Localized self-trapping in two-dimensional molecular lattice with interaction between Wannier–Mott excitons and phonon lattice*

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We investigate the interactions of lattice phonons with Wannier–Mott exciton, the exciton that has a large radius in two-dimensional molecular lattice, by the method of continuum limit approximation, and obtain that the self-trapping can also appear in two-dimensional molecular lattice with a harmonic and nonlinear potential. The exciton effect on molecular lattice does not distort the molecular lattice but only makes it localized and the localization can also react, again through phonon coupling, to trap the energy and prevents its dispersion.

Keywords: self-trapping, Wannier–Mott exciton, two-dimensional molecular lattice, phonon
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1. Introduction

The first application of the localized theory of the nonlinear lattice to the biological field was in 1973. Davydov proposed a novel mechanism for the localization and transport of vibrational energy in protein.[1] Referring to the simplified structure of an α-helix region of protein, this mechanism can be described classically as follows. Vibrational energy of the stretching oscillators that is localized on the helix, acts as distorting the structure of the helix through a phonon coupling. The helical distortion reacts, again through phonon coupling, to trap the energy and prevents its dispersion. This effect is called self-localization or self-trapping.

In the following decades the biological mechanism was studied in detail by Davydov and his colleagues, and made significant progress. The effects of the phonon coupling on the transport of single exciton in the helical molecular chain were discussed in the study of the solitons in molecular system,[2,3] and obtained the conclusion that the exciton transferred along this structure as a soliton. Soon afterwards, biology and quantum mechanics,[4] quantum theory of muscular contraction,[5] soliton and energy transferring along protein molecules,[6] soliton bioenergetics, the mechanism of muscle contraction,[7] etc. achieved many studying fruits. The more perfect soliton theory of molecular system was found. This soliton is known as Davydov's soliton.

The polaron suggested by Landau[8] and studied by many scholars[9−12] has been used over the past half-century to denote a wide variety of excitations that are self-localized through interactions with lattice phonons. But Davydov's soliton is an exciton not a polaron, and it corresponds only to a polaron that is (i) large so that the continuum limit approximation is justified, (ii) acoustic because the self-localization arises from interactions with acoustic modes of the lattice, and (iii) weakly coupled because the anharmonic energy is small compared with the phonon bandwidth.

From the 1970s to the 1990s, the Davydov's solitons in nonlinear molecular lattice were studied to the full. In 1982, Scott modified Davydov's model and added ten dipole–dipole coupling terms to represent the helical symmetry, and gave the conclusion that such solitons should appear under normal physiological conditions through numerical method and the continuum limit approximation.[13] Lomdahl and Ker pointed out that the random displacements produced by thermal motions were so much larger than the displacements needed to form the coherent soliton pattern that the solitons could not be formed at the temperature relevant to biological procedure.[14] Wang *et al.* obtained that the exact equations could reduce to

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the usual nonlinear Schrödinger equation in the continuum limit approximation, when they studied the Davydov's theory of energy transferring in biological molecular system.[15] They also discussed initial states and the soliton formation process. The time scale and the length scale that govern soliton coherence properties were determined. In 1992, Scott systematically studied the behaviour of Davydov's soliton,[16] and formed more perfect theoretical system of Davydov's soliton. Soon afterwards, the thermal stability of Davydov's soliton was studied to the full.[17−19]

In the 21st century, the Hamiltonian and the wave function in the Davydov theory have simultaneously been improved and extended, based on some physical and biological grounds and on the results from other models. The equations of motion for the improved Davydov model with a quasicoherent two-quantum state and a new interaction term in the Hamiltonian describe bioenergy transport along the molecular chains in protein molecules by a soliton mechanism. Some elementary properties of the soliton, including the nonlinear coupling energy and the greatly increased binding energy of the soliton, are also given. The results obtained suggest that the model could be a candidate for a bioenergy transport mechanism in protein molecules.[20] The two-dimensional localized modes around a soliton have been investigated by using an extension of the Su–Shrieffer–Heeger model, in which is included a nonlinear term of electron–phonon interaction. The results show that there appears an additional localized mode, and the two modes obtained in the previous work without the nonlinear term disappear. Furthermore, the frequencies of the modes are shifted and their localizations are changed after turning on the nonlinear term.[21] Coherent excitons at different orientation arrangements of local transition dipole moments in circular light-harvesting complexes,[22] factors influencing entanglement of two excitons in a coupled exciton–photon system,[23] and the effect of interchain coupling on a biexciton in organic polymers[24] have also been investigated, and the conclusions can also reflect the interaction between exciton and photon in molecular lattice, which inspires the further study. Recently, the interactions of lattice phonons with Frenkel exciton, which has a small radius in a two-dimensional discrete molecular lattice, have been investigated by the virtue of the quasi-discreteness approximation and the method of multiple-scale, and obtained that the self-trapping can also appear in the two-dimensional discrete molecular lattice with a harmonic and nonlinear potential. The exciton effect on the molecular lattice does not distort it but only causes it to be localized, which enables it to react again through phonon coupling to trap the energy and prevent its dispersion.[25] This paper focus on the study of interactions of lattice phonons with Wannier–Mott exciton, by the method of continuum limit approximation in Ref. [26].

2. Self-trapping in a two-dimensional isotropic harmonic molecular lattice

We first consider a two-dimensional isotropic harmonic molecular lattice. By taking into account the interaction between the lattice and its nearest-neighbours, the Hamiltonian of the system with a harmonic potential is given by

$$H = H_{\rm ex} + H_{\rm ph} + H_{\rm ex-ph}, \tag{1}$$

where $H_{\rm ex}$ is the Hamiltonian describing the exciton energy and given by

$$H_{\rm ex} = \left\{ J_l \sum_{l,n} \left[|\psi_{l,n}|^2 - \psi^*_{l,n} \left(\psi_{l+1,n} + \psi_{l-1,n} \right) \right] + J_n \sum_{l,n} \left[|\psi_{l,n}|^2 - \psi^*_{l,n} \left(\psi_{l,n+1} + \psi_{l,n-1} \right) \right] \right\}, \tag{2}$$

with $\psi_{l,n}$ being a wave function of the exciton at $(l,\ n)$th site, J_l and J_n denoting the nearest neighbour dipole–dipole coupling energies along the l direction and the n direction, respectively.

The Hamiltonian describing phonon energy is given by

$$H_{\rm ph} = \sum_{l,n} \left[\frac{p^2_{l,n}}{2m} + \frac{1}{2} k_l \left(u_{l+1,n} - u_{l,n} \right)^2 + \frac{1}{2} k_n \left(u_{l,n+1} - u_{l,n} \right)^2 \right], \tag{3}$$

where m, $u_{l,n}$ and $p_{l,n}$ denote the mass, the displacement and the momentum, respectively, k_l and k_n are coupling coefficients along the l direction and the n direction, respectively.

The exciton–phonon interaction Hamiltonian is

$$H_{\mathrm{ex-ph}} = \sum_{l,n} \left[\chi_l \left|\psi_{l,n}\right|^2 \left(u_{l+1,n} - u_{l,n}\right) + \chi_n \left|\psi_{l,n}\right|^2 \left(u_{l,n+1} - u_{l,n}\right) \right], \tag{4}$$

where χ_l and χ_n describe the parameters of the strength of the interaction between the exciton and phonon along the l direction and the n direction, respectively. When the molecular lattice is isotropic lattice, $J_l = J_n = 2J$, $k_l = k_n = k$, and $\chi_l = \chi_n = \chi$, we have

$$\begin{aligned} H &= H_{\mathrm{ex}} + H_{\mathrm{ph}} + H_{\mathrm{ex-ph}} \\ &= J \sum_{l,n} \left[4 \left|\psi_{l,n}\right|^2 - \psi^*_{l,n} \left(\psi_{l+1,n} + \psi_{l-1,n} + \psi_{l,n+1} + \psi_{l,n-1}\right) \right] \\ &\quad + \sum_{l,n} \left[\frac{p^2_{l,n}}{2m} + \frac{1}{2} k \left(u_{l+1,n} - u_{l,n}\right)^2 + \frac{1}{2} k \left(u_{l,n+1} - u_{l,n}\right)^2 \right] \\ &\quad + \chi \sum_{l,n} \left[\left|\psi_{l,n}\right|^2 \left(u_{l+1,n} + u_{l,n+1} - 2u_{l,n}\right) \right]. \end{aligned} \tag{5}$$

The nonlinear vibration equation of the system is obtained by $\dot{p}_{l,n} = \ddot{u}_{l,n} = -\partial H / \partial u_{l,n}$ and $\mathrm{i}\dot{\psi}_{l,n} = \partial H / \partial \psi^*_{l,n}$

$$\begin{aligned} m\ddot{u}_{l,n} &= k \left(u_{l+1,n} + u_{l-1,n} + u_{l,n+1} + u_{l,n-1} - 4u_{l,n}\right) + \chi \left(2 \left|\psi_{l,n}\right|^2 - \left|\psi_{l-1,n}\right|^2 - \left|\psi_{l,n-1}\right|^2 \right), \\ \mathrm{i}\dot{\psi}_{l,n} &= -J \left(\psi_{l+1,n} + \psi_{l-1,n} + \psi_{l,n+1} + \psi_{l,n-1} - 4\psi_{l,n}\right) + \chi \left(u_{l+1,n} - u_{l,n} + u_{l,n+1} - u_{l,n}\right) \psi_{l,n}. \end{aligned} \tag{6}$$

First, let $x_l = la, y_n = na$, $u_{l,n} = u\left(x_l, y_n, t\right)$ and $\psi_{l,n} = \psi\left(x_l, y_n, t\right)$, $(n = 1, 2, \ldots, N-1)$. $u_{0,n} = u_{l,0} = u_{0,N} = u_{N,0} = \psi_{0,N} = \psi_{N,0} = 0$ means $u_{l\pm1,n} = u\left(x_l \pm a, y_n, t\right)$, $u_{l,n\pm1} = u\left(x_l, y_n \pm a, t\right)$, $\psi_{l\pm1,n} = \psi\left(x_l \pm a, y_n, t\right)$, $\psi_{l,n\pm1} = \psi\left(x_l, y_n \pm a, t\right)$, and here a is lattice constant. When $x_l \to x, y_n \to y, u_{l,n} \to u\left(x, y, t\right)$, $\psi_{l,n} \to \psi\left(x, y, t\right)$, Eqs. (2) can be transform into the following equations:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{ka^2}{m} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) &= \frac{a\chi}{m} \left(\frac{\partial \left|\psi\right|^2}{\partial x} + \frac{\partial \left|\psi\right|^2}{\partial y} \right) + O\left(a^3\right), \\ \mathrm{i}\frac{\partial \psi}{\partial t} &= -Ja^2 \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + a\chi \left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \right) \psi + O\left(a^3\right). \end{aligned} \tag{7}$$

Let $v_0^2 = ka^2/m$, $\Lambda = Ja^2, \Delta = a\chi/m$, $\Delta = -m\Delta = -a\chi$, and eliminate small variable $O\left(a^3\right)$, then Eqs. (3) can be rewritten as

$$\begin{aligned} &\frac{\partial^2 u}{\partial t^2} - v_0^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = \Delta \left(\frac{\partial \left|\psi\right|^2}{\partial x} + \frac{\partial \left|\psi\right|^2}{\partial y} \right), \\ &\mathrm{i}\frac{\partial \psi}{\partial t} + \Lambda \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + \Delta \left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \right) \psi = 0. \end{aligned} \tag{8}$$

Assuming the solution to be stationary, i.e. $\dot{u} = 0$, we have

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial y} = -\frac{\Delta}{v_0^2} \left|\psi\right|^2, \tag{9}$$

which is corresponding to lattice distortion, and Eq. (8) can be rewritten as

$$\mathrm{i}\frac{\partial \psi}{\partial t} + \Lambda \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + \gamma \left|\psi\right|^2 \psi = 0, \tag{10}$$

where $\gamma = -2a^2\chi^2/mv_0^2$. Equation (10) is a nonlinear Schrodinger equation and has the following solution:

$$\psi = B \operatorname{sech} \eta \sqrt{\left(x - vt\right)^2 + \left(y - vt\right)^2} \cdot \mathrm{e}^{\mathrm{i}(qx + qy - \omega t)}. \tag{11}$$

Thus, Eq. (8) has the following solutions:

$$\begin{aligned} u &= A \tanh \eta \sqrt{\left(x - vt\right)^2 + \left(y - vt\right)^2}, \\ \psi &= B \operatorname{sech} \eta \sqrt{\left(x - vt\right)^2 + \left(y - vt\right)^2} \cdot \mathrm{e}^{\mathrm{i}(qx + qy - \omega t)}, \end{aligned} \tag{12}$$

where $\eta = \sqrt{(\omega - \Lambda q^2)/\Lambda}, A = -(\beta/v_0^2)\sqrt{2\left(\omega - \Lambda q^2\right)/\gamma}$, $B = \sqrt{2\left(\omega - \Lambda q^2\right)/\gamma}$, and $v = 2\Lambda q$. Solutions (12) can be shown in Fig. 1.

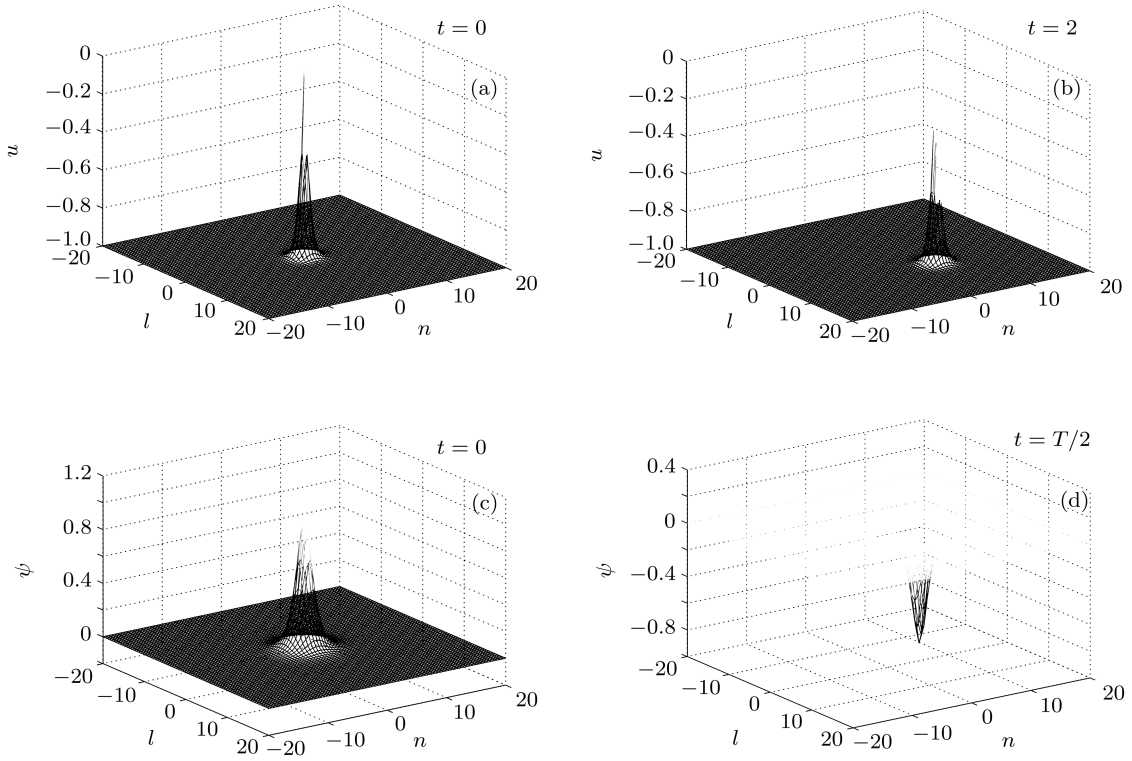


Fig. 1. Localized modes in two-dimensional molecular lattice, (a) motional bright soliton in molecular lattice $t = 0$, (b) motional bright soliton in molecular lattice $t = T/2$, (c) motional exciton–breathers $t = 0$, and (c) motional exciton–breathers $t = T/2$.

From Fig. 1 it follows that motional bright soliton can exist in a two-dimensional isotropic molecular lattice with the interactions of excitons with phonons in the continuum limit approximation, while Davydov's solitons can be transformed into exciton–breathers and move in a molecular lattice. The difference from the conclusion in one-dimensional molecular lattice is that the exciton effect on molecular lattice does not distort molecular lattice but only makes it localized and the localization can also react again through phonon coupling to trap the energy and prevents its dispersion.

3. Self-trapping in a two-dimensional isotropic anharmonic molecular lattice

We first consider a two-dimensional isotropic molecular lattice with a cubic nonlinear potential. By taking into account the interactions between the lattice and its nearest-neighbours, the Hamiltonian of the system is given by

$$H_{\rm ph} = \frac{1}{2}\sum_{l,n}\left[\frac{p_{l,n}^2}{m} + k\left(u_{l+1,n}-u_{l,n}\right)^2 + k\left(u_{l,n+1}-u_{l,n}\right)^2 + \frac{2}{3}\alpha k\left(u_{l+1,n}-u_{l,n}\right)^3 + \frac{2}{3}\alpha k\left(+u_{l,n+1}-u_{l,n}\right)^3\right]. \quad (13)$$

If the lattice distortion keeps the same form as Eq. (9), and through the procedure the same as the above, we obtain

$$u = C\tanh\eta\sqrt{(x-vt)^2+(y-vt)^2},$$
$$\psi = B\,\mathrm{sech}\,\eta\sqrt{(x-vt)^2+(y-vt)^2}\cdot \mathrm{e}^{\mathrm{i}(qx+qy-\omega t)}, \quad (14)$$

where $C = \alpha A/3v_1$, and v_1 is a parameter. Solution (14) can also be shown in Fig. 1. The result is the same as that in a two-dimensional isotropic harmonic molecular lattice with the interactions of excitons with phonons in the continuum limit approximation. We also investigate the conditions of the molecular lattices separately with a quartic potential and a cubic & quartic potential, and obtain the same conclusions.

4. Conclusions

In this paper we investigate the interactions of lattice phonons with Wannier–Mott exciton, the exciton that has a small radius in a two-dimensional isotropic molecular lattice, in the continuum limit approximation, and obtain the following conclusions.

(i) When the interactions of lattice phonons with Wannier–Mott excitons are taken into account, the self-trapping (or self-localization) can also appear in a two-dimensional isotropic molecular lattice. Motional bright soliton can exist in a two-dimensional isotropic molecular lattice with the interactions of excitons with phonons in the continuum limit approximation, while Davydov's solitons can be transformed into exciton–breathers and move in a molecular lattice.

(ii) The difference from the conclusion in a one-dimensional molecular lattice[26] is that the exciton effect on molecular lattice does not distort molecular lattice but only makes it localized.

(iii) Considering the two-dimensional isotropic molecular lattice separately with a cubic nonlinear potential, a quartic nonlinear potential, and a cubic & quartic potential, the conclusions are same as those in the two-dimensional isotropic molecular lattice with a harmonic potential.

Therefore, we conclude that the self-trapping can also appear in a two-dimensional isotropic molecular lattice with a harmonic and nonlinear potential. The exciton effect on molecular lattice does not distort molecular lattice but only makes it localized and the localization can also react again through phonon coupling to trap the energy and prevents its dispersion.

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