Nonadiabatic effects in a soliton ground state of an extended Jahn-Teller system in one dimension

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We have investigated conditions for the existence and for the stability of a soliton ground state of the Fulton-Gouterman-transformed extended one-dimensional Jahn-Teller model with low electron density against quantum fluctuations of optical phonons. The Jahn-Teller band splitting occurs but the respective gap is narrowed by the self-trapping effect modified by quantum fluctuations and by many-phonon effects due to the participation of phonons in the electron transfer. The electron transfer parameter T_R is reduced by the self-trapping effect which is further modified by the effects of complex squeezing parameters. These effects determine then the value of the strength of the parameter $\overline{\Omega}=\Omega/T_R$, which is a measure of the influence of the quantum fluctuations. We have shown that the electron channels are coupled due to the participation of the phonons, which couple the original electron levels, in the electron transfer. However, the dominating contribution of these phonons is diagonal and the coupling of the channels becomes negligible if the change of the phonon wave vector by the scattering with an electron at the distance of the soliton width is negligible. Under these conditions, the problem of the Fulton-Gouterman quantum ground state of the Jahn-Teller model becomes qualitatively equivalent to the related problem of a Holstein polaron (a soliton of the nonlinear Schrödinger equation). The soliton ground state is shown to be unstable against quantum fluctuations for weak electron-phonon coupling and for $\overline{\Omega}>\frac{2}{3}\kappa^3$ ($\kappa=\lambda^{-1}$ is an inverse soliton width). The fluctuations compete the self-trapping polaron effect: For $\overline{\mu}<\mu_{\rm crit}$, $\overline{\mu}$ an effective coupling constant, $\overline{\mu}=\alpha^2\exp\Gamma(r,\theta)/4\Omega^2T$, the stability of the soliton of the nonlinear Schrödinger equation describing the traveling lattice distortion is destroyed. The soliton was found to be stable only for a sufficiently strong effective electron-phonon coupling $\overline{\mu}>\mu_{\rm crit}$. Because the soliton effect on the phonon displacements couples with the squeezing effect through Γ (or $\overline{\mu}$), the nonadiabatic effects are either amplified, if the net effect of squeezing decreases $\overline{\mu}$, or weakened, if the net effect of squeezing increases $\overline{\mu}$. The latter case can occur if the phonon displacement and/or the squeezing parameter are complex quantities. The many-phonon effects are shown to contribute only for large quantum fluctuations $\overline{\Omega}>2\kappa^2$ beyond the validity of the above condition for the use of the perturbation theory. The soliton ground state with $\lambda>(2T/3\Omega)^{1/3}$ is destabilized by the quantum fluctuations. [S0163-1829(96)09629-4]

I. INTRODUCTION

Traveling electron-phonon bound states accompanied by a lattice distortion (polarons, solitons) are relevant for understanding various physical effects. Nonadiabatic (quantum) effects in these systems become important if the scales of phonon and electron energies are comparable, i.e., the ratios $\hbar\Omega/T$ (T an intersite electron transfer matrix element) for a low electron density or $\hbar\Omega/E_F$ (E_F Fermi energy) for a high electron density are not too small. In high-T_c oxides, e.g., there is a typical local Jahn-Teller (JT) configuration:[1] a degenerate electron level at each Cu^{2+} ion lattice site surrounded by a high-symmetry O^{2-} ionic configuration. A similar, although a little more complicated situation is also in C_{60} compounds which indicates the necessity to investigate nonadiabatic effects in the electron-phonon interaction in a Jahn-Teller system.[2] Recently, a theory of nonadiabatic superconductivity by Pietronero and co-workers appeared which emphasized the role of nonadiabatic effects due to very small Fermi energy in all high-T_c superconductors.[3]

In contrast to the lattice of Jahn-Teller molecules, the quantum effects in $E\otimes e$ Jahn-Teller system and in an equivalent two-site (dimer) one are well understood: A fully exact analytical treatment of the $E\otimes e$ Jahn-Teller effect has not yet been done and only a combination of unitary transformations and the variational principle was applied.[4] There is a similar state of affairs also in the analysis of the electron- (or molecular-exciton-) phonon interaction in a periodic lattice in spite of a long-standing effort since the early days of solid states physics:[5,6] The analytical results on the ground state of the electron-(exciton-) phonon system in a one-dimensional lattice have been achieved by a combination of variational principle and unitary transformations.[7–11]

Fulton and Gouterman[12] (FG) obtained important new results on two-level and equivalent two-site (dimer) problems with a reflection symmetry by applying a nonlinear unitary transformation. It has been used in exciton-phonon and dimer problems starting from the pioneering work by Shore and Sander[7] in combination with the variational principle. The FG transformation exactly diagonalizes two-level Hamiltonians of the above-mentioned problems[13] and reduces substantially the transfer probability between levels. In a combination with the variational approach it yields the lowest ground states,[7,14,15] e.g., also for local problems with a coherent two-phonon (squeezed) phonon trial wave function (Ref. 16 and references therein). It leads to a peculiar structure of the excited-spectra–exotic states[15,17,18] for phonon subsystems. The generalization of the FG approach to problems with translation symmetry done by Wagner[19] appeared to be equivalent to the Bloch formalism. It has been applied, e.g., to the formulation of the theory of excitonic solitons.[14,20]

We shall investigate a model system specified in the Sec. II: a degenerate electron level at each lattice site interacting with optical phonons (i) via coupling to the respective electron densities and (ii) via phonon-assisted transitions between the levels. Due to the presence of interaction (i), our model contains intrinsically the problem of the Holstein polaron in one dimension (1D) (in the adiabatic approximation a soliton of a nonlinear Schrödinger equation) and, in addition, there is an e-ph term responsible for the coupling of the split JT levels.

The aim of the present study is (a) to specify the physical mechanism which makes the JT model qualitatively different from the case yielding a soliton and to find conditions for the existence of a soliton ground state and (b) to investigate the nonadiabatic effects in a soliton ground state for the Holstein-like extended Jahn-Teller model.

In this respect we shall focus on (i) a modification of the self-trapping due to the complex displacements and complex squeezing parameters (the variational functions for the displacements are supposed to account for the electron effect), (ii) a modification of the soliton ground state of our model for the case of phonons weakly scattered during their transfer at the distance of the soliton width, and (iii) an investigation of the stability of the soliton ground state against the quantum fluctuations included in (i) and (ii) (Sec. IV).

In Sec. III, we shall investigate the physical mechanism of the channel coupling when applying the transformations of the Fulton-Gouterman type to the extended Jahn-Teller Hamiltonian. We shall generalize the FG transformation in such a way that the dominating diagonal part of the transformed Hamiltonian will then represent the problem of a modified Holstein polaron suitable for variational calculations of the ground state. The condition for neglecting the nondiagonal part will be specified.

Investigations of the coherent and squeezing phenomena by Zheng[21] and Feinberg *et al.*[9] within the Holstein model brought interesting new features for the transfer probability of electrons: While the transfer probability was reduced by the self-trapping effect, $\widetilde{T}<T$ (the ratio $\Omega/\widetilde{T}$ therefore increased and the system became more sensitive to quantum fluctuations), the squeezing effect enhanced the transfer probability for real displacements of the coherent states.

We shall treat this problem using a generalized variational ansatz for the coherent and squeezed phonons, taking complex displacements as variational functions and complex squeezing parameters. The variational ansatz for the electron wave function is chosen to be compatible with known analytical results of the adiabatic approach to the related electron-phonon problem. The soliton ground state of the electron- (molecular-exciton-) phonon problem in the adiabatic approximation was found to be a soliton of the nonlinear Schrödinger equation.[6,8,11,14,22,23] We shall use the respective soliton solution as an electron variational wave function with the inverse width of the soliton as a variational parameter. At a certain stage of the calculations it is necessary to specify the electron dispersion law, for our case of small electron density as a quadratic one near the bottom of the conduction band. The case of high electron density is of interest for high-T_c superconductors mentioned above and will not be investigated here.

In general, quantum fluctuations are known to play a significant role for a weak electron-phonon coupling:[24] They destroy the adiabatic ground state. Therefore, in our case, one can expect nonadiabatic effects to play a significant role for weak electron-phonon couplings.

II. HAMILTONIAN

The Hamiltonian of the Jahn-Teller electron-phonon system on a 1D lattice is

$$H=\sum_n \left[\Omega\left(\sum_{i=1,2} b_{in}^\dagger b_{in}+1\right)+\frac{\alpha}{2}(c_{2n}^\dagger c_{2n}-c_{1n}^\dagger c_{1n})\times(b_{1n}^\dagger+b_{1n})-\frac{\beta}{2}(c_{1n}^\dagger c_{2n}+c_{2n}^\dagger c_{1n})(b_{2n}^\dagger+b_{2n})-T(c_{1,n+1}^\dagger c_{1n}+c_{2,n+1}^\dagger c_{2n}+\text{H.c.})\right]\equiv H_0+H_T. \quad (1)$$

Here, the optical phonons $i=1,2$ are dispersionless, $c_{jn},c_{jn}^\dagger$ are electron annihilation and creation operators related to two degenerate levels, $j=1,2$, respectively, and $\hbar=1$. The first interaction term related to the difference of the electron densities at two levels causes the splitting of the degenerate level; the second interaction term represents phonon-assisted transitions between the levels. Transitions between levels 1 and 2 of two neighbor sites $c_{1,n+1}^\dagger c_{2n}+\text{H.c.}$ are not allowed. It is evident that the respective one-level problem turns to the problem of the Holstein polaron.[6]

It is convenient to rewrite Hamiltonian (1) in the ''spin'' representation of electrons:

$$H=\sum_n \left[\Omega\left(\sum_{i=1,2} b_{in}^\dagger b_{in}+1\right)+\alpha(b_{1n}^\dagger+b_{1n})\sigma_{zn}-\beta(b_{2n}^\dagger+b_{2n})\sigma_{xn}-T(R_1+R_{-1})I_n\right], \quad (2)$$

where $c_{1n}^\dagger c_{1n}+c_{2n}^\dagger c_{2n}=I_n$, and

$$\sigma_{xn}=\frac{1}{2}(c_{1n}^\dagger c_{2n}+c_{2n}^\dagger c_{1n}),$$

$$\sigma_{yn}=\frac{1}{2i}(c_{2n}^\dagger c_{1n}-c_{1n}^\dagger c_{2n}), \quad (3)$$

$$\sigma_{zn}=\frac{1}{2}(c_{2n}^\dagger c_{2n}-c_{1n}^\dagger c_{1n}).$$

The Pauli matrices σ_{kn} are related by $[\sigma_{in},\sigma_{jn}]=i\sigma_{k,n}$, $i,j,k=x,y,z$; I_n is a unit 2×2 matrix. R_n is an operator of translation in a lattice space; it is defined by $R_nO_m=O_{m+n}$

and $R_1^N = I$, $R_n \phi_n(k) = \exp(ikn)\phi_n(k)$.[19] Hamiltonian (2) is a two-level multisite two-phonon Hamiltonian with translation symmetry.

III. GROUND STATE

A. Extended Fulton-Gouterman transformation

The FG transformations will be applied in three steps: (1) a transformation which diagonalizes the local two-level e-ph problem, (2) a transformation which diagonalizes a dominant term of the transfer part of the Hamiltonian, and (3) the generalized FG (Bloch) transformation for the diagonalization of the translation-invariant electron lattice problem.

The ground state of the system given by the model above will be chosen in the form of the translation-invariant Fulton-Gouterman variational ansatz

$$\Psi_{\mathrm{FG}}(k) = N^{-1/2} \sum_n \exp(ikna) U_n D(n) S(n) \Phi(n) |0\rangle, \tag{4}$$

where $\Phi(n)$ is an electron amplitude vector of a two-level local state,

$$\Phi(n) = \begin{pmatrix} f(n) \\ g(n) \end{pmatrix}. \tag{4a}$$

The amplitudes $f(n), g(n)$ are variational functions which are to be determined. In Eq. (4), $|0\rangle$ is the electron and phonon vacuum state. Bloch electron wave vectors are $k = (2\pi/L)n$, $n = \pm 1, \ldots, \pm N/2$, $L = Na$, where a is a lattice constant. Further, $D(n)$ and $S(n)$ are phonon parts of the variational ansatz representing unitary operators for coherent states,

$$D(n) = \exp \frac{1}{\sqrt{N}} \sum_{q, i=1,2} [\gamma_{iq}(n) b_{iq}^\dagger - \gamma_{iq}^*(n) b_{iq}], \tag{5a}$$

and for squeezed states,

$$S(n) = \exp \frac{1}{\sqrt{N}} \sum_{q, i=1,2} [\zeta_i(n) b_{iq}^{\dagger 2} - \zeta_i^*(n) b_{iq}^2]. \tag{5b}$$

Here, the displacements $\gamma_{iq}(n)$ and the parameters of squeezing $\zeta_i(n) = r_i \exp(-i\theta_i)$, $i = 1,2$, and their complex conjugates are variational functions which are to be determined as well. The n dependence of ζ_i will be neglected: This dependence is expected to be much weaker than that of $\gamma_{iq}(n)$ and would make the variational problem too complicated. The ansatz (4a) is a generalization of the adiabatic ansatz of the polaron theory with either γ_{iq} n independent or periodically n dependent. The n dependence of $\gamma_{iq}(n)$ accounts for an effect of electrons on the phonon variational parameters. Further, the operator $U_n \equiv U_{n2} U_{n1}$ with

$$U_{ni} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ G_{ni} & -G_{ni} \end{pmatrix}, \quad G_{ni} = \exp(i\pi b_{in}^\dagger b_{in}), \tag{6}$$

is a unitary operator of a local Fulton-Gouterman transformation, $G_{ni}^2 = 1$. Evidently, U_{n1} diagonalizes the local part of the Hamiltonian (2),

$$\widetilde{H}_{0n} = U_{n1}^{-1} H_{0n} U_{n1} = \Omega \left(\sum_{i=1,2} b_{in}^\dagger b_{in} + 1 \right) + \alpha (b_{1n}^\dagger + b_{1n}) I_n - \beta (b_{2n}^\dagger + b_{2n}) G_{n1} \sigma_{zn}, \tag{7}$$

due to $\widetilde{\sigma}_{xn} \equiv U_{n1}^{-1} \sigma_{xn} U_{n1} = G_{n1} \sigma_{zn}$, $\widetilde{\sigma}_{zn} \equiv U_{n1}^{-1} \sigma_{zn} U_{n1} = \sigma_{xn}$, and $U_{n1}^{-1} (b_{1n}^\dagger + b_{1n}) U_{n1} = (b_{1n}^\dagger + b_{1n}) \sigma_{xn}$, where σ_{in}, $i = x, y, z$ are Pauli matrices, related to the site n. Besides the shifts of the phonon operators related to α and β, the effect of e-ph interactions is represented by a highly nonlinear way through the operator G_{n1}, Eq. (6) in the last term of (7). This indicates the presence of many-phonon effects respected by the ansatz for the wave function, Eqs. (4) and (5). The nonlinear periodic term mediates multiple oscillations of an electron between two levels due to the assistance of phonons 1 and coupling to phonons 2.

The respective transformation of the hopping term of the lattice Jahn-Teller Hamiltonian in (2),

$$V_{n,1} \equiv U_{n1}^{-1} R_1 U_{n1} = U_{n1}^{-1} U_{n+1,1} = \frac{1}{2} (1 + G_{n1} G_{n+1,1}) I_n + \frac{1}{2} (1 - G_{n1} G_{n+1,1}) \sigma_{xn} = V_{n,-1}, \tag{8}$$

yields a nondiagonal form. When applying further the unitary transformation U_{n2} we get for the terms of the local Hamiltonian (7)

$$U_{n2}^{-1} (b_{2n}^\dagger + b_{2n}) U_{n2} = (b_{2n}^\dagger + b_{2n}) \sigma_{xn},$$

$$\widetilde{\sigma}_{zn} = U_{n2}^{-1} \sigma_{zn} U_{n2} = \sigma_{xn},$$

and for the transfer part (8)

$$\widetilde{V}_{n1} = U_{n2}^{-1} V_{n1} U_{n+1,2} = \frac{1}{4} [(1 + G_{n1} G_{n+1,1}) I_n + (1 - G_{n1} G_{n+1,1}) G_{n2} \sigma_{zn}][(1 + G_{n2} G_{n+1,2}) I_n + (1 - G_{n2} G_{n+1,2}) \sigma_{xn}] = \widetilde{V}_{n,-1} \equiv \widetilde{V}_n. \tag{9}$$

According to (9) channels 1 and 2 are coupled due to the participation of phonons 2 in the transfer introduced by the Fulton-Gouterman transformation (9). While in the initial Hamiltonian (2) phonons 2 mediate local transitions between channels 1 and 2 (for given n) due to the transformation (9) the nondiagonality is revealed due to the hopping transfer of phonons 2. However, the dominant contribution of phonons 2 in (9) is diagonal.

In the continuum approximation the nondiagonal term in (9) yields, under account of $G_2^2(x) = 1$,

$$1 - G_2(x) \left(G_2(x) + \frac{dG_2(x)}{dx} a + \frac{1}{2} \frac{d^2 G_2(x)}{dx^2} a^2 \right) = -\frac{1}{2} G_2(x) \frac{d^2 G_2(x)}{dx^2} a^2 = -\frac{1}{2} G_2(\overline{x}) \frac{d^2 G_2(\overline{x})}{d\overline{x}^2} \kappa^2. \tag{10}$$

Here, we introduced the dimensionless quantities $\overline{x}=sx$ and $\kappa=as$ as defined below [Eqs. (22a) and (22b)]. s is an extent of the localization of a soliton used here as a relevant length measure and defined by the ansatz (20) for the electron amplitude. Expression (10) is negligibly small if the change of the phonon wave vector due to the scattering at the electron at the distance of a soliton width κ^{-1} fulfills the condition $(\Delta\overline{q}\kappa)^2 \ll 1$. This condition for $\Delta\overline{q}$ is respectively weakened by the fact that the inverse soliton width $\kappa \ll 1$. Then, the nondiagonal part (10) can be neglected and the diagonal part of Eq. (9) in this case yields

$$\widetilde{V}_n \approx \frac{1}{2}(1+G_{n,1}G_{n+1,1})I_n + \frac{1}{2}(1-G_{n,1}G_{n+1,1})G_{n,2}\sigma_{zn}. \tag{9$'$}$$

In the momentum representation we get, with the use of (7)–(9), the Hamiltonian (2) in the form

$$H=\sum_q \left[\Omega\left(\sum_{i=1,2} b_{iq}^\dagger b_{iq}+1\right)+\frac{1}{\sqrt{N}}\sum_n \{\alpha[b_{1q}^\dagger \exp(iqna)+b_{1q}\exp(-iqna)]I_n-\beta[b_{2q}^\dagger \exp(iqna) + b_{2q}\exp(-iqna)]G_{n,1}I_n\}\right] - T\frac{1}{\sqrt{N}}\sum_n \{\widetilde{V}_n[R_1^{(\mathrm{ph})}\exp[i(p_{n+1}-p_n)]+R_{-1}^{(\mathrm{ph})}\exp[-i(p_{n+1}-p_n)]]\}. \tag{11}$$

Here, $q=(2\pi/N)m$, $m=\pm 1,\pm 2,\ldots \pm N/2$, and $b_{iq}=1/\sqrt{N}\,\Sigma_n \exp(iqna)b_{in}$, $i=1,2$. In Eq. (11) we introduced the electron momentum operators p_n which apply to the electron amplitudes f_n, $\exp[i(p_{n+1}-p_n)]f_n=f_{n+1}$. The operators $R_{\pm 1}^{(\mathrm{ph})}$ apply to the phonon part of the wave function.

B. Self-trapping effect with complex displacement and squeezing parameters

The aim of this section is to calculate the ground state energy of the Hamiltonian (11) with the reduced phonon transfer term (9′) for weakly scattered phonons 2 and find an effective self-trapping in the framework of the Fulton-Gouterman variational ansatz (4). Let us first transform the Hamiltonian (11) by the unitary operators $D(n)$ and $S(n)$ defined by (5a,b); $\widetilde{H}(n)=S(n)^{-1}D(n)^{-1}HD(n)S(n)$. The result for the Hamiltonian density $\widetilde{H}(n)$ reads as follows:

$$\widetilde{H}(n)=\sum_q \Bigg(\Omega\sum_{i=1,2}\left\{\cosh(4r_i)\left[b_{iq}^\dagger b_{iq}+\frac{1}{2}+|\widetilde{\gamma}_{iq}(n)|^2+\widetilde{\gamma}_{iq}(n)b_{iq}^\dagger+\widetilde{\gamma}_{iq}^*(n)b_{iq}\right]+\frac{1}{2}\sinh(4r_i)\{e^{-i\theta_i}[b_{iq}+\widetilde{\gamma}_{iq}(n)]^2+\mathrm{H.c.}\}\right\}$$
$$+\frac{\alpha}{\sqrt{N}}\{\{\cosh(2r_1)(b_{1q}^\dagger+\widetilde{\gamma}_{1q}^*)+e^{-i\theta_1}\sinh(2r_1)[b_{1q}+\widetilde{\gamma}_{1q}(n)]\}\exp(iqna)+\mathrm{H.c.}\}I_n-\frac{\beta}{\sqrt{N}}\{\{\cosh(2r_2)(b_{2q}^\dagger+\widetilde{\gamma}_{2q}^*)$$
$$+e^{-i\theta_2}\sinh(2r_2)[b_{2q}+\widetilde{\gamma}_{2q}(n)]\}\exp(iqna)+\mathrm{H.c.}\}\widetilde{G}_{n,1}I_n\Bigg)-T\widetilde{V}_n\{\widetilde{R}_1^{(\mathrm{ph})}\exp[i(p_{n+1}-p_n)]$$
$$+\widetilde{R}_{-1}^{(\mathrm{ph})}\exp[-i(p_{n+1}-p_n)]\}. \tag{12}$$

In Eq. (12) we defined

$$\widetilde{\gamma}_{iq}(n)=\gamma_{iq}(n)\cosh 2r_i+\gamma_{iq}^*(n)e^{i\theta_i}\sinh 2r_i. \tag{13a}$$

Evidently, the respective inverse transformation reads

$$\gamma_{iq}(n)=\widetilde{\gamma}_{iq}(n)\cosh 2r_i-\widetilde{\gamma}_{iq}^*(n)e^{i\theta_i}\sinh 2r_i, \quad i=1,2. \tag{13b}$$

For the evaluation of expression (12) we used formulas (A1)–(A5) of Appendix A. Further, $\widetilde{R}_{\pm 1}^{(\mathrm{ph})}$ is given by (A5)–(A7).

Using formulas (A5)–(A8) for the averaging of the transfer term in (12) over the phonon part of the wave function (4), we obtain exactly

$$\widetilde{T}(n)=T\langle 0_{\mathrm{ph}}|\widetilde{V}_n\widetilde{R}_{\pm 1}^{\mathrm{ph}}|0_{\mathrm{ph}}\rangle=\frac{T}{4}\exp[-W(n)]\left\{\left[1+\frac{1}{2}[\epsilon_1(n)+\epsilon_1^*(n)]\right]I_n+\left[1-\frac{1}{2}[\epsilon_1(n)+\epsilon_1^*(n)]\right]\exp(-2|\gamma_{2n}(n)|^2)\sigma_{zn}\right\}$$
$$\times\left\{\left[1+\frac{1}{2}[\epsilon_2(n)+\epsilon_2^*(n)]\right]I_n+\left[1-\frac{1}{2}[\epsilon_2(n)+\epsilon_2^*(n)]\right]\sigma_{xn}\right\}, \tag{14}$$

where, in the continuum representation, we have according to (A6) and (A7),

$$W(x)=\frac{1}{2\sqrt{N}}a^2\sum_{q,i=1,2}\left\{\left[\mathrm{Re}\left(e^{-i\,\theta_i/2}\frac{d\gamma_{iq}}{dx}\right)\right]^2 e^{-4r_i}+\left[\mathrm{Im}\left(e^{-i\,\theta_i/2}\frac{d\gamma_{iq}}{dx}\right)\right]^2 e^{4r_i}\right\}. \tag{14a}$$

and, according to (A8),

$$\epsilon_i(n)=\exp\left[-\frac{1}{2}(|\tilde{\gamma}_{i,n}(n)|^2+|\tilde{\gamma}_{i,n}(n+1)|^2+|\tilde{\gamma}_{i,n+1}(n)|^2+|\tilde{\gamma}_{i,n+1}(n+1)|^2)-\tilde{\gamma}_{i,n}(n+1)\tilde{\gamma}^*_{i,n}(n)-\tilde{\gamma}_{i,n+1}(n+1)\tilde{\gamma}^*_{i,n+1}(n)\right]. \tag{14b}$$

Here, $\tilde{\gamma}_{i,m}(n)=(1/\sqrt{N})\Sigma_q\tilde{\gamma}_{i,q}(n)\exp(iqma)$ is a nonlocal expression. In the continuum limit it becomes local as $\epsilon_i(n)$, Eq. (14b), tends to

$$\epsilon_i(n)\rightarrow\epsilon_i(x)=\epsilon_i^*(x)=\exp[-4|\tilde{\gamma}_i(x)|^2]. \tag{14c}$$

From Eq. (14), it is evident that the participation of phonons in the transfer opens a gap $\Delta=\langle f|\Delta(x)|f\rangle$, where

$$\Delta(x)=\frac{T}{2}\exp[-W(x)]\{1-\exp[-4|\tilde{\gamma}_1(x)|^2]\}\exp[-2|\tilde{\gamma}_2(x)|^2]\{1+\exp[-4|\tilde{\gamma}_2(x)|^2]\}. \tag{15}$$

The gap Δ represents a joint effect of phonons 1 and 2, coupled to the electron transfer term, to the band splitting in the extended Jahn-Teller model. Both bands are coupled due to the participation of phonons 2 in the transfer [Eq. (10)], unless this contribution could be neglected for weakly scattered phonons.

In what follows we shall investigate the case of a soliton, i.e., either the one-level case of a Holstein polaron, $\beta=0$, or a qualitatively equivalent reduced case with negligible coupling (10) of channels 1 and 2 (a modified Holstein polaron).

We shall go over to the continuum $(p_{n+1}-p_n\rightarrow pa)$ and expand into series $\exp(\pm ipa)$ near the bottom of the lower band [specified by $\sigma_{z1}=1$ in (14)], near $k=0$. (For the upper band the expansion would be performed near $k=\pi/a$). Then, using the formulas (A9)–(A12), we obtain for the effective density of the Hamiltonian (12) as an average in the FG state (4) [$\sigma_{z1}=1$ in (14)]

$$\begin{aligned}\langle\Psi_{\rm FG}|\tilde{H}(x)|\Psi_{\rm FG}\rangle=&\frac{\Omega}{2}\sum_i\cosh4r_i+\frac{1}{\sqrt{N}}\sum_{i,q}\langle\tilde{u}_{iq}|\Omega\cosh4r_i+\tilde{T}a^2A^\dagger A|\tilde{u}_{iq}\rangle+\frac{\Omega}{2}\sinh4r_i(\langle f|\tilde{\gamma}_{iq}e^{-i\theta_i}|\tilde{u}_{iq}\rangle+\langle\tilde{u}_i|\tilde{\gamma}^*_{iq}e^{\theta_i}|f\rangle)\\&+\alpha\frac{1}{\sqrt{N}}\sum_q\{\cosh2r_1[\langle\tilde{u}_{1q}|\exp(-iqx)|f\rangle+\text{ H.c.}]+\sinh2r_1[e^{i\theta_1}\langle\tilde{u}_{1q}|\exp(iqx)|f\rangle+\text{H.c.}]\}\\&-\beta\frac{1}{\sqrt{N}}\sum_q\{\cosh2r_2[\langle\tilde{u}_{2q}|\exp(-iqx)\exp[-2|\tilde{\gamma}_1(n)|^2]|f\rangle+\text{H.c.}]\\&+\sinh2r_2[e^{i\theta_2}\langle\tilde{u}_{2q}|\exp(-iqx)\exp[-2|\tilde{\gamma}_1(n)|^2]|f\rangle+\text{H.c.}]\}+\langle f|\tilde{T}(x)|f\rangle\langle f|-2+(ap)^2|f\rangle.\end{aligned} \tag{16}$$

In Eq. (16) the auxiliary states

$$|\tilde{u}_{iq}\rangle=|\tilde{\gamma}_{iq}f\rangle \tag{17}$$

were defined, where $\tilde{\gamma}_{iq}(n)$ are given by Eq. (13a).

The confinement to small electron momenta p made it possible for us to express part of the averaged Hamiltonian (16) in a convenient compact form by the use of the operator

$$A=\frac{1}{f}\frac{df}{dx}-ip.$$

An identity $A|f\rangle=0$ is evidently fulfilled: It allows an interpretation of A as a soliton annihilation operator and simplifies the calculation of the related matrix elements in the next section. The operator A was introduced by Nagy[22] and was used with convenience in a variational problem of a free electron interacting with acoustic phonons.

In the last term of Eq. (16) we decoupled the electron term, which was approved if $\tilde{T}$ varies much more slowly with x than $f(x)$. The reduced transfer matrix element of $\tilde{T}$, Eqs. (14)–(14c), reads

$$\begin{aligned}T_R\equiv\langle f|\tilde{T}(x)|f\rangle=&\frac{T}{2}\langle f|\exp[-W(x)]\\&\times(1+\exp[-4|\tilde{\gamma}_1(x)|^2]+\{1-\exp[-4|\tilde{\gamma}_1(x)|^2]\}\\&\times\exp[-2|\tilde{\gamma}_2(x)|^2])|f\rangle,\end{aligned} \tag{18}$$

where $W(x)$ is given by Eq. (14a). The coefficient of T, Eq. (18), represents the reduction due to the self-trapping polaron effect modified by the squeezing, Eq. (14a), and a reduction by exponential factors stemming from many-phonon effects if $\gamma_2\neq0$. Consequently, the respective effective mass is modified according to $m^{*-1}=2a^2\langle f|\tilde{T}(x)|f\rangle$. If $\beta=0$, then $\gamma_2(x)=0$ and $T_R=T\langle f|\exp[-W(x)]|f\rangle$. Formula (14a) for $W(x)$ brings a generalization of the effective self-trapping effect found by Zheng[21] and Feinberg *et al.*[9] for the Holstein polaron in the framework of coherent and squeezed states with real displacements γ_{iq} and a real parameter of squeezing, $\theta_i=0$. Evidently, the generalization to complex parameters brings a new term in the exponent which grows $\propto e^{r_i}$ and introduces a θ_i dependence. For the final effect, however, an explicit evaluation of $\gamma_{iq}(x)$ or $\tilde{\gamma}_{iq}(x)$, Eq. (13), is necessary and will be performed in the next section.

The classical case $r_i=\theta_i=0$ reduces to the problem solved by Brizhik *et al.*[11] This case of a polaron resembles also the problem of the acoustic polaron as it was presented by Nagy.[22] These facts lead us to the choice of the variational ansatz for the respective local electron amplitude $f(x)$, Eq. (4a), in a form compatible with the known adiabatic solution for the ground state of the electron (exciton) in the Holstein model[6] and in the Davydov model[8] which imply the nonlinear Schrödinger equation for the electron amplitude $f(x)$. The respective adiabatic solution reads

$$f_{\rm ad}(sx)=(as_{\rm ad})^{1/2}\frac{1}{\sqrt{2}}{\rm sech}(s_{\rm ad}x),\quad as_{\rm ad}=\frac{\alpha_{\rm ad}^2}{4\Omega^2T}\equiv\mu_{\rm ad}, \tag{19}$$

$as_{\rm ad}$ being a dimensionless inverse soliton width and T a bandwidth parameter. The adiabatic approximation in the above-mentioned models was approved for large T. An analogous result for the exciton-acoustic phonon adiabatic ground state was obtained, e.g., by Venzl and Fischer[23] and by Nagy in his generalized adiabatic variational approach.[22] It should be noted that the soliton solution (19) breaks the translational invariance of the problem. As is known, it can be restored by introducing an arbitrary constant x_0 into the argument of $f(sx)$ as $f[s(x-x_0)]$.

IV. STABILITY OF THE SOLITON AGAINST QUANTUM FLUCTUATIONS

The aim of this section is to investigate the stability of a ground state with a localized solution of the type (19) with respect to quantum phonon fluctuations included in the Hamiltonian (16) with $T(x)$, Eq. (14), diagonal ($\beta=0$) or, equivalently, with the negligible nondiagonal term (10) when the related conditions found above are fulfilled. To this purpose, we shall assume the shape of the electron amplitude $f(sx)$ of the quantum ground state (4a) in a form similar to (19),

$$f(sx)=(as)^{1/2}\frac{1}{\sqrt{2}}{\rm sech}(sx), \tag{20}$$

taking s as an electron variational parameter, and minimize the energy (16) with respect to the electron and phonon variational parameters $\kappa=as$ and $\tilde{\gamma}_{iq}(x),\tilde{\gamma}_{iq}^*(x)$.

In view of the form of the averaged energy (16) it is convenient to minimize it with respect to the auxiliary states $|\tilde{u}_{iq}\rangle$ Eq. (17). This way of minimization is not quite exact as in expression (16) there occur also $\tilde{\gamma}_{iq},\tilde{\gamma}_{iq}^*$ explicitly. However, this effect can be accounted for by iteration of the γ_{iq}'s at the end. Then, from

$$\frac{\partial\langle H/T_R\rangle}{\partial\langle\tilde{u}_{iq}|}=0, \tag{21}$$

we get operator equations for $|\tilde{u}_{iq}\rangle$,

$$(\bar{\Omega}\cosh 4r_1+\kappa^2\bar{A}^\dagger\bar{A})|\tilde{u}_{1q}\rangle+\bar{\alpha}\left[\cosh 2r_1\exp\left(-i\bar{q}\frac{\bar{x}}{\kappa}\right)+\sinh 2r_1e^{i\theta_1}\exp\left(i\bar{q}\frac{\bar{x}}{\kappa}\right)\right]|f\rangle=0, \tag{22a}$$

$$(\bar{\Omega}\cosh 4r_2+\kappa^2\bar{A}^\dagger\bar{A})|\tilde{u}_{2q}\rangle-\bar{\beta}\left[\cosh(2r_2)\exp\left(-i\bar{q}\frac{\bar{x}}{\kappa}\right)+\sinh(2r_2)e^{i\theta_2}\exp\left(i\bar{q}\frac{\bar{x}}{\kappa}\right)\exp\left(-\frac{i\bar{q}\bar{x}}{\kappa}-2|\tilde{\gamma}_1(\bar{x})|^2\right)\right]|f\rangle=0. \tag{22b}$$

Here, we went over to dimensionless variables by rescaling the Hamiltonian $\tilde{H}=H/T_R$, Eq. (21), and consequently also the variables $\bar{\Omega}=\Omega/T_R$, $\bar{\alpha}=\alpha/T_R$, $\bar{\beta}=\beta/T_R$, where T_R was defined by Eq. (18). Further, we define $sx=\bar{x}$, $p=s\bar{p}$, and $\bar{A}=sA$ in order to eliminate s from the function $f(sx)=f(\bar{x})$. We introduced also the dimensionless quantities $\kappa=sa$, $\bar{q}=qa$. From Eqs. (22) we can find $\gamma_{iq}(\bar{x})$. The result is

$$\gamma_{1q}(\bar{x})=-\bar{\alpha}\exp\left(-i\bar{q}\frac{\bar{x}}{\kappa}\right)[\bar{\Omega}\cosh 4r_1+\bar{q}^2-2\kappa^2(1-\tanh^2\bar{x})-i2\bar{q}\kappa\tanh\bar{x}]^{-1}, \tag{23a}$$

$$\gamma_{2q}(\bar{x})=\bar{\beta}\exp\left(-i\bar{q}\frac{\bar{x}}{\kappa}-2|\tilde{\gamma}_1(\bar{x})|^2\right)\left[\bar{\Omega}\cosh 4r_2+\bar{q}^2-2\kappa^2(1-\tanh^2\bar{x})+2i\kappa\left(\bar{q}-i\kappa\frac{d}{dx}|\tilde{\gamma}_1(x)|^2\right)\tanh\bar{x}\right.$$
$$\left.-4i\kappa\left(\bar{q}\frac{d}{dx}|\tilde{\gamma}_1(x)|^2-i\kappa\frac{d^2}{dx^2}|\tilde{\gamma}_1(x)|^2\right)\right]^{-1}. \tag{23b}$$

The $\bar{x}$ dependence of the nonperiodic part of $\tilde{\gamma}_{iq}(\bar{x})$ represents the localizing influence of a soliton on phonons at the soliton width scale κ^{-1}.

There remains to minimize the energy (16) with respect to the electron variational parameter κ defined above.

Let us substitute the functions (22) into the mean energy (16). The result reads, up to order $\bar{\alpha}^2$ and $\bar{\beta}^2$,

$$E(\kappa;r_1,r_2;\theta_1,\theta_2;\overline{\alpha,\beta,\Omega})=\langle\Psi_{\rm FG}|\widetilde{H}|\Psi_{\rm FG}\rangle=\frac{\overline{\Omega}}{2}\sum_i \cosh 4r_i-2+\langle f|a^2\overline{p^2}|f\rangle-\frac{\overline{\alpha^2}}{\overline{\Omega}\sqrt{N}}\sum_q \langle f|Q_q|f\rangle$$
$$-\frac{\overline{\beta^2}}{\overline{\Omega}\sqrt{N}}\sum_q \langle f|\exp[-2|\widetilde{\gamma}_1(x)|^2]Q_q\exp[-2|\widetilde{\gamma}_1(x)|^2]|f\rangle. \tag{24}$$

In Eq. (24) we defined

$$Q_q=\overline{\Omega}(\overline{\Omega}+\overline{q^2}-2\overline{q\kappa p}+\kappa^2\overline{A^\dagger A})^{-1}. \tag{25}$$

This quantity is rewritten into a more suitable form in Appendix B. There its mean value $\langle f|Q_q|f\rangle$ is also calculated, which appears in Eq. (24).

The exponential reduction of the last term in (24) enhances the energy of the ground state. This reduction is due to a decrease of the transition probability between two split levels by the self-trapping due to phonons $i=1$ nonlinearly coupled to phonons $i=2$.

In order to make $E(\kappa;r_1,r_2;\theta_1,\theta_2,\overline{\alpha,\beta,\Omega})$, Eq. (24), more suitable for variational calculations, we shall simplify it for small $\overline{\alpha}$ and β or for small κ. We expect a weak x dependence of $W(x)$ and of $|\gamma_i(x)|^2$ given by (23a) and (23b) and write

$$T_R=T\langle f|\exp[-W(x)]\tfrac{1}{2}[1+\exp[-4|\widetilde{\gamma}_1(x)|^2]+\{1-\exp[-4|\widetilde{\gamma}_1(x)|^2]\}\exp[-2|\widetilde{\gamma}_2(x)|^2]]|f\rangle$$
$$\approx T\exp[-\langle f|W(x)-\ln\tfrac{1}{2}(\{1+\exp[-4|\widetilde{\gamma}_1(x)|^2]\}+\{1-\exp[-4|\widetilde{\gamma}_1(x)|^2]\}\exp[-2|\widetilde{\gamma}_2(x)|^2])|f\rangle b]\equiv T\exp(-\Gamma). \tag{26}$$

Here, the dominant term of Γ is κ independent [see Eqs. (23)] and the remaining terms are slowly varying with κ for κ small; therefore we shall consider Γ as κ independent. Evidently, for $\beta=0$, $\Gamma=\langle f|W(x)|f\rangle$. Similarly, we assume

$$\langle f|\sum_q \exp[-2|\widetilde{\gamma}_1(x)|^2]Q_q\exp[-2|\widetilde{\gamma}_1(x)|^2]|f\rangle\approx\sum_q \langle f|Q_q|f\rangle\exp[-4\langle f||\widetilde{\gamma}_1(x)|^2|f\rangle]. \tag{27}$$

In Eq. (27) the integration over q can be performed by the use of the relation

$$\frac{1}{\sqrt{N}}\frac{\overline{\alpha^2}}{\Omega\Omega}\sum_q=\frac{\alpha^2}{\Omega^2T_R}\frac{a}{2\pi}\int_{-\pi/a}^{\pi/a}dq\equiv\frac{\mu_R}{\pi}\int_{-\pi}^{\pi}d\overline{q},\quad \mu_R=\frac{\alpha^2}{2\Omega^2T_R}\equiv\mu\exp\Gamma, \tag{28}$$

Γ was given by (26) and $\mu=\alpha^2/2\Omega^2T$.

In Eq. (27), $\widetilde{\gamma}_1(x)$ is given by (14a) and (23a). Evidently, the exponential reduction factor in (27) reads

$$|\widetilde{\gamma}_{1q}|^2=|\gamma_{1q}|^2\cosh 4r_1-\frac{1}{2}\sinh 4r_1(\gamma_{1q}^{*2}e^{i\theta}+\gamma_{1q}^2e^{-i\theta}), \tag{28a}$$

where

$$|\gamma_{1q}|^2=\overline{\alpha^2}\{[\overline{\Omega}+\overline{q^2}-2\kappa^2(1-\overline{\tanh^2x)}]^2+4\overline{q^2}\kappa^2\overline{\tanh^2x}\}^{-1}, \tag{28b}$$

$$\gamma_{1q}^2=\overline{\alpha^2}\exp\left(-2i\frac{\overline{qx}}{\kappa}\right)[\overline{\Omega}+\overline{q^2}-2\kappa^2(1-\overline{\tanh^2x)}-i2\overline{q\kappa}\overline{\tanh x}]^{-2}, \tag{28c}$$

and

$$\gamma_{1q}^{*2}e^{i\theta}+\gamma_{1q}^2e^{-i\theta}=2\overline{\alpha^2}\{[\overline{\Omega}+\overline{q^2}-2\kappa^2(1-\overline{\tanh^2x)}]^2+4\overline{q^2}\kappa^2\overline{\tanh^2x}\}^{-2}$$
$$\times(\cos(2\overline{qx/}\kappa-\theta_1)\{[\overline{\Omega}+\overline{q^2}-2\kappa^2(1-\overline{\tanh^2x)}]^2-4\overline{q^2}\kappa^2\overline{\tanh^2x}\}$$
$$+2\sin(2\overline{qx/}\kappa-\theta_1)\overline{q\kappa}\overline{\tanh x}[\overline{\Omega}+\overline{q^2}-2\kappa^2(1-\overline{\tanh^2x)}]). \tag{28d}$$

In the case of the Holstein polaron, $\beta=0$, Eq. (23b) implies $\gamma_2(x)=0$ and $\epsilon_2(x)=1$ [Eqs. (15b) and (23b)], and, according to Eq. (14), the problem becomes diagonal exactly. Then, with the use of Eqs. (25)–(28), Eq. (24) yields

$$E(\kappa;r_1,r_2;\theta_1,\theta_2;\mu,\overline{\Omega})-\frac{\overline{\Omega}}{2}\sum_i\cosh 4r_i+2=\frac{1}{3}\kappa^2-\frac{\mu}{\pi}\int_{-\pi}^{\pi}d\overline{q}\langle f|Q_q|f\rangle. \tag{29}$$

Here, $\overline{\mu}=\mu\exp(\Gamma)$. The matrix element $\langle f|Q_q|f\rangle$ is calculated in Appendix B. Details of the integration over $\overline{q}$ in (29) are presented in Appendix C.

According to Appendix C, Eq. (29) yields finally

$$E_{\min}\equiv E(\kappa;r_1,r_2;\theta_1,\theta_2;\mu,\overline{\Omega})-\frac{\overline{\Omega}}{2}\sum_{i=1,2}\cosh 4r_i+2$$
$$=\frac{1}{3}\kappa^2-\frac{2\overline{\mu}}{(1+\overline{\Omega}/\kappa^2)^{1/2}}\left\{\frac{\kappa}{3}+\frac{\delta}{\kappa}+\frac{\delta^2}{2\kappa}-\frac{\delta^2}{(\pi^2+\delta^2)}+\frac{2\delta}{\pi}\arctan\frac{\pi}{\delta}+\frac{1}{4\pi}[S(\kappa,\delta)-S(\kappa,-\delta)]\right\}. \quad (30)$$

We defined [see (C3)]

$$S(\kappa,\delta)\equiv S(1,\kappa,\delta)=\left[4\kappa\frac{\kappa+\delta}{2\kappa+\delta}+(\delta+2\kappa)\left(1+\frac{\delta}{\kappa}\right)+\frac{\delta^2}{2\kappa+\delta}\right]\arctan\frac{\pi}{\delta+2\kappa},$$

and $\delta=\delta(\kappa,\overline{\Omega})=(\kappa^2+\overline{\Omega})^{1/2}-\kappa$. Numerical evaluations of $E(\kappa,\overline{\Omega},\overline{\mu})$, Eq. (30), are plotted in Figs. 1(a), 1(b) and 2, with $\overline{\mu}$ defined in (29) and $\overline{\Omega}=\Omega/T_R$ as parameters, and $r_i=\theta_i=0$. $E(\kappa,\overline{\Omega},\overline{\mu})$ exhibits a minimum for $\kappa=\kappa_{\min}(\overline{\Omega},\overline{\mu})$ only for a sufficiently large $\overline{\mu}$, $\overline{\mu}>\mu_{\text{crit}}(\overline{\Omega})$. As we utilized the soliton bare ansatz (20) for the evaluation of (29), the terms with δ there are considered as perturbations, $\delta<\frac{1}{3}\kappa^2$ or $\overline{\Omega}<\frac{2}{3}\kappa^3+\frac{1}{9}\kappa^4$.

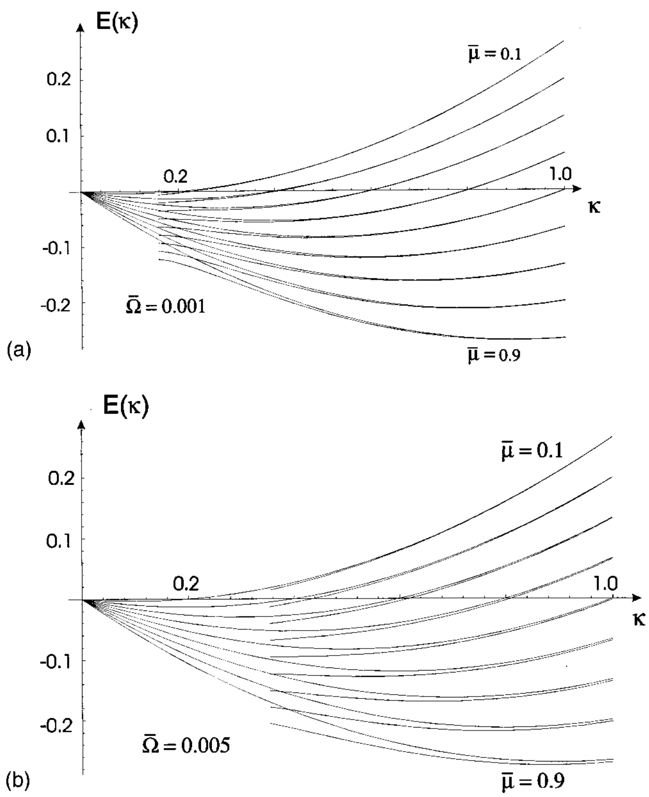

FIG. 1. (a) Energy $E(\kappa,\overline{\mu})$, Eq. (27), in the adiabatic case and in the quantum case for $\kappa^3>\overline{\Omega}=\Omega/T$, $\overline{\Omega}=0.001$, $\overline{\mu}=0.1$, 0.2,…,0.9, $r_i=\theta_i=0$, $i=1,2$. For the adiabatic curves $E(\kappa=0,\overline{\mu})=0$. The term $\exp(-2J)$ in (27) contributes for $2\kappa^2<\overline{\Omega}$, i.e., beyond the scope of validity of the perturbation theory, $\overline{\Omega}\leq\kappa^3$. The curves are not plotted in this region. (b) The same for $\overline{\Omega}=0.005$.

The dependence of $\kappa_{\min}\equiv\kappa(\overline{\Omega},\overline{\mu})$ is plotted in Fig. 3. The phase diagram $(\overline{\mu},\overline{\Omega})$ is shown in Fig. 4. A line $\overline{\mu}_{\text{crit}}(\overline{\Omega})$ of critical coupling parameters results: At $\overline{\mu}(\overline{\Omega})>\mu_{\text{crit}}(\overline{\Omega})$ the electron-phonon interaction gives rise to a finite soliton width $\lambda(\overline{\Omega})=\kappa^{-1}(\overline{\Omega})$. If $\overline{\mu(\Omega)}<\mu_{\text{crit}}(\overline{\Omega})$, then the quantum fluctuations destabilize the soliton.

In order to get the adiabatic limit of (30) and compare it with the Holstein result (19) we have to have a clear definition of μ in Eq. (29) for the adiabatic case. If in the classical Hamiltonian the coefficient of the interaction term is α_{ad}, then by transformation to quantum normal phonons it becomes $\alpha\rightarrow\alpha_{\text{ad}}/\sqrt{2}$. Our choice $\alpha/2$ as the respective coefficient in (1) yields $\alpha_{\text{ad}}/2\rightarrow\alpha/(2\sqrt{2})$. Then, the adiabatic limit of Eq. (30) yields

$$E_{\text{ad}}(\kappa,\overline{\mu}_{\text{ad}})+2=\langle f|\kappa^2\overline{p}^2-\overline{\mu}_{\text{ad}}\sum_q Q_q|f\rangle=\frac{1}{3}\kappa^2-\frac{2}{3}\overline{\mu}_{\text{ad}}\kappa. \quad (31)$$

By minimization of (31) with respect to κ, we obtain for the adiabatic ground state finally

$$\kappa_{\text{ad}}=as_{\text{ad}}=\overline{\mu}_{\text{ad}}=\alpha^2\exp(\Gamma_{\text{ad}})/4\Omega^2T=\frac{\mu}{2}\exp(\Gamma_{\text{ad}})$$
$$=\mu_{\text{ad}}\exp(\Gamma_{\text{ad}}), \quad (32)$$

There, Eqs. (14a) and (26) imply

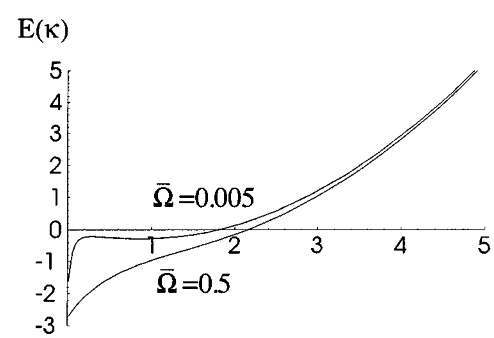

FIG. 2. Energy $E(\kappa,\overline{\mu})$ for $\overline{\mu}=1.8$ and $\overline{\Omega}=0.5$, 0.005, $r_i=\theta_i=0$.

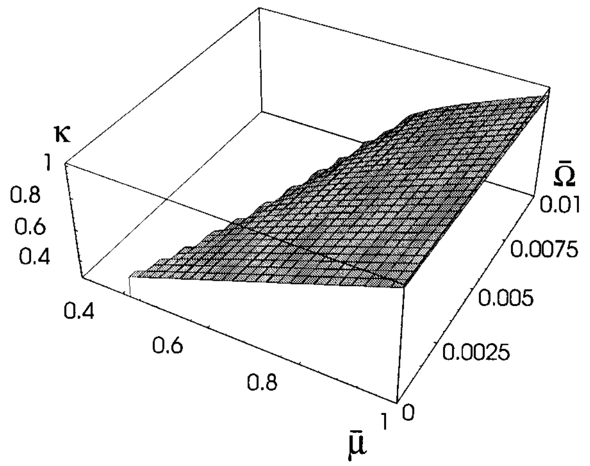

FIG. 3. Inverse width of the soliton κ vs $\overline{\mu}$ and $\overline{\Omega}$. Note that the adiabatic curve ($\overline{\Omega}=0$) starts at $\overline{\mu}_{\rm crit}^{\rm ad}\neq 0$.

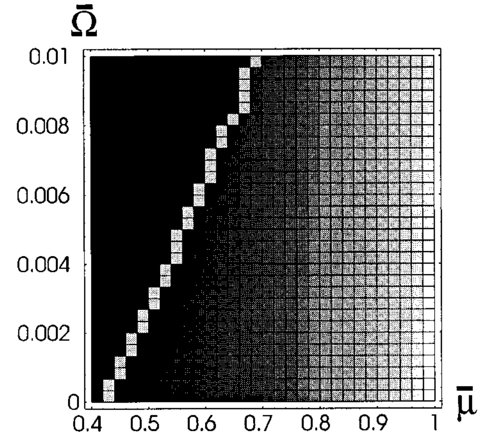

FIG. 4. Phase diagram $\overline{\mu}$ vs $\overline{\Omega}$. View of the surface in Fig. 3 from above. The dark region of the soliton instability is separated from the region of stability by the curve $\mu_{\rm crit}(\overline{\Omega})$.

$$\Gamma_{\rm ad}=\frac{1}{2\sqrt{N}}a^2\sum_{q,i}\left\langle f\left|\left|\frac{d\gamma_{iq}}{dx}\right|^2\right|f\right\rangle.$$

Using (32) we obtain for the dimensionless adiabatic ground state energy (31)

$$E_{\rm ad}(\mu_{\rm ad})+2\exp(-\Gamma_{\rm ad})=-\frac{\mu_{\rm ad}^2}{3}\exp(\Gamma_{\rm ad})$$
$$=-\frac{\alpha^4}{48\Omega^4T^2}\exp(\Gamma_{\rm ad}). \qquad (33)$$

The preexponential term is identical with the corresponding result by Holstein.[6] It is evident that the self-trapping effect lowers the soliton ground state energy (33) and increases κ, Eq. (32); i.e., it lowers the soliton width which means increasing of the soliton stability.

If $\beta\neq 0$, then instead of $\overline{\mu}$ in Eq. (30) we have

$$\overline{\mu}\rightarrow\mu_R\left(1+\frac{\overline{\beta^2}}{\overline{\alpha^2}}\exp(-2\mu_R J)\right), \qquad (34)$$

where

$$J\equiv J(\kappa,\overline{\Omega},r_1,\theta_1)=\frac{\overline{\Omega}T}{\pi}\int_{-\infty}^{\infty}\frac{d\overline{x}}{\cosh^2\overline{x}}\int_0^{\pi}d\overline{q}\left(\left\{\left[1+\frac{\overline{q}^2}{\overline{\Omega}}-\frac{2\kappa^2}{\overline{\Omega}}(1-\tanh^2\overline{x})\right]^2+\frac{4\kappa^2\overline{q}^2}{\overline{\Omega}}\tanh^2\overline{x}\right\}^{-1}\cosh 4r_1\right.$$
$$-\frac{1}{2}\sinh 4r_1\left\{\left[1+\frac{\overline{q}^2}{\overline{\Omega}}-2\frac{\kappa^2}{\overline{\Omega}}(1-\tanh^2\overline{x})\right]^2+4\frac{\overline{q}^2\kappa^2}{\overline{\Omega}}\tanh^2\overline{x}\right\}^{-2}$$
$$\times\left(\cos(2\overline{q}\overline{x}/\kappa-\theta_1)\left\{\left[1+\frac{\overline{q}^2}{\overline{\Omega}}-2\frac{\kappa^2}{\overline{\Omega}}(1-\tanh^2\overline{x})\right]^2-4\frac{\overline{q}^2\kappa^2}{\overline{\Omega}}\tanh^2\overline{x}\right\}\right.$$
$$\left.\left.+2\sin(2\overline{q}\overline{x}/\kappa-\theta_1)\overline{q}\kappa\tanh\overline{x}\left[1+\frac{\overline{q}^2}{\overline{\Omega}}-\frac{2\kappa^2}{\overline{\Omega}}(1-\tanh^2\overline{x})\right]\right)\right). \qquad (35)$$

The integral J, Eq. (35) diverges ($J\rightarrow+\infty$) for $\overline{\Omega}<2\kappa^2$; therefore in the region relevant for the nonadiabatic contributions to the soliton ground state the contribution of the exponential term in (34) is zero. On the other hand, this contribution is finite for $\overline{\Omega}>2\kappa^2$, i.e., out of the region of soliton stability.

V. CONCLUSION

Generally, the extended Jahn-Teller Hamiltonian (1) does not admit the Fulton-Gouterman ground state with a localized (soliton) electron amplitude. The reason is that phonons 2 which in the original Hamiltonian (1) couple the JT levels participate also in the transfer of electrons due to many-phonon effects. If the change of the phonon wave vector due to their scattering at electrons during the transfer at a distance of a soliton width is small, then this effect was shown to be negligible. Then the problem becomes effectively a one-level problem qualitatively equivalent to the problem of a Holstein polaron with parameters renormalized due to phonons 2: The reduction factor $\exp[-W(x)]$ is additionally reduced [see Eq. (26)]. For this case, one can summarize following results.

(i) Expression (15) related to the band splitting implies that the gap is opened by the interaction of the electron states with phonons 1 during their transfer in the lattice and a simultaneous coupling to phonons 2. The gap is narrowed by the self-trapping effect—the self-trapping is further modified by the quantum effects discussed next.

(ii) The soliton ground state is affected by quantum fluctuations: The measure of the influence is the ratio of the phonon and electron energy scales, $\overline{\Omega}=\Omega/T_R$. This ratio is modified by the self-trapping effect determined by the complex displacements and complex squeezing parameters: The self-trapping polaron effect given by Eqs. (26) and (14a) reduces the bandwidth T by a factor which includes a joint effect of electrons on the phonon displacements $\gamma_{iq}(n)$ and of the squeezing. It consists of two competing contributions (14a): (1) a term

$$\left[\mathrm{Re}\left(\frac{d\gamma_{iq}}{dx}e^{-i\theta_i/2}\right)\right]^2 e^{-4r_i}$$

weakens the self-trapping, and (2) a term

$$\left[\mathrm{Im}\left(\frac{d\gamma_{iq}}{dx}e^{-i\theta_i/2}\right)\right]^2 e^{4r_i}$$

competing with (i) enhances the self-trapping.

Evidently, the effect (2) is present if at least one of $\mathrm{Im}\gamma_{iq}(x)$ or θ_i is nonzero. Equations (23a) and (23b) imply that $\mathrm{Im}\gamma_{iq}$ contributes if $\kappa\neq 0$ and $q\neq 0$, simultaneously.

Nonadiabatic effects due to $\overline{\Omega}$ become evident if one compares the result (30) with the adiabatic one (31). In Eq. (30), there are nonadiabatic contributions related to $\delta(\kappa,\overline{\Omega})$ ($\delta\to 0$ if $\overline{\Omega}\to 0$). The perturbation theory used for the calculation of the energy (30) is valid only for $\delta<\kappa^2/3$, i.e., when accounting for the definition of δ, Eq. (30), for $\overline{\Omega}<\frac{2}{3}\kappa^3+\frac{1}{9}\kappa^4$. From the numerical evaluation of the formula (30) plotted in Figs. 1(a) and 1(b) we see that the curves exhibit local minima which represent soliton ground states. These minima disappear for small $\overline{\mu}=\mu\exp(\Gamma)$. As Γ enhances the effective interaction $\overline{\mu}$, it stabilizes the soliton due to the respective decrease of the soliton width $\lambda=\kappa^{-1}$, ($\kappa\propto\overline{\mu}$). In the Figs. 1(a) and 1(b) the energies in the region of small κ are not plotted as this region is beyond the validity of our perturbation theory.

Nonadiabatic effects compete the self-trapping: For a weak effective e-ph coupling $\overline{\mu}<\mu_{\mathrm{crit}}$ they destroy the stability of the soliton: the minimum of the ground state energy disappears [Figs. 1(a) and 1(b)]. Above the critical coupling they shift the minimum of the ground state energy $E(\kappa)$, Eq. (30), to lower values of $\kappa_{\min}$ (higher values of the width of the soliton λ).

(iii) Further, the contribution of the many-phonon effects, $\propto\beta^2$ in (34), is zero for $\overline{\Omega}<2\kappa^2$. On the other hand, they are shown to contribute for $\overline{\Omega}>2\kappa^2$, i.e., out of the region of the stability of the soliton against the quantum fluctuations discussed above.

From Fig. 3 and from the phase diagram at Fig. 4 we see also a shift of the $\mu_{\mathrm{crit}}(\overline{\Omega})$ to higher values with increasing $\overline{\Omega}$. There exists a line of $\mu_{\mathrm{crit}}(\overline{\Omega})$ increasing with $\overline{\Omega}$ above which the soliton remains stable (Fig. 4). Let us note that we did not perform a numerical analysis of the ground state energy for r_i, $\theta_i=0$ as the respective set of equations for the ground state would be too complicated and the respective corrections relatively very small.

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APPENDIX A

For calculation of the mean value of the Hamiltonian (11) in the state (4) we need the following transformations:

$$D(\gamma)S(\zeta)=S(\zeta)D(\tilde{\gamma}),\quad \tilde{\gamma}=\gamma\cosh(2r)+\gamma^* e^{i\theta}\sinh(2r),$$
$$\zeta=re^{i\theta},\quad \text{(A1)}$$

$$D^{-1}(\tilde{\gamma}_{iq}(n))b_{iq}D(\tilde{\gamma}_{iq}(n))=b_{iq}+\tilde{\gamma}_{iq}(n),\quad i=1,2, \quad \text{(A2)}$$

$$S^{-1}(\zeta_i)b_{iq}S(\zeta_i)=b_{iq}\cosh 2r_i+b_{iq}^{\dagger}e^{i\theta}\sinh 2r_i,\quad \text{(Ref. 25)}, \quad \text{(A3)}$$

$$S^{-1}(\zeta_i(n))D^{-1}(\gamma_{iq}(n))p_nD(\gamma_{iq}(n))S(\zeta_i(n))$$
$$=p_n+i\frac{1}{\sqrt{N}}\sum_q\sum_{i=1,2}\left[\frac{d\gamma_{iq}}{dn}\cosh 2r_i-\frac{d\gamma_{iq}^*}{dn}e^{-i\theta}\sinh 2r_i\right]b_{iq}^{\dagger}+\mathrm{H.c.}, \quad \text{(A4)}$$

$$\tilde{R}_1^{(ph)}=S^{-1}(\zeta_i(n))D^{-1}(\gamma_{iq}(n))R_1^{(ph)}D(\gamma_{iq}(n))S(\zeta_i(n))$$
$$=S^{-1}(\zeta_i(n))D(\gamma_{iq}(n))^{-1}D(\gamma_{iq}(n+1))S(\zeta_i(n))S^{-1}(\zeta_i(n))S(\zeta_i(n+1)), \quad \text{(A5)}$$

where

$$S^{-1}(\zeta_i(n))D^{-1}(\gamma_{iq}(n))D(\gamma_{iq}(n+1))S(\zeta_i(n+1))$$
$$=\exp\left(-\frac{1}{2\sqrt{N}}\sum_{q,i}\left\{\frac{1}{4}[e^{-i\theta/2}\Gamma_{iq}(n)+\text{H.c.}]^2e^{-4r_i}-\frac{1}{4}[e^{-i\theta/2}\Gamma_{iq}(n)-\text{H.c.}]^2e^{4r_i}\right\}\right)$$
$$\times\exp\frac{1}{\sqrt{N}}\sum_{i,q}\{[[\Gamma_{iq}(n)-\Gamma^*_{iq}(n)e^{-i\theta}]b^\dagger_{iq}+[\Gamma_{iq}(n)e^{i\theta}-\Gamma^*_{iq}(n)]b_{iq}]e^{2r_i}$$
$$+[[\Gamma_{iq}(n)+\Gamma^*_{iq}(n)e^{-i\theta}]b^\dagger_{iq}-[\Gamma_{iq}(n)e^{i\theta}+\Gamma^*_{iq}(n)]b_{iq}]e^{-2r_i}\} \tag{A6}$$

and

$$\langle 0|S(\zeta_i(n))^{-1}S(\zeta_i(n+1))|0\rangle=\exp\left\{-\frac{a^2}{\sqrt{N}}\sum_i\left[\left(\frac{dr_i}{dx}\right)^2+r_i^2\left(\frac{d\theta_i}{dx}\right)^2\right]\right\}=1, \tag{A7}$$

as we suppose r_i and θ_i to be independent of x.

In (A6) we defined $\Gamma_{iq}(n)=\gamma_{iq}(n+1)-\gamma_{iq}(n)$.

Calculation of the phonon mean value of (14) leads to

$$\epsilon_1(n)\equiv\langle 0_{n+1},0_n|D_n^{-1}(\tilde{\gamma}_{1n}(n))D_{n+1}^{-1}(\tilde{\gamma}_{1n}(n))S_n^{-1}S_{n+1}^{-1}(-1)^{b^\dagger_{1,n+1}b_{1,n+1}}(-1)^{b^\dagger_{1,n}b_{1,n}}S_nS_{n+1}D_n(\tilde{\gamma}_{1n}(n+1))$$
$$\times D_{n+1}(\tilde{\gamma}_{1n+1}(n+1))|0_n,0_{n+1}\rangle$$
$$=\sum_{m_n=0}^{\infty}(-1)^{m_n}|_g\langle\tilde{\gamma}_{1n}(n)|m_n\rangle|^2\sum_{l_{n+1}=0}^{\infty}(-1)^{l_{n+1}}{}_g\langle\tilde{\gamma}_{1,n+1}(n)|l_{n+1}\rangle\langle l_{n+1}|\tilde{\gamma}_{1,n+1}(n+1)\rangle_g$$
$$=\exp\left\{-\frac{1}{2}[|\tilde{\gamma}_{1n}(n)|^2+|\tilde{\gamma}_{1n}(n+1)|^2+|\tilde{\gamma}_{1,n+1}(n)|^2+|\tilde{\gamma}_{1,n+1}(n+1)|^2]-\tilde{\gamma}_{1n}(n+1)\tilde{\gamma}^*_{1n}(n)\right.$$
$$\left.-\tilde{\gamma}_{1,n+1}(n+1)\tilde{\gamma}^*_{1,n+1}(n)\right\}, \tag{A8}$$

where

$$\tilde{\gamma}_m(n)=\frac{1}{\sqrt{N}}\sum_q\tilde{\gamma}_q(n)\exp(iqma).$$

Evaluation of expression (A8) has been obtained using the formulas (A9)–(A11). They read[25]

$$\langle 0|D^{-1}S^{-1}(-1)^{b^\dagger b}SD|0\rangle\equiv{}_g\langle\gamma|(-1)^{b^\dagger b}|\gamma>_g$$
$$=\sum_{n=0}^{\infty}(-1)^n|\langle n|\gamma\rangle_g|^2, \tag{A9}$$

where $|\gamma\rangle_g=SD|0\rangle=S|\gamma\rangle$ and,[26]

$$\langle n|\gamma\rangle_g=\frac{1}{(n!\mu)^{1/2}}\left(\frac{\nu}{2\mu}\right)^{n/2}H_n\left(\frac{\gamma}{(2\mu\nu)^{1/2}}\right)$$
$$\times\exp\left(-\frac{|\gamma|^2}{2}+\frac{\nu^*\gamma^2}{2\mu}\right). \tag{A10}$$

Here $\mu=\cosh 2r$, $\nu=e^{-i\theta}\sinh 2r$, $|\mu|^2-|\nu|^2=1$, and H_n are Hermitian polynomials. [The squeezing parameter μ used in the formula (A10) does not occur more so that it does not interfere with the parameter of effective interaction μ defined by Eq. (28)].

By the calculation of (A9) with the use of (A11), the following formula is necessary:[27]

$$\sum_{k=0}^{\infty}\frac{t^k}{k!}H_{k+m}(x)H_{k+n}(y)=(1-4t^2)^{-(m+n+1)/2}\exp\left[\frac{4txy-4t^2(x^2+y^2)}{1-4t^2}\right]\sum_{k=0}^{\min(m,n)}2^{2k}k!\binom{m}{n}$$
$$\times\binom{n}{k}t^kH_{m-k}\left(\frac{x-2ty}{\sqrt{1-4t^2}}\right)H_{n-k}\left(\frac{y-2tx}{\sqrt{1-4t^2}}\right),\quad |t|<\frac{1}{2}. \tag{A11}$$

In our calculations we use continuum versions of the above formulas when replacing $na \rightarrow x$,

$$\gamma_{iq}(n+1) - \gamma_{iq}(n) \rightarrow \frac{d\gamma_{iq}(x)}{dx} a. \tag{A12}$$

APPENDIX B

In Eq. (25) we defined an operator Q_q which can be rewritten as

$$\begin{aligned} Q_q &= \overline{\Omega}(\overline{\Omega} + \kappa^2 - 2\overline{q}\overline{\kappa p} + \kappa^2 \overline{A^\dagger A})^{-1} \\ &= 1 - \frac{\overline{q^2}}{(\overline{\Omega} + \kappa^2)^{1/2}} \mathrm{Re} \int_0^\infty dt \exp\{-t[(\kappa^2 + \overline{\Omega})^{1/2} \\ &\quad + i(\overline{q} - \overline{\kappa p})]\}. \end{aligned} \tag{B1}$$

This form is suitable for calculation of the mean value of (B1) which appears in Eqs. (24), (27), and (28), with the use of a simple formula $\langle f|e^{i\kappa tp}|f\rangle = \kappa t/\sinh(\kappa t)$, where $f(x) = (1/\sqrt{2})\mathrm{sech} x$. It yields

$$\begin{aligned} \langle f|Q_q|f\rangle &= 1 - \frac{\overline{q^2}}{2\kappa(\overline{\Omega} + \kappa^2)^{1/2}} \\ &\quad \times \mathrm{Re}\Psi^{(1)}\left(1 + \frac{(\kappa^2 + \overline{\Omega})^{1/2} - \kappa + i\overline{q}}{2\kappa}\right) \qquad \text{(B2)} \\ &= 1 - \frac{\overline{q^2}}{2\kappa(\overline{\Omega} + \kappa^2} \\ &\quad \times \mathrm{Re}\left[\frac{1}{2z^2} - \frac{\pi^2}{2\sinh^2(\pi z)} - iz\sum_{l=1}^{\infty} \frac{l}{(l^2 + z^2)}\right], \end{aligned}$$

where $z = \{\overline{q} - i[(\kappa^2 + \overline{\Omega})^{1/2} - \kappa]\}/2\kappa$. The digamma function $\Psi^{(1)}(1+x)$ Ref. 28 in Eq. (B2) was rewritten by using the following identities

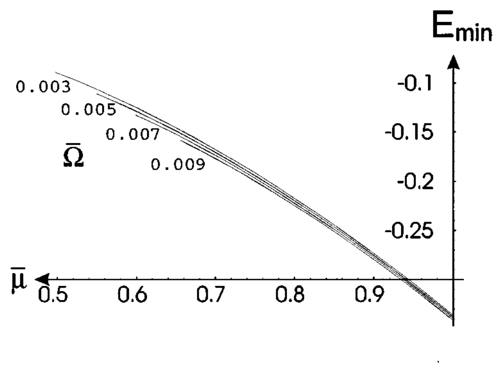

FIG. 5. Ground state energy $E(\kappa_{\min}, \overline{\mu})$ for $\overline{\Omega} < \kappa^3$.

$$\Psi^{(1)}(1+x) = -\Psi^{(1)}(-x) - \pi^2/\sinh^2(\pi x), \tag{B3}$$

$$\Psi^{(1)}(-x) = \frac{1}{x^2} + \sum_{l=1}^{\infty} \frac{1}{(x+l)^2}, \tag{B4}$$

$$\frac{\pi^2}{\sinh^2(\pi x)} = \frac{1}{x^2} - 2\sum_{l=1}^{\infty} \frac{1}{(x^2+l^2)} + 4x^2 \sum_{l=1}^{\infty} \frac{1}{(x^2+l^2)^2}, \tag{B5}$$

and

$$\sum_{l=1}^{\infty} \frac{1}{x^2 + l^2} = \left(\coth x - \frac{1}{\pi x}\right)\frac{\pi}{2x}. \tag{B6}$$

APPENDIX C

In Eq. (24) there is to evaluate $\int_{-\pi}^{\pi} d\overline{q} \overline{\langle f|Q_q|f\rangle}$ where the integrand is given by (B2)–(B6). It is possible to perform it exactly:

$$\begin{aligned} \frac{1}{\pi}\int_{-\pi}^{\pi} d\overline{q}\overline{\langle f|Q_q|f\rangle} &= \frac{1}{\pi}\int_{-\pi}^{\pi} d\overline{q}\Bigg[1 - \frac{\overline{q^2}}{2\kappa(\overline{\Omega}+\kappa^2)^{1/2}}\mathrm{Re}\Bigg\{\frac{2\kappa^2}{(\overline{q}-i\delta)^2} - \frac{\pi^2}{2\sinh^2[(\pi/2\kappa)(\overline{q}-i\delta)]} \\ &\quad - i\left(\frac{\overline{q}-i\delta}{2\kappa}\right)\sum_{l=1}^{\infty}\frac{l}{\{l^2+[(\overline{q}-i\delta)/2\kappa]^2\}^2}\Bigg\}\Bigg] \\ &= \frac{1}{\pi}\int_{-\pi}^{\pi} d\overline{q}\Bigg[1 - \frac{\overline{q^2}}{2\kappa(\overline{\Omega}+\kappa^2)^{1/2}}\Bigg\{\frac{2\kappa^2}{\overline{q}^2+\delta^2} - \frac{4\kappa^2\delta^2}{(\overline{q}^2+\delta^2)^2}\frac{\pi}{2}\mathrm{Re}\frac{1}{\sinh^2[\pi(\overline{q}-i\delta)/2\kappa]} \\ &\quad + \frac{1}{2}\mathrm{Re}\left(\frac{i\overline{q}+\delta}{2\kappa}\right)\sum_{l=1}^{\infty}\frac{d}{dl}\frac{1}{\{l^2+[(\overline{q}-i\delta)/2\kappa]^2\}}\Bigg\}\Bigg], \end{aligned} \tag{C1}$$

where $\delta=[(\kappa^2+\overline{\Omega})^{1/2}-\kappa]$. Expression (C1) except for the last term is easy to obtain as

$$2\left(1+\frac{\overline{\Omega}}{\kappa^2}\right)^{-1/2}\left[\frac{\delta}{\kappa}+\frac{2\delta}{\pi}\arctan\frac{\pi}{\delta}-\frac{\delta^2}{\pi^2+\delta^2}+\frac{\delta^2}{2\kappa}+\frac{\kappa}{3}\right].$$

The integration of the last term of (C1) can be performed exactly by simple but lengthy calculations. We obtain

$$-\frac{1}{2\pi}\left(1+\frac{\overline{\Omega}}{\kappa^2}\right)^{-1/2}\sum_{l=1}^{\infty}\frac{d}{dl}[S(l,\kappa,\delta)-S(l,\kappa,-\delta)], \tag{C2}$$

where

$$S(l,\kappa,\delta)=\left[4\kappa l^2\frac{\kappa l+\delta}{2\kappa l+\delta}+\left(l+\frac{\delta}{\kappa}\right)(\delta+2\kappa l)+\frac{l\delta^2}{2\kappa l+\delta}\right]\times\arctan\frac{\pi}{\delta+2\kappa l}.$$

If we use the convenience of expression (C2) for integration over l instead of the summation, we obtain

$$(\mathrm{C2})\approx\frac{1}{2\pi}\left(1+\frac{\overline{\Omega}}{\kappa^2}\right)^{-1/2}[S(1,\kappa,\delta)-S(1,\kappa,-\delta)]. \tag{C3}$$

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