp\left(-\sum_{k=1}^{2} W_k\right).$$

The system of homogeneous linear equations (C1a) and (C1b) has a nontrivial solution only if its determinant is equal to zero, i.e.,

$$\begin{vmatrix} E - J - L(\lambda_1 + \lambda_2 + \nu) & -L(\lambda_1 - \lambda_2) \\ -L(\lambda_1 - \lambda_2) & E - J - L(\lambda_1 + \lambda_2 - \nu) \end{vmatrix} = 0\,. \tag{C2}$$

The equation (C2) has two solutions,

$$E_1 = J + L\left(\lambda_1 + \lambda_2\right) + L\sqrt{\left(\lambda_1 - \lambda_2\right)^2 + \nu^2}, \tag{C3}$$

$$E_2 = J + L\left(\lambda_1 + \lambda_2\right) - L\sqrt{\left(\lambda_1 - \lambda_2\right)^2 + \nu^2}. \tag{C4}$$

Then the values (C3) and (C4) give the next expression for the excitation energy:

$$\Delta E = E_2 - E_1 = -2L\sqrt{\left(\lambda_1 - \lambda_2\right)^2 + \nu^2}, \tag{C5}$$

where we have considered the case $K = 0$, as energetically the most advantageous one.

Further, when inserting $E = E_1$ in the equations (C1a) and (C1b), multiplying (C1a) by κ_1 and (C1b) by κ_2, and adding them, we obtain the next expression:

$$\begin{aligned} E_1 &= J + L\left[\kappa_1^2\left(\lambda_1 + \lambda_2 + \nu\right) + 2\kappa_1\kappa_2\left(\lambda_1 - \lambda_2\right) + \kappa_2^2\left(\lambda_1 + \lambda_2 - \nu\right)\right] \\ &= J + L\sum_{i,j,\Delta}\lambda_{i,j,\Delta}\kappa_i\kappa_j \exp\left(-\sum_{k=1}^{2}\left(W_k + \left(\left[1 - (-1)^{\delta_k^0}\right] + \left[1 - (-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right)\right). \end{aligned} \tag{C6}$$

The values of energy E_1, as given by (C3) and by (C6), are equal in the ground state. Therefore,

$$\begin{aligned} &\exp\left(-\sum_{k=1}^{2} W_k\right)\left(\lambda_1 + \lambda_2 + \sqrt{\left(\lambda_1 - \lambda_2\right)^2 + \nu^2}\right) \\ &= \sum_{i,j,\Delta}\lambda_{i,j,\Delta}\kappa_i\kappa_j \exp\left(-\sum_{k=1}^{2}\left(W_k + \left(\left[1 - (-1)^{\delta_k^0}\right] + \left[1 - (-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right)\right). \end{aligned} \tag{C7}$$

Because $\lambda_1 > 1$ and $\lambda_2 > 0$, the expression (C7) leads to

$$\mu \geq \cos(K) \exp\left(-\sum_{k=1}^{2} W_k\right) T/(4\hbar\omega) > 0\,,$$

provided that $\cos(K) > 0$.

Further, it can be easily proved that (C7) is equivalent to

$$\sqrt{(\lambda_1 - \lambda_2)^2 + \nu^2} = \nu\left(\kappa_1^2 - \kappa_2^2\right) + (\lambda_1 - \lambda_2)\, 2\kappa_1\kappa_2. \tag{C8}$$

One has $\lambda_1 = \lambda_2$ for $\zeta_2(0) = 0$. Then we come to the equality $\nu = \nu\left(\kappa_1^2 - \kappa_2^2\right)$ from the expression (C8), and this implies that $\kappa_1^2 = 1$ and $\kappa_2^2 = 0$ is for $\zeta_2(0) = 0$.

We can easily obtain from (15)

$$\begin{aligned}\kappa_2 \sum_{j,\Delta} \lambda_{1,j,\Delta}\kappa_j \exp\left(-\sum_{k=1}^{2}\left(\left[1-(-1)^{\delta_k^0}\right] + \left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right) \\ = \kappa_1 \sum_{j,\Delta} \lambda_{2,j,\Delta}\kappa_j \exp\left(-\sum_{k=1}^{2}\left(\left[1-(-1)^{\delta_k^0}\right] + \left[1-(-1)^{\delta_k^{0\pm1}}\right]\right)\zeta_k(0)\,\zeta_k(1)\right)\end{aligned} \tag{C9}$$

which is equivalent to

$$2\kappa_1\kappa_2\nu = \left(\kappa_1^2 - \kappa_2^2\right)(\lambda_1 - \lambda_2)\,. \tag{C10}$$

From the expressions (C8) and (C10), we come to

$$\kappa_1^2 - \kappa_2^2 = \frac{\nu}{\sqrt{(\lambda_1 - \lambda_2)^2 + \nu^2}}, \tag{C11}$$

which leads to the next conclusion: if $\zeta_1(0) \neq 0$, then $\zeta_2(0) = 0$ is equivalent to $\kappa_2 = 0$.

If $\zeta_2(0) = 0$, then $B_1 = 0$. This statement can be proved as follows: Because

$$\begin{aligned}B_1 = \zeta_1(0)\cos(K)\,\frac{T}{2\hbar\omega}\exp\left(-\sum_{k=1}^{2} W_k\right)\Big[2\left(\kappa_1^2 + \kappa_2^2\right)\left(e^{-4x_1} + e^{-4x_1-4x_2}\right) \\ + 4\left(\kappa_2^2 - \kappa_1^2\right)e^{-4x_1-2x_2} + 4\kappa_1\kappa_2\left(e^{-4x_1} - e^{-4x_1-4x_2}\right)\Big],\end{aligned}$$

where $x_1 = \zeta_1(0)\,\zeta_1(1)$ and $x_2 = \zeta_2(0)\,\zeta_2(1)$, we obtain the relation $B_1 = 0$ for $\zeta_2(0) = 0$, i.e., for $x_2 = 0$. We have used here $\kappa_1^2 = 1$ and $\kappa_2^2 = 0$, which are valid in the case that $\zeta_2(0) = 0$, as it has been proved above.

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