Properties of ground state and anomalous quantum fluctuations in one-dimensional polaron–soliton systems—the effects of electron-two-phonon interaction and non-adiabatic quantum correlations*

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Based on the Holstein model Hamiltonian of one-dimensional molecular crystals, by making use of the expansion approach of the correlated squeezed-coherent states of phonon instead of the two-phonon coherent state expansion scheme, the properties of the ground state and the anomalous quantum fluctuations are investigated in a strongly coupled electron–phonon system with special consideration of the electron-two-phonon interaction. The effective renormalization ($\widetilde{\alpha}_i$) of the displacement of the squeezed phonons with the effect of the squeezed-coherent states of phonon and both the electron-displaced phonon and the polaron-squeezed phonon correlations have been combined to obtain the anomalous quantum fluctuations for the corrections of the coherent state. Due to these non-adiabatic correlations, the effective displacement parameter $\widetilde{\alpha}_i$ is larger than the ordinary parameter $\alpha_i^{(0)}$. In comparison with the electron-one-phonon interaction (g) corrected as $\widetilde{\alpha}_i g$, we have found the electron-two-phonon interaction (g_1) corrected as $\widetilde{\alpha}_i^2 g_1$ is enhanced significantly. For this reason, the ground state energy ($E_0^{(2)}$) contributed by the electron-two-phonon interaction is more negative than the single-phonon case ($E_0^{(1)}$) and the soliton solution is more stable. At the same time, the effects of the electron-two-phonon interaction greatly increase the polaron energy and the quantum fluctuations. Furthermore, in a deeper level, we have considered the effect of the polaron-squeezed phonon correlation (f-correlation). Since this correlation parameter $f > 1$, this effect will strengthen the electron-one and two-phonon interactions by $f\widetilde{\alpha}_i g$ and $f^2\widetilde{\alpha}_i^2 g_1$, respectively. The final results show that the ground state energy and the polaron energy will appear more negative further and the quantum fluctuations will gain further improvement.

Keywords: correlated squeezed-coherent state expansion, electron-two-phonon interaction, non-adiabatic correlations and renormalized phonon displacement, anomalous quantum fluctuations, polaron-squeezed phonon correlation

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1. Introduction

The study of the behaviour of electron–phonon coupled systems has long been an active research subject in condensed matter physics. The coupling of electron with the lattice vibrations noticeably changes the characteristics of both electrons and phonons. Furthermore, it leads to a number of interesting effects and phenomena such as superconductivity, electron driven instabilities (charge density wave (CDW)), polaron and bipolaron to occur.[1−6] In fact, in the strongly coupled case, each electron drives a lattice deformation with itself in a coherent way, which is called small polaron, severely localized in its own potential well. In the intermediately and strongly coupled regions, the electron–phonon interaction enhances the localization of polaron and local pairs, thereby causing some important effects on the ground state properties, the quantum fluctuations and the binding energy of polaron in the interaction systems. However, while the behaviours of electron–phonon coupled system in the weakly coupled region have been well studied, the behaviours of electron–phonon coupled systems in the strongly coupled regions and intermediately coupled regions are still lacking in research, which is due to the failure of perturbation theory. Fortunately, the concept of coherent state is introduced to describe the lattice part of the quantum states involved in polaron states. The relevant study in this field has been done by Zheng and Feinberg.[7,8] They proposed a vari-

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ational wave function of two-phonon coherent state for the lattice ground state of the electron–phonon systems in these coupled ranges. However, the influence of the squeezed effect of the phonons on polaron state and the correlation effects among the coherent and squeezed states of phonons, in particular the effect of electron-two-phonon interaction, were not taken into consideration in the ansatz of state conceived by Zheng and Feinberg *et al.*[7−10] Therefore, it is still an approximate treatment. Because of this, for these problems, no important progress has been made in the past twenty years.[7−22] In recent years, the realization of one-dimensional material provides us an opportunity to investigate the polaron–soliton states in one-dimensional molecular crystals. As a typical model in research, Holstein model Hamiltonian has been widely used in a lot of fields such as condensed matter, molecular physics, high polymer material, and DNA. Also, there have been a number of valuable results. Recently, one has made use of an expansion of the electron–ion interaction potential at equilibrium position, including the third-order displacement, to obtain the electron-two-phonon interaction, then used that as the initial base to study the properties of the ground state for the electron–phonon coupled systems.[20−25] It is thought that one has achieved an outcome for the properties of ground and excitation states in the one-dimensional molecular crystals. Also, they have further improved the variational methods in terms of the coherent state expansion. However, these existing studies have not considered the influence of the "squeezed state", so they certainly ignore the necessary amendments of the research results. Therefore, it becomes our important and interesting research subject, based on the picture of coherent state and squeezed state in quantum optics, to look into much deeper levels, within a strongly coupled electron–phonon system, to find out the whole picture of the squeezed characteristics of the polaron–soliton states and the full spectrum of the properties of the ground state and to explore how to truly describe these characteristics and properties, especially, with considering the presence of electron-two-phonon interaction.

To modify the coherent state approximation in the intermediately coupled range and the strongly coupled range, it is necessary to take into account the strong non-adiabatic quantum fluctuation induced by polaron motion which is due to the action of the phonon squeezing. Its straightforward result leads to the strong non-adiabatic anomalous phonon fluctuation in the strongly coupled electron–phonon system. In our present work, based on the concept of the squeezed-coherent state in quantum optics,[26−28] taking the electron-two-phonon interaction into account, instead of using the two-phonon coherent state expansion approach, we use the expansion of the correlated squeezed coherent states of phonons to study the properties of the ground state, the quantum fluctuations and the binding energy of the polaron in a one-dimensional Holstein polaron system. In order to obtain the anomalous non-adiabatic phonon fluctuation in the coupled system, we have considered some important corrections here as follows:

1) The effects of the displacement and the squeezing of the phonons not only occur simultaneously, but are also influenced mutually and related to each other closely, so that the effect of the displacement-squeezed phonon correlation makes an important contribution to the strongly coupled system. The straightforward result coming from this correlated effect is the renormalized correction to the displacement action of the phonons through the squeezing and the related quantum effects on the polaron characteristics.

2) In the case of small polaron, the displacement of phonon and the changing states of the hopping electron motion also occur simultaneously and they are related more closely, so the correlation between the displaced phonon and the hopping electron will bring a new correction to the polaron–soliton state.

3) It is well known that the squeezing of phonons is induced by the motion of polarons, but when the phonons are squeezed, the polaron state should also be affected at the same time in accordance with the physical law of action–counteraction. That is to say, the squeezing of phonons and the change of the polaron states occur simultaneously, they are dependent on and closely related to each other in the coupled electron–phonon system, especially in the intermediately coupled regime and the strongly coupled regime. Therefore, the states formed by the physical mechanism should be reasonably described by a unified wave functional state ansatz, but not be resolved into individual steps of factorized operators as presented by Zheng *et al.*[7−9,12−15]

The rest of this paper is arranged as follows. In Section 2, based on the expansion of the correlated squeezed-coherent states of phonon, with taking

the electron-two-phonon interaction into account, the electron-displaced phonon correlation and the renormalization correction of the phonon displacement with the effect of the squeezed-coherent states of phonon, we obtain the self-consistent nonlinear Schrödinger equation for the polaron–soliton state, the polaron–soliton solutions and the ground state properties for the coupled electron–phonon systems. On this base we pay more attention in Section 3 to the discussion over the effect of the polaron-squeezed phonon correlation on the properties of ground state. In Section 4 we study further the quantum fluctuations and polaron binding energy in one-dimensional polaron–soliton system. We draw some important conclusions and perform discussion in Section 5 finally.

2. Nonlinear equation of polaron–soliton state and the effects of the electron-two-phonon interaction

Taking into account the effect of third-order displacement of the expansion of the electron–ion potential at equilibrium position, i.e. the electron-two-phonon interaction, the Holstein's Hamiltonian for a coupled electron–phonon system in one-dimensional molecular crystal reads

$$\begin{aligned} H = & -t\sum_i (c_i^\dagger c_{i+1} + c_i^\dagger c_{i-1}) + \omega \sum_i b_i^\dagger b_i \\ & + g\sum_i c_i^\dagger c_i (b_i^\dagger + b_i) + g_1 \\ & \times \sum_i c_i^\dagger c_i (b_i^\dagger b_i^\dagger + b_i b_i), \end{aligned} \tag{1}$$

where $c_i^\dagger$ (c_i) is electron creation (annihilation) operator, $b_i^\dagger$ (b_i) is phonon creation (annihilation) operator, t denotes the hopping strength, g the electron-one-phonon coupling constant, and g_1 the electron-two-phonon coupling constant.

First of all, we consider only the effects of the electron-two-phonon interaction. By virtue of the expansion of the phonon coherent states, the variational wave function Φ_0 for the coupled electron–phonon system takes the form of

$$|\Phi_0\rangle = \sum_l \Psi_l c_l^\dagger D|0\rangle, \tag{2}$$

where

$$D = \exp\left[\sum_i \alpha_i^{(1)}(b_i^\dagger - b_i)\right], \quad |\Psi_1\rangle = \sum_i \Psi_i c_i^\dagger |0\rangle, \tag{3}$$

with Ψ_i and $\alpha_i^{(1)}$ being the variational parameters to be determined, $|0\rangle$ denoting the vacuum state of coupled electron–phonon system.

In this manner, the energy of the ground state of the system will be given by

$$\begin{aligned} E_{(0)} = & \langle\Psi_1|D^{-1}HD|\Psi_1\rangle / \langle\Psi_1|\Psi_1\rangle \\ = & \frac{1}{\sum_l \Psi_l^2}\Big\{ - t\sum_i (\Psi_i\Psi_{i+1} + \Psi_i\Psi_{i-1}) \\ & + \omega \sum_{i_1} \Psi_{i_1}^2 \sum_i {\alpha_i^{(1)}}^2 + 2g\sum_i \alpha_i^{(1)}\Psi_i^2 \\ & + 2g_1 \sum_i {\alpha_i^{(1)}}^2 \Psi_i^2 \Big\}. \end{aligned} \tag{4}$$

From the variational equation

$$\frac{\partial E_{(0)}}{\partial \alpha_k^{(1)}} = \frac{2g}{\sum_l \Psi_l^2}\Psi_k^2 + \frac{4g_1\alpha_k^{(1)}}{\sum_l \Psi_l^2}\Psi_k^2 + 2\omega\alpha_k^{(1)} = 0, \tag{5}$$

we can obtain the following solution:

$$\alpha_k^{(1)} = -\frac{g\Psi_k^2}{\omega + 2g_1\Psi_k^2}, \tag{6}$$

where $\alpha_k^{(1)}$ is the bare displacement parameter of phonon.

In order to consider the correction to the effect of phonon squeezing, notice that the hopping electron state and the phonon displacement appear simultaneously and they are closely related to each other in the polaron–soliton systems (non-adiabatic effect), i.e. there exists the correlation between the electron state and phonon displacement (electron-displaced phonon correlation). In place of the two-phonon coherent state representation, we take the correlated representation of U-operator as

$$U = \exp\left\{\sum_i [r(b_i^2 - {b_i^\dagger}^2) - \alpha_i^{(1)}(b_i^\dagger - b_i)c_i^\dagger c_i]\right\}. \tag{7}$$

As is well noted, for the strongly coupled case, the squeezed state of phonons and the phonon displacement also occur simultaneously and they are mutually coupled in an interacting system. This non-adiabatic correlation effect influences both the displacement of the squeezed phonon and the polaron state and its straightforward effect resulting from correlated representation (7) leads to the renormalization of the phonon displacement[23]

$$\alpha_i^{(1)} \to \widetilde{\alpha}_i^{(1)} = \frac{\mathrm{e}^{2r} - 1}{2r}\alpha_i^{(1)}.$$

Therefore, the decoupled form of U implies a new renormalized displacement $\widetilde{\alpha}_i^{(1)}$. Go a step further, in contrast to the variational wave function of two-phonon coherent state given by Zheng *et al.*, based on the concept of squeezed-coherent state $|\widetilde{\alpha}_i^{(1)}, r\rangle = U_{\rm s}(r)D(\widetilde{\alpha}_i^{(1)})|0\rangle_{\rm b}$,[26] in the present work we use the expansion of the correlated squeezed-coherent states of phonon in a decoupled form

$$|\Phi\rangle = \sum_l \Psi_l U_{\rm s}(r) D(\widetilde{\alpha}_i^{(1)}) c_l^\dagger |0\rangle, \tag{8}$$

where $U_{\rm s}(r)$ is the squeezing operator of phonon, r is the squeeze parameter,

$$U_{\rm s} = \exp\left[\sum_i r(b_i^2 - b_i^{\dagger 2})\right], \tag{9}$$

and

$$D(\widetilde{\alpha}_i^{(1)}) = \exp\left[\sum_i \widetilde{\alpha}_i^{(1)}(b_i^\dagger - b_i)c_i^\dagger c_i\right]. \tag{10}$$

With this result, noting that $U = U_{\rm s}(r)D(\widetilde{\alpha}_i^{(1)})$ we find

$$U^{-1} b_i U = \widetilde{b}_i + \widetilde{\alpha}_i c_i^\dagger c_i, \tag{11}$$

where the new effective displacement of the squeezed phonon $\widetilde{\alpha}_i$ is

$$\begin{aligned} \widetilde{\alpha}_i &= \widetilde{\alpha}_i^{(1)} \cosh 2r + \widetilde{\alpha}_i^{(1)^*} \sinh 2r = \alpha_0 \eta_0 \alpha_i^{(1)}, \\ \left(\alpha_0 \right. &= \left. \cosh 2r + \sinh 2r, \quad \eta_0 = \frac{{\rm e}^{2r} - 1}{2r}\right), \\ \widetilde{b}_i &= b_i \cosh 2r + b_i^\dagger \sinh 2r. \end{aligned} \tag{12}$$

To avoid the difficulty in solving the nonlinear equation, considering ${\rm e}^{-4r}\widetilde{\alpha}_i^2 \ll 1$, as a reasonable approximation we have

$$\begin{aligned} & {}_{\rm b}\langle 0|U^{-1} c_i^\dagger c_{i+1} U|0\rangle_{\rm b} \\ &= {}_{\rm b}\langle 0|c_i^\dagger c_{i+1} {\rm e}^{-[\widetilde{\alpha}_i(\widetilde{b}_i^\dagger - \widetilde{b}_i) - \widetilde{\alpha}_{i+1}(\widetilde{b}_{i+1}^\dagger - \widetilde{b}_{i+1})]}|0\rangle_{\rm b} \\ &\approx c_i^\dagger c_{i+1} {\rm e}^{-\frac{1}{2}\widetilde{\alpha}_i^2 {\rm e}^{-4r}} \approx c_i^\dagger c_{i+1}. \end{aligned} \tag{13}$$

In this manner, including the corrections to the correlation between electron and displaced phonon and the new effective phonon displacement, finally, the ground state energy of the coupled electron–phonon systems will be rewritten in the form of

$$\begin{aligned} E_0 &= \langle \Psi_1 | U H U^{-1} | \Psi_1 \rangle / \langle \Psi_1 | \Psi_1 \rangle \\ &= \frac{1}{\sum_l \Psi_l^2} \{ -t \sum_i (\Psi_i \Psi_{i+1} + \Psi_i \Psi_{i-1}) \\ &\quad + \omega \sum_{i_1} \Psi_{i_1}^2 \sum_i (2\widetilde{\alpha}_i^2 + \sinh^2 2r) + 2g \sum_i \widetilde{\alpha}_i \Psi_i^2 \\ &\quad + 2g_1 \sum_i (2\widetilde{\alpha}_i^2 \Psi_i^2 + \sinh 2r \cosh 2r) \}. \end{aligned} \tag{14}$$

To investigate the properties of ground state and the quantum fluctuation, in this paper we use the scheme of solving the nonlinear equation. From the variational equation

$$\frac{\partial E_0}{\partial \Psi_k} = 0, \tag{15}$$

we can have

$$\begin{aligned} & t(\Psi_{k+1} + \Psi_{k-1}) - 2g\widetilde{\alpha}_k \Psi_k - 2(\omega + 2g_1)\widetilde{\alpha}_k^2 \Psi_k \\ & - \Psi_k \sum_i \Psi_i [t(\Psi_{i+1} + \Psi_{i-1}) \\ & - 2g\widetilde{\alpha}_i \Psi_i - 2(\omega + 2g_1)\widetilde{\alpha}_i^2 \Psi_i] = 0. \end{aligned} \tag{16}$$

Using the continuous approximation

$$\begin{aligned} & \Psi_k \to \Psi, \Psi_{k+1} + \Psi_{k-1} = \frac{{\rm d}^2\Psi}{{\rm d}x^2} + 2\Psi, \\ & \sum_i \Psi_i^2 = \int_{-\infty}^{+\infty} \Psi^2(x) {\rm d}x = 1, \end{aligned} \tag{17}$$

equation (16) can be transformed as follows:

$$\frac{{\rm d}^2\Psi}{{\rm d}x^2} + \frac{2A}{1 + A_1\Psi^2}\Psi^3 - \frac{A\widetilde{A}_1}{(1 + A_1\Psi^2)^2}\Psi^5 = A_0\Psi, \tag{18}$$

where

$$\begin{aligned} A_0 &= \int_{-\infty}^{+\infty} \Psi \left[\frac{{\rm d}^2\Psi}{{\rm d}x^2} + \frac{2A}{1 + A_1\Psi^2}\Psi^3 \right. \\ &\quad \left. - \frac{A\widetilde{A}_1}{(1 + A_1\Psi^2)^2}\Psi^5\right] {\rm d}x, \\ A_1 &= \frac{2g_1}{\omega}, \quad A = \frac{g^2(\alpha_0\eta_0)}{\omega t}, \\ \widetilde{A}_1 &= \frac{2(\omega + 2g_1)(\alpha_0\eta_0)}{\omega}. \end{aligned} \tag{19}$$

From Eqs. (18) and (19), based on the continuous approximation, the energy of the ground state turns out to be

$$\widetilde{E} = \varepsilon_0(r) - 2t - A_0 t, \tag{20}$$

where

$$\varepsilon_0(r) = \omega \sinh^2 2r + 2g_1 \sinh 2r \cosh 2r. \tag{21}$$

From these new results, we have found that, on the one hand, equations (18) and (19) form a self-consistent and closed system of equations which are different from those in Refs. [16] and [20]. On the other hand, the electron-displaced phonon correlation and the electron-two-phonon interaction increase greatly itself nonlinearity of the nonlinear equation. In the

other deeper levels, the squeezed-coherent state effect of phonon and the renormalization correction of phonon displacement strengthen the electron–phonon interaction, as a result, the solitary wave nature of the coupled system has some new physical connotations.

2.1. Ground state of the polaron–soliton systems when $g_1 = 0$

If $g_1 = 0$, equation (18) will be reduced into

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} + 2A\Psi^3 - 2(\alpha_0\eta_0)A\Psi^5 = A_0^{(1)}\Psi. \tag{22}$$

In place of the Ψ^3-nonlinear equation, considering the electron-displaced phonon correlation, we now arrive at the Ψ^5-nonlinear equation. Using the boundary condition

$$\Psi|_{x\to\pm\infty} = 0, \quad \Psi_x|_{x\to\pm\infty} = 0, \tag{23}$$

we have

$$\Psi_x^2 = \Psi^2(a_0 + a_1\Psi^2 + a_2\Psi^4), \tag{24}$$

where $a_0 = A_0^{(1)}$, $a_1 = -A$, and $a_2 = \frac{2}{3}(\alpha_0\eta_0)A$. Instead of the sech-type solitary wave, the solitary solution of Eq. (22) is

$$\Psi^{(1)}(x) = \frac{1}{[(\alpha_1+\beta_1) + 2\beta_1\sinh^2\sqrt{a_0}(x-x_0)]^{1/2}}, \tag{25}$$

with

$$\alpha_1 = -\frac{a_1}{2a_0}, \quad \beta_1 = \frac{1}{2a_0}(a_1^2 - 4a_0a_2)^{1/2}. \tag{26}$$

By using the normalization for the solitary wave function, we have

$$\alpha_1 = \frac{\eta_1}{\sqrt{a_0}\tanh\eta_1}, \quad \eta_1^2 = a_2 > 0, \quad \left(\eta_1 = \frac{\beta_1}{\alpha_1}\right) \tag{27}$$

and the localization of soliton L_1

$$L_1 = -\frac{2\eta_1}{a_1}\coth\eta_1. \tag{28}$$

From the above results, then we have

$$A_0^{(1)} = a_0 = \frac{a_1^2}{4a_2}\tanh^2\sqrt{a_2}. \tag{29}$$

As the result of the electron-one-phonon interaction only, the ground state energy of the polaron–soliton systems is explicitly

$$E_0^{(1)} = \varepsilon_0(r) - 2t - \frac{a_1^2 t}{4a_2}\tanh^2\sqrt{a_2}. \tag{30}$$

Note that $\alpha_1 + \beta_1 \approx -a_2/a_1$, since $a_1 < 0$ and $a_2 > 0$, the stability condition of soliton solution (25)

$$\alpha_1 + \beta_1 > 0, \quad \beta_1 > 0, \tag{31}$$

is satisfied fully.

2.2. Ground state with the electron-two-phonon interaction in the coupled electron–phonon system

When $g_1 \neq 0$, noting that $2g_1 < \omega$, $\Psi^2 < 1$, and $A_1\Psi^2 \ll 1$, as a reasonable nonlinear expansion approximation to Eq. (15), the result is readily shown to be

$$\begin{aligned}\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} &- A_0\Psi + 2A\Psi^3 - (2AA_1 + A\widetilde{A}_1)\Psi^5 \\ &+ 2A_1(AA_1 - A\widetilde{A}_1 - 2A_0A_1^2)\Psi^7 \\ &- 3A_1^2(2AA_1 - A\widetilde{A}_1 - A_0A_1^2)\Psi^9 = 0. \end{aligned}\tag{32}$$

Obviously, Ψ^5-term in Eq. (32) represents the first-order effect of electron-two-phonon interaction (g_1), Ψ^7-nonlinear term the second-order effect and so on. We now take only the first-order effect for this interaction into account ($g_1 \approx -0.01 \sim -0.2$), then the nonlinear equation of Ψ takes the form as

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} - A_0^{(2)}\Psi + 2A\Psi^3 - (2AA_1 + A\widetilde{A}_1)\Psi^5 = 0. \tag{33}$$

With regard to the boundary condition (23), one obtains

$$\Psi_x^2 = \Psi^2(b_0 + b_1\Psi^2 + b_2\Psi^4), \tag{34}$$

where

$$b_0 = A_0^{(2)}, \quad b_1 = -A, \quad b_2 = \frac{1}{3}(A\widetilde{A}_1 + 2AA_1). \tag{35}$$

For the existence of the solitary wave solution, the stable condition

$$\beta_2^2 = \frac{1}{4b_0^2}(b_1^2 - 4b_0b_2) > 0$$

must hold. Obviously, if $g_1 < 0$, this condition is satisfied sufficiently, and then equation (34) has the solitary wave solution

$$\Psi^{(2)}(x) = \frac{1}{[(\alpha_2+\beta_2) + 2\beta_2\sinh^2\sqrt{b_0}(x-x_0)]^{1/2}}, \tag{36}$$

with

$$\alpha_2 = -\frac{b_1}{2b_0}, \quad \beta_2 = \frac{1}{2b_0}(b_1^2 - 4b_0b_2)^{1/2}. \tag{37}$$

In a similar manner, using the normalization condition of $\Psi^{(2)}$ we obtain

$$\alpha_2 = \frac{\eta_2}{\sqrt{b_0}\tanh\eta_2}, \quad \eta_2^2 = b_2 > 0, \quad \left(\eta_2 = \frac{\beta_2}{\alpha_2}\right), \tag{38}$$

while the soliton localization L_2

$$L_2 = -\frac{2\eta_2}{b_1}\coth\eta_2, \tag{39}$$

and

$$b_0 = A_0^{(2)} = \frac{b_1^2}{4b_2}\tanh^2\sqrt{b_2}. \tag{40}$$

By the way, we find the energy of the ground state to be

$$E_0^{(2)} = \varepsilon_0(r) - 2t - \frac{b_1^2 t}{4b_2}\tanh^2\sqrt{b_2}, \tag{41}$$

the existence condition of the stable soliton solution is

$$\alpha_2 + \beta_2 > 0, \quad \beta_2 > 0. \tag{42}$$

Since $\alpha_2 + \beta_2 \approx -b_2/b_1$, but $b_2 > 0$ and $b_1 = -A < 0$, then the above stable condition is satisfied fully. Particularly, it should be noticed that

$$b_2 = a_2 + \frac{4g_1}{3\omega}(1 + \alpha_0\eta_0)A,$$

when $g_1 < 0$, which leads to $b_2 < a_2$, $E_0^{(2)} < E_0^{(1)}$, and $L_2 < L_1$. That is to say, when we consider the effects of the electron-two-phonon interaction including the correction of the new effective phonon displacement $\widetilde{\alpha}_i$ and the correlation between electron and displaced phonon (non-adiabatic), the energy of the ground state of the polaron–soltion systems changes to a more negative value, the stable condition of soliton solution is surely fully filled.

3. Effects of the correlation between polaron state and squeezed phonon state

As expected, the squeezed state of the phonon and the polaron state occur simultaneously and they are dependent on each other and related closely to the electron–phonon interaction process. It is simply stated that there exists the quantum correlation between the polaron state and the squeezed phonon state (polaron-squeezed phonon correlation), therefore, the correlated representation should be corrected as

$$|\Phi\rangle = \sum_l \Psi_l \widetilde{U} c_l^+ |0\rangle, \tag{43}$$

with

$$\widetilde{U} = U_{\rm s}(r)D(\widetilde{\alpha}, f),$$
$$D(\widetilde{\alpha}, f) = \exp\left[\sum_i f\widetilde{\alpha}_i(b_i^\dagger - b_i)c_i^\dagger c_i\right], \tag{44}$$

where f denotes the new variational parameter of the polaron-squeezed phonon correlation. Using

$$\widetilde{U}^{-1} b_i \widetilde{U} = \widetilde{b}_i + f\widetilde{\alpha}_i c_i^\dagger c_i,$$
$$\widetilde{U}^{-1} c_i^\dagger \widetilde{U} = c_i^\dagger {\rm e}^{-f\widetilde{\alpha}_i e^{-2r}(b_i^\dagger - b_i)}, \tag{45}$$

we obtain the energy of the ground state as

$$\begin{aligned}\widetilde{E}_0 &= \langle\Psi_1|\widetilde{U}^{-1}H\widetilde{U}|\Psi_1\rangle/\langle\Psi_1|\Psi_1\rangle \\ &= \frac{1}{\sum_l \Psi_l^2}\Big\{ - t\sum_i {\rm e}^{-\frac{1}{2}f^2\widetilde{\alpha}_i^2 e^{-4r}}(\Psi_i\Psi_{i+1} + \Psi_i\Psi_{i-1}) \\ &\quad + \omega\sum_i (2f^2\widetilde{\alpha}_i^2\Psi_i^2 + \sinh^2 2r) + 2g\sum_i f\widetilde{\alpha}_i\Psi_i^2 \\ &\quad + 2g_1\sum_i (2f^2\widetilde{\alpha}_i^2\Psi_i^2 + \sinh 2r\cosh 2r)\Big\}. \end{aligned} \tag{46}$$

Further, the parameter f can be determined by the variational equation

$$\frac{\partial\widetilde{E}_0}{\partial f} = 0. \tag{47}$$

As a result, we have

$$\begin{aligned} & f\Big[t\sum_i \widetilde{\alpha}_i^2 {\rm e}^{-4r}{\rm e}^{-\frac{1}{2}f^2\widetilde{\alpha}_i^2 {\rm e}^{-4r}}(\Psi_i\Psi_{i+1} + \Psi_i\Psi_{i-1}) \\ & + 4\sum_i (2g_1 + \omega)\widetilde{\alpha}_i^2\Psi_i^2\Big] + 2g\sum_i \widetilde{\alpha}_i\Psi_i^2 = 0. \end{aligned} \tag{48}$$

Since $\frac{1}{2}f^2\widetilde{\alpha}_i^2{\rm e}^{-4r} \ll 1$, equation (48) can be approximated as

$$\begin{aligned} & \frac{1}{2}t\sum_i \widetilde{\alpha}_i^4 {\rm e}^{-8r}(\Psi_i\Psi_{i+1} + \Psi_i\Psi_{i-1})f^3 \\ & - \Big[t\sum_i \widetilde{\alpha}_i^2 {\rm e}^{-4r}(\Psi_i\Psi_{i+1} + \Psi_i\Psi_{i-1}) \\ & + 4\sum_i (2g_1 + \omega)\widetilde{\alpha}_i^2\Psi_i^2\Big] f - 2g\sum_i \widetilde{\alpha}_i\Psi_i^2 = 0. \end{aligned} \tag{49}$$

By the continuous approximation, equation (49) reduces into

$$af^3 - bf + c = 0, \tag{50}$$

where

$$\begin{aligned} a &= \frac{1}{2}t{\rm e}^{-8r}\int_{-\infty}^{+\infty} \frac{g^4(\alpha_0\eta_0)^4}{\omega^4(1 + A_1\Psi^2)^4}\Psi^9 \\ &\quad \times \Big\{\Big[- \frac{2A}{1 + A_1\Psi^2}\Psi^3 + \frac{A\widetilde{A}_1}{(1 + A_1\Psi^2)^2}\Psi^5 \\ &\quad + A_0\Psi\Big] + 2\Psi\Big\}{\rm d}x, \end{aligned} \tag{51}$$

$$b = t\,\mathrm{e}^{-4r}\int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)^2}{\omega^2(1+A_1\Psi^2)^2}\Psi^5 \times\left\{\left[-\frac{2A}{1+A_1\Psi^2}\Psi^3+\frac{A\widetilde{A}_1}{(1+A_1\Psi^2)^2}\Psi^5 + A_0\Psi\right]+2\Psi\right\}\mathrm{d}x+4(\omega+2g_1) \times\int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)^2}{\omega^2(1+A_1\Psi^2)^2}\Psi^6\mathrm{d}x, \quad (52)$$

$$c = 2\int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)}{\omega(1+A_1\Psi^2)}\Psi^4\mathrm{d}x. \quad (53)$$

By considering the random phase approximation

$$-t\sum_i \mathrm{e}^{-\frac{1}{2}f^2\widetilde{\alpha}_i^2\mathrm{e}^{-4r}}(\Psi_i\Psi_{i+1}+\Psi_i\Psi_{i-1}) \approx -t\langle\Psi_1|\mathrm{e}^{-\frac{1}{2}f^2\widetilde{\alpha}_i^2\mathrm{e}^{-4r}}|\Psi_1\rangle \times\sum_i(\Psi_i\Psi_{i+1}+\Psi_i\Psi_{i-1}), \quad (54)$$

we obtain, for the result of the quantum tunnel effect of the polaron,

$$\widetilde{t} = t\langle\Psi_1|\mathrm{e}^{-\frac{1}{2}f^2\widetilde{\alpha}_i^2\mathrm{e}^{-4r}}|\Psi_1\rangle \doteq t\left[1-\frac{1}{2}\mathrm{e}^{-4r}f^2\int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)^2}{\omega^2(1+A_1\Psi^2)^2}\Psi^6\mathrm{d}x\right]. \quad (55)$$

At the same time, A and A_1 are corrected as

$$A\to A' = \frac{g^2(\alpha_0\eta_0)}{\omega\widetilde{t}}f, \qquad \widetilde{A}_1\to\widetilde{A}_1' = \frac{2(\omega+2g_1)(\alpha_0\eta_0)}{\omega}f, \quad (56)$$

respectively. Later $f=f^{(1)}$, $\widetilde{t}=t^{(1)}$, $A'=A^{(1)}$, $\widetilde{A}_1'=\widetilde{A}_1^{(1)}$, and $\widetilde{E}_0^{(1)}$ are related to the electron-one-phonon interaction and $f=f^{(2)}$, $\widetilde{t}=t^{(2)}$, $A'=A^{(2)}$, $\widetilde{A}_1'=\widetilde{A}_1^{(2)}$, and $\widetilde{E}_0^{(2)}$ to the electron-two-phonon interaction, respectively.

3.1. Polaron-squeezed phonon correlation effects when $g\neq 0$ and $g_1=0$

When $g_1=0$, the solitary wave function satisfies the following nonlinear equations

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2}+2A^{(1)}\Psi^3-2f^{(1)}(\alpha_0\eta_0)A^{(1)}\Psi^5=\widetilde{A}_0^{(1)}\Psi, \quad (57)$$

and

$$\Psi_x^2=\Psi^2(\widetilde{a}_0+\widetilde{a}_1\Psi^2+\widetilde{a}_2\Psi^4), \quad (58)$$

under boundary condition (23), where $\widetilde{a}_0=\widetilde{A}_0^{(1)}$, $\widetilde{a}_1=-A^{(1)}$, $\widetilde{a}_2=\frac{2}{3}f^{(1)}\alpha_0\eta_0A^{(1)}$, and $A^{(1)}=[g^2(\alpha_0\eta_0)/\omega t^{(1)}]f^{(1)}$. Correspondingly, we obtain the solitary solution to be

$$\widetilde{\Psi}^{(1)}(x)=\frac{1}{[(\widetilde{\alpha}_1+\widetilde{\beta}_1)+2\widetilde{\beta}_1\sinh^2\sqrt{\widetilde{a}_0}(x-x_0)]^{1/2}}, \quad (59)$$

where $\widetilde{\alpha}_1=-\widetilde{a}_1/2\widetilde{a}_0$ and $\widetilde{\beta}_1=(1/2\widetilde{a}_0)(\widetilde{a}_1^2-4\widetilde{a}_0\widetilde{a}_2)^{1/2}$. As a result, we obtain further

$$\widetilde{L}_1=-\frac{2\widetilde{\eta}_1}{\widetilde{a}_1}\coth\widetilde{\eta}_1,\quad \widetilde{\eta}_1^2=\widetilde{a}_2>0, \quad (60)$$

and

$$\widetilde{A}_0^{(1)}=\widetilde{a}_0=\frac{\widetilde{a}_1^2}{4\widetilde{a}_2}\tanh^2\sqrt{\widetilde{a}_2}. \quad (61)$$

Thus, the energy of the ground state in the polaron–soliton system is corrected as

$$\widetilde{E}_0^{(1)}=\varepsilon_0(r)-2t^{(1)}-\frac{\widetilde{a}_1^2t^{(1)}}{4\widetilde{a}_2}\tanh^2\sqrt{\widetilde{a}_2}. \quad (62)$$

3.2. Polaron-squeezed phonon correlation effects when $g\neq 0$ and $g_1\neq 0$

Including the electron-two-phonon interaction in the first-order correction, the nonliear solitary equation becomes

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2}+2A^{(2)}\Psi^3-(2A^{(2)}A_1+A^{(2)}\widetilde{A}_1^{(2)})\Psi^5=\widetilde{A}_0^{(2)}\Psi, \quad (63)$$

and

$$\Psi_x^2=\Psi^2(\widetilde{b}_0+\widetilde{b}_1\Psi^2+\widetilde{b}_2\Psi^4), \quad (64)$$

where

$$\widetilde{b}_0=\widetilde{A}_0^{(2)},\quad \widetilde{b}_1=-A^{(2)},$$
$$\widetilde{b}_2=\frac{1}{3}(A^{(2)}\widetilde{A}_1^{(2)}+2A^{(2)}A_1),$$
$$A^{(2)}=\frac{g^2(\alpha_0\eta_0)}{\omega t^{(2)}}f^{(2)},$$

and

$$\widetilde{A}_1^{(2)}=\frac{2(\omega+2g_1)(\alpha_0\eta_0)}{\omega}f^{(2)}.$$

Likewise, the solitary solution can be expressed as

$$\widetilde{\Psi}^{(2)}(x)=\frac{1}{[(\widetilde{\alpha}_2+\widetilde{\beta}_2)+2\widetilde{\beta}_2\sinh^2\sqrt{\widetilde{b}_0}(x-x_0)]^{1/2}}, \quad (65)$$

where

$$\widetilde{\alpha}_2=-\frac{\widetilde{b}_1}{2\widetilde{b}_0}\quad\text{and}\quad\widetilde{\beta}_2=\frac{1}{2\widetilde{b}_0}(\widetilde{b}_1^2-4\widetilde{b}_0\widetilde{b}_2)^{1/2}.$$

Furthermore, we obtain

$$\widetilde{L}_2=-\frac{2\widetilde{\eta}_2}{\widetilde{b}_1}\coth\widetilde{\eta}_2,\quad \widetilde{\eta}_2^2=\widetilde{b}_2>0, \quad (66)$$

and

$$\widetilde{A}_0^{(2)}=\widetilde{b}_0=\frac{\widetilde{b}_1^2}{4\widetilde{b}_2}\tanh^2\sqrt{\widetilde{b}_2}. \quad (67)$$

Therefore, the ground state energy of the polaron–soliton system is corrected as

$$\widetilde{E}_0^{(2)}=\varepsilon_0(r)-2t^{(2)}-\frac{\widetilde{b}_1^2t^{(2)}}{4\widetilde{b}_2}\tanh^2\sqrt{\widetilde{b}_2}. \quad (68)$$

4. Quantum fluctuations and binding energy of the polaron due to the effects of electron-two-phonon interaction and polaron-squeezed phonon correlation

By using the polaron-squeezed phonon correlation representation $\widetilde{U}$, the phonon coordinate q_i and momentum p_i

$$q_i = \sqrt{\frac{\hbar}{2m\omega}}(b_i^\dagger + b_i), \quad p_i = \mathrm{i}\sqrt{\frac{\hbar\omega m}{2}}(b_i^\dagger - b_i), \quad (69)$$

can be, respectively, transformed to

$$\widetilde{U}q_i\widetilde{U}^{-1} = \sqrt{\frac{\hbar}{2m\omega}}[(b_i^\dagger + b_i)\mathrm{e}^{2r} - 2f\widetilde{\alpha}_i c_i^\dagger c_i], \quad (70)$$

$$\widetilde{U}p_i\widetilde{U}^{-1} = \mathrm{i}\sqrt{\frac{\hbar\omega m}{2}}(b_i^\dagger - b_i)\mathrm{e}^{2r}. \quad (71)$$

Thus, from these results, we find the mean-square fluctuations of q_i and p_i to be

$$\langle \Phi|\Delta^2\widetilde{q}|\Phi\rangle = \frac{\hbar}{2m\omega}\mathrm{e}^{4r}[1 + 4\mathrm{e}^{-4r}\langle\Delta^2\widetilde{n}\rangle], \quad (72)$$

$$\langle \Phi|\Delta^2\widetilde{p}|\Phi\rangle = \frac{\hbar\omega m}{2}\mathrm{e}^{-4r}, \quad (73)$$

and the uncertainty between the phonon coordinate and momentum reads

$$\langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle = \frac{\hbar^2}{4}[1 + 4\mathrm{e}^{-4r}\langle\Delta^2\widetilde{n}\rangle], \quad (74)$$

in which the electron density quantum fluctuation is

$$\langle\Delta^2\widetilde{n}\rangle = 2\sum_i f^2\widetilde{\alpha}_i^2\Psi_i^2 - \sum_i f^2\widetilde{\alpha}_i^2\Psi_i^4. \quad (75)$$

Using the continuous approximation, $\langle\Delta^2\widetilde{n}\rangle$ can be rewritten in the following form

$$\langle\Delta^2\widetilde{n}\rangle = f^2\left[2\int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)^2}{\omega^2(1+A_1\Psi^2)^2}\Psi^6\mathrm{d}x - \int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)^2}{\omega^2(1+A_1\Psi^2)^2}\Psi^8\mathrm{d}x\right]. \quad (76)$$

At the same time, the energy of the polaron $\widetilde{E}_\mathrm{p}$ is related to the effects of the effective displacement of the squeezed phonon and the polaron-squeezed phonon correlation, especially to the electron-two-phonon interaction and the result is

$$\widetilde{E}_\mathrm{p} = -\sum_i\langle\Psi_1|(f\widetilde{\alpha}_i c_i^\dagger c_i)^2|\Psi_1\rangle\hbar\omega = -2\hbar\omega f^2\int_{-\infty}^{+\infty}\frac{g^2(\alpha_0\eta_0)^2}{\omega^2(1+A_1\Psi^2)^2}\Psi^6\mathrm{d}x. \quad (77)$$

5. Discussion and conclusion

Based on the Holstein model Hamiltonian, by using the expansion approach to the correlated squeezed-coherent states of phonon, instead of using the variational wave function of the two-phonon coherent states, we can analytically solve the model polaron–soliton system in one-dimensional molecular crystals. Particularly, including the electron-two-phonon interaction, the displacement-squeezed phonon correlation with the effect of the squeezed-coherent states of phonon and both the electron-displaced phonon and the polaron-squeezed phonon correlations are combined to obtain the anomalous quantum fluctuations for the corrections of the coherent states. Note that

$$\widetilde{\alpha}_i = \alpha_i^{(1)}\alpha_0\eta_0,$$

and

$$\alpha_i^{(1)} = -g\Psi_i^2/\omega + 2g_1\Psi_i^2.$$

The term $\widetilde{\alpha}_i(b_i^\dagger + b_i)c_i^\dagger c_i$ clearly refers to the electron–phonon interaction with the displacement-squeezed phonon correlation (η_0), the effect of the squeezed-coherent states of phonon (α_0) and the electron-displaced phonon correlation, while the term $f\widetilde{\alpha}_i(b_i^\dagger + b_i)c_i^\dagger c_i$ means that the polaron-squeezed phonon correlation is considered as further correction. In view of the non-adiabatic correlations the properties of the ground state, both the electron density and the phonon coordinate quantum fluctuations and the polaron energy are studied in the strongly coupled electron–phonon system. Through the following discussion and analysis, some new important results and improvements will be shown clearly and recognized firmly.

As is well known, the two-phonon state is a coherent state with the squeezed-phonon character. In the strongly coupled case, each electron carries a strong lattice deformation in a coherent way. The "squeezing" effect of phonon is deeply related to the anomalous lattice fluctuation induced by the electron motion in the intermediately and strongly coupled systems. Therefore, the reasonable approximation aiming to strongly couple the electron–phonon systems can be attributed to how to solve the anomalous quantum fluctuation of the phonons. For this reason, we

have stated the quantum uncertainty of the phonon coordinate as follows:

$$\langle \Delta^2 q\rangle = \langle \Delta^2 q\rangle^{(0)}[\mathrm{e}^{4r} + 4\langle \Delta^2 \widetilde{n}\rangle],$$

where

$$\langle \Delta^2 q\rangle^{(0)} = \hbar/2m\omega.$$

Obviously, besides the corrective term e^{4r} from the two-phonon coherent state, we also find that the anomalous lattice fluctuation term $4\langle \Delta^2 \widetilde{n}\rangle$ is due to the coupling with electron density fluctuation. Noting that

$$\langle \Delta^2 n\rangle = 2\sum_i \widetilde{\alpha}_i^2 \Psi_i^2 - \sum_i \widetilde{\alpha}_i^2 \Psi_i^4,$$
$$\langle \Delta^2 \widetilde{n}\rangle = 2\sum_i f^2 \widetilde{\alpha}_i^2 \Psi_i^2 - \sum_i f^2 \widetilde{\alpha}_i^2 \Psi_i^4,$$

and

$$\widetilde{\alpha}_i = \alpha_0 \eta_0 \alpha_i^{(1)} \gg \alpha_i^{(1)},$$

we have

$$\langle \Delta^2 n\rangle \gg \langle \Delta^2 n\rangle_{\alpha_i^{(1)}},$$

where

$$(\langle \Delta^2 n\rangle_{\alpha_i^{(1)}} = \alpha_i^{(1)}(\langle n^2\rangle_0 - \langle n\rangle_0^2),$$

and

$$\langle n\rangle_0 = \frac{1}{N}\sum_i \langle 0 \mid c_i^\dagger c_i \mid 0\rangle).$$

In fact, from the numerical result one finds that $4\langle \Delta^2 n\rangle \gg \mathrm{e}^{4r}$. Consequently, the anomalous quantum fluctuation $\langle \Delta^2 n\rangle$ caused by the non-adiabatic correlations is the main contribution of the phonon coordinate fluctuation. At the same time, as a result of the anomalous lattice fluctuation $\langle \Delta^2 q\rangle$, the phonon coordinate–momentum quantum fluctuation $\langle \Delta^2 p\rangle\langle \Delta^2 q\rangle \gg \hbar^2/4$ due to $4\langle \Delta^2 n\rangle \gg \mathrm{e}^{4r}$.

From Figs. 1 and 2 we can see that with the evolution of the phonon squeezing, $\langle \Delta^2 n\rangle$ greatly increases due to $\widetilde{\alpha}_i^2$ increasing quickly but Ψ_i^2 trends to come down with the evolution of phonon squeezing. Since the increase of the phonon energy destroys the stability of the soliton state, we encounter a certain maximum constant; while $\langle \Delta^2 p\rangle\langle \Delta^2 q\rangle$ also increases quickly with the phonon squeezing increasing and a maximum peak occurs, afterward it comes down to a certain constant due to Ψ_i^2 decreasing. In particular, the electron-two-phonon interaction significantly increases the anomalous quantum fluctuations $\langle \Delta^2 n\rangle^{(2)} \gg \langle \Delta^2 n\rangle^{(1)}$, $\langle \Delta^2 p\rangle\langle \Delta^2 q\rangle^{(2)} \gg \langle \Delta^2 p\rangle\langle \Delta^2 q\rangle^{(1)}$ as shown in Fig. 1 and Fig. 2 respectively.

The non-adiabatic correlations obviously strengthen the electron–phonon interaction. In fact, since $\widetilde{\alpha}_i \gg \alpha_i^{(1)}$, the electron-one-phonon interaction $\alpha_i^{(1)} g$ is corrected as $\widetilde{\alpha}_i g$, while the electron-two-phonon interaction $\alpha_i^{(1)} g_1$ as $\widetilde{\alpha}_i^2 g_1$. Therefore, based on the anomalous quantum fluctuation caused by the non-adiabatic correlations, the ground state energy is greatly reduced to more negative ($E_0 \ll E_0(\alpha_i^{(1)})$), at the same time the binding energy of polaron ($E_\mathrm{p} \ll E_\mathrm{p}(\alpha_i^{(1)})$) in the polaron–soliton system increases as shown in Fig. 3 and Fig. 4 respectively.

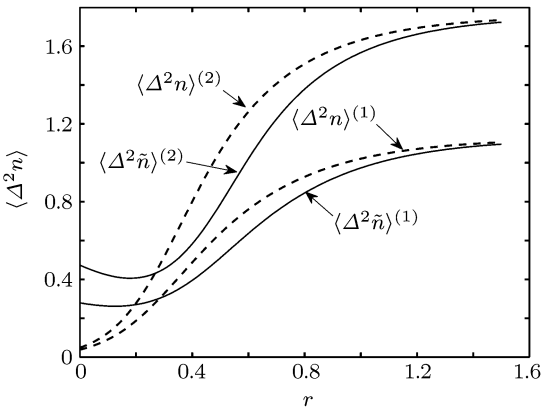


Fig. 1. Fluctuations of electron density versus r at $\omega = 1.0$, $t = 1.0$, $g = 1.0$ and $g_1 = -0.1$, with $\langle \Delta^2 n\rangle^{(1),(2)}$ denoting the electron-one-phonon interaction and electron-two-phonon interaction without the f-correlation parameter and $\langle \Delta^2 \widetilde{n}\rangle^{(1),(2)}$ referring to the one with the f-correlation parameter.

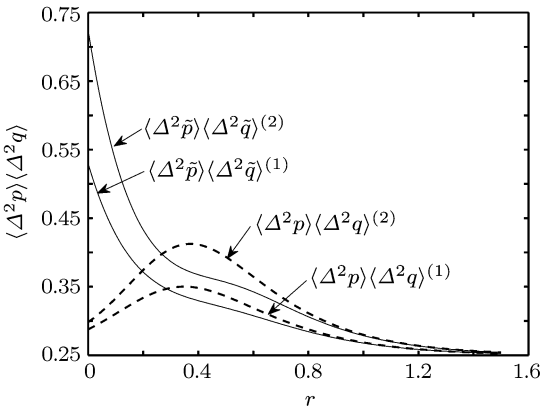


Fig. 2. Quantum fluctuations of phonon coordinate-momentum versus r at $\omega = 1.0$, $t = 1.0$, $g = 1.0$, and $g_1 = -0.1$, with $\langle \Delta^2 p\rangle\langle \Delta^2 q\rangle^{(1),(2)}$ denoting the electron-one-phonon interaction and electron-two-phonon interaction without the f-correlation parameter and $\langle \Delta^2 \widetilde{p}\rangle\langle \Delta^2 \widetilde{q}\rangle^{(1),(2)}$ referring to the one with the f-correlation parameter.

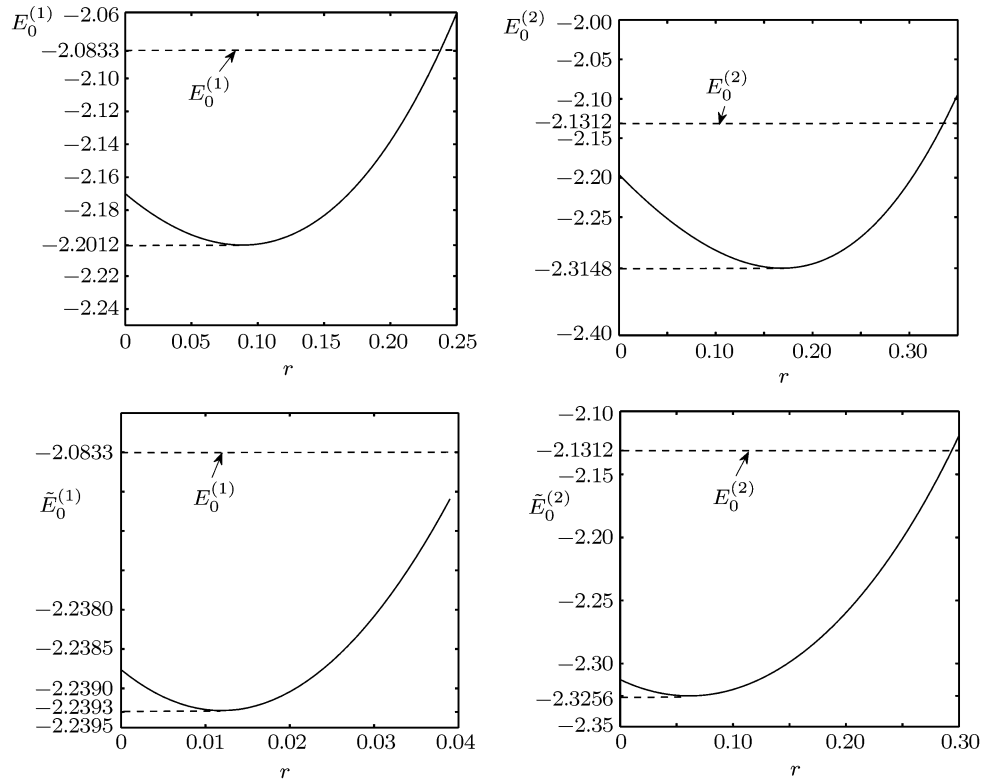


Fig. 3. Dependences of energy of the ground state on the squeezed parameter r at $\omega = 1.0$, $t = 1.0$, $g = 1.0$, and $g_1 = -0.1$, with $E_0^{(1),(2)}$ denoting the electron-two phonon interaction without the f-correlation parameter and $\widetilde{E}_0^{(1),(2)}$ referring to the one with the f-correlation parameter. However the single-phonon (two-phonon) energy of ground state in Refs. [20] and [22] is only $E_{(0)}^{(1)} = -2.0833$ ($E_{(0)}^{(2)} = -2.1312$).

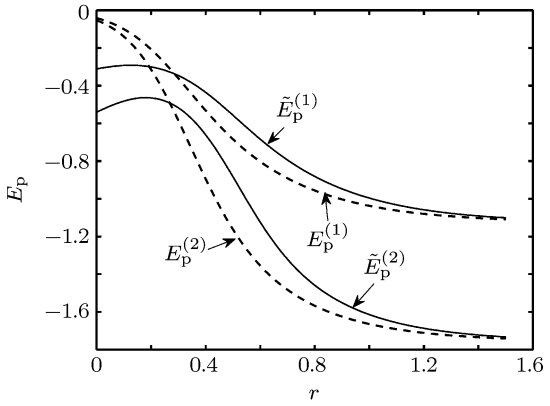


Fig. 4. The polaron energy as a function of r at $\omega = 1.0$, $t = 1.0$, $g = 1.0$, and $g_1 = -0.1$, where $E_{\rm p}^{(1),(2)}$ stand for the electron-one-phonon interaction and electron-two-phonon interaction without the f-correlation parameter, while $\widetilde{E}_{\rm p}^{(1),(2)}$ with the f-correlation parameter, respectively.

Furthermore, the effect of the electron-two-phonon interaction restricts the increase of phonon energy $\varepsilon_0(r)$ with the further enhancement of phonon squeezing, so that there exists a minimun ground state energy ($r^{(2)} < r^{(1)}$). Particularly, since $\widetilde{\alpha}_i^2 g_1 \gg \alpha_i^{(1)} g_1$, $E_0^{(2)} \ll E_0^{(1)}$ as shown in Fig. 3. As a comparison ($t = 1.0, \omega = 1.0, g = 1.0, g_1 = -0.1$),

$$E_0^{(1)} = -2.2012, \quad (r^{(1)} \sim 0.09),$$
$$E_0^{(2)} = -2.3148, \quad (r^{(2)} \sim 0.17),$$

and for the polaron-squeezed phonon correlation,

$$\widetilde{E}_0^{(1)} = -2.2393, \quad (r^{(1)} \sim 0.01),$$
$$\widetilde{E}_0^{(2)} = -2.3256, \quad (r^{(2)} \sim 0.05).$$

When these correlations are not considered, $E_{(0)}^{(1)} = -2.0833$ and $E_{(0)}^{(2)} = -2.1312$.[20,22] Thus we have the relative corrections $\delta_0 = (E_0^{(2)} - E_0^{(1)})/E_0^{(2)} \approx 0.051$ and $\delta_{(0)} = (E_{(0)}^{(2)} - E_{(0)}^{(1)})/E_{(0)}^{(2)} \approx 0.0015$, respectively.

On the other hand, the polaron energy is related deeply to the non-adiabatic correlations $\widetilde{\alpha}_i^2$ and Ψ_i^2. As the phonon squeezing increases, $|E_{\rm p}|$ will noticeably increase due to $\widetilde{\alpha}_i^2 \gg \alpha_i^{(1)}$, finally $E_{\rm p}$ arrives at a certain minimum constant due to Ψ_i^2 coming down. Equally, in consequence of the electron-two-phonon interaction, $E_{\rm p}^{(2)} \ll E_{\rm p}^{(1)}$ as shown in Fig. 4. It should be noted particularly that when $g_1 < 0$,

$$b_2 = a_2 + \frac{4g_1}{3\omega}(1 + \alpha_0\eta_0)A < a_2,$$

so

$$\beta_2^2 = \frac{1}{4b_0^2}(b_1^2 - 4b_0b_2) > 0$$

is satisfied enough so that the stable soliton solution exists in Eq. (33) and $L^{(2)} < L^{(1)}$; conversely if $g_1 > 0$, then $\beta_2^2 < 0$, so it does not have a soliton solution.

The polaron-squeezed phonon correlation is an important non-adiabatic effect in the present work. From Eq. (48) and Eq. (49), we can estimate approximately the parameter f of polaron-squeezed phonon correlation as

$$f \approx \frac{g\sum_i \widetilde{\alpha}_i \Psi_i^2}{2\sum_i(\omega + 2g_1)\widetilde{\alpha}_i^2\Psi_i^2}, \tag{78}$$

which is related to the evolutions of $\widetilde{\alpha}_i$ and $\Psi_i(r)$. When $r = 0$, f will be

$$f_0 \approx \frac{g\sum_i \alpha_i^{(1)}\Psi_i^2}{2\sum_i(\omega + 2g_1)\alpha_i^{(1)^2}\Psi_i^2} > 1. \tag{79}$$

Including the f-correlation effect, $\alpha_i^{(1)}g \to (f\widetilde{\alpha}_i)g$, $\alpha_i^{(1)^2}g_1 \to (f^2\widetilde{\alpha}_i^2)g_1$. When r is not larger, since $f^{(1),(2)} > 1$, this effect further strengthens the electron–phonon interaction. But with the increase of the phonon squeezing, the squeezed-phonon effects will destroy the stable polaron–soliton state due to the phonon energy increasing, thus weakening the f-correlation effect, i.e. $f^{(1),(2)} < 1$. As a result, it further lightens the electron–phonon interaction. In particular, when $f \ll 1$, the effect of the polaron-squeezed phonon correlation will disappear as seen in Fig. 5.

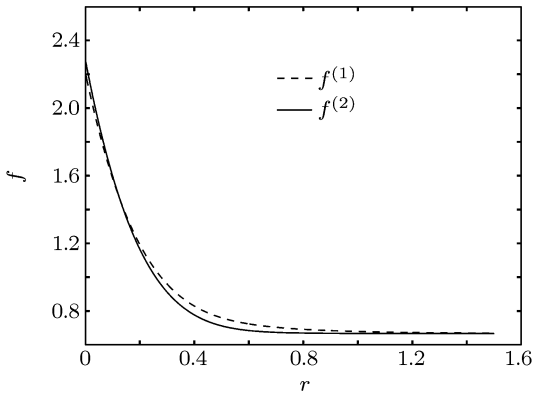


Fig. 5. Variations of polaron-squeezed phonon correlation with squeezing parameter r at $\omega = 1.0, t = 1.0, g = 1.0$ and $g_1 = -0.1$, where $f^{(1),(2)}$ denote the electron-one-phonon interaction and electron-two-phonon interaction, respectively.

On the other hand, considering

$$\psi_i^2 \approx \frac{B}{4}\,\mathrm{sech}^2\,\frac{\sqrt{B}}{2} < 1, \quad \frac{B}{4} = \frac{g^2}{4\omega t} < 1,$$

thus,

$$\frac{1}{2}f^2\widetilde{\alpha}_i^2\mathrm{e}^{-4r} \approx \frac{g^6\mathrm{e}^{-4r}(\alpha_0\eta_0)^2}{32\omega^2t^2(\omega + g_1\psi_i)^2}f^2 \ll 1. \tag{80}$$

Noting that $g^2/4\omega t < 1$ due to $\Psi_i^2 < 1$. When r is small, although $f > 1$, $(\alpha_0\eta_0)^2\mathrm{e}^{-4r} \sim 1.0$, so that $\frac{1}{2}f^2\widetilde{\alpha}_i^2\mathrm{e}{-}4r \ll 1$; when r evolves to a larger value and $(\alpha_0\eta_0)^2\mathrm{e}^{-4r} > 1$, but at the same time $f \ll 1$ and then we still have $\frac{1}{2}f^2\widetilde{\alpha}_i^2\mathrm{e}^{-4r} \ll 1$. Therefore, the non-adiabatic polaron-squeezed correlation assures the satisfaction of the condition of the strongly coupled approximation. With the evolution of the phonon squeezing, the effect of polaron-squeezed phonon correlation significantly enhances the quantum fluctuations, i.e., $\langle\Delta^2\widetilde{n}\rangle^{(i)} \gg \langle\Delta^2 n\rangle^{(i)}$ and $\langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(i)} \gg \langle\Delta^2 p\rangle\langle\Delta^2 q\rangle^{(i)}$ $(i = 1, 2)$, in particular, $\langle\Delta^2\widetilde{n}\rangle^{(2)} > \langle\Delta^2\widetilde{n}\rangle^{(1)}$ and $\langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(2)} > \langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(1)}$ as shown in Figs. 1 and 2. However as the phonon squeezing increases further, since the increase of phonon energy will weaken the polaron–phonon correlation, $\langle\Delta^2\widetilde{n}\rangle^{(i)} < \langle\Delta^2 n\rangle^{(i)}$, $\langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(i)} < \langle\Delta^2 p\rangle\langle\Delta^2 q\rangle^{(i)}$ and finally, $\langle\Delta^2\widetilde{n}\rangle^{(i)} \sim \langle\Delta^2 n\rangle^{(i)}$, $\langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(i)} \sim \langle\Delta^2 p\rangle\langle\Delta^2 q\rangle^{(i)}$. Particularly, we always have $\langle\Delta^2\widetilde{n}\rangle^{(2)} > \langle\Delta^2\widetilde{n}\rangle^{(1)}$ and $\langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(2)} \sim \langle\Delta^2\widetilde{p}\rangle\langle\Delta^2\widetilde{q}\rangle^{(1)}$.

In addition, the polaron-squeezed phonon correlation results in leading to more important correction for the ground state energy, i.e. it noticeably lowers the ground state energy to a more negative value, such as $\widetilde{E}_0^{(1)} < E_0^{(1)}$, $\widetilde{E}_0^{(2)} < E_0^{(2)}$ and $\widetilde{E}_0^{(2)} < \widetilde{E}_0^{(1)}$. As for the binding energy of polaron, with the phonon squeezing evolution, $\widetilde{E}_{\mathrm{p}}^{(1)} < E_{\mathrm{p}}^{(1)}$, $\widetilde{E}_{\mathrm{p}}^{(2)} < E_{\mathrm{p}}^{(2)}$ and $\widetilde{E}_{\mathrm{p}}^{(2)} < \widetilde{E}_{\mathrm{p}}^{(1)}$. In the final stage of the evolution of the phonon squeezing, $\widetilde{E}_{\mathrm{p}}^{(1)} \sim E_{\mathrm{p}}^{(1)}$, $\widetilde{E}_{\mathrm{p}}^{(2)} \sim E_{\mathrm{p}}^{(2)}$ particularly, $\widetilde{E}_{\mathrm{p}}^{(2)} < \widetilde{E}_{\mathrm{p}}^{(1)}$.

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