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Spatially periodic solutions of a continuous nonlinear polaron model on a ring

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Abstract. Spatially periodic solutions (cnoidal waves) for excitations of a molecular-crystal model with the dispersion term on a diatomic molecule ring are found. The relative displacement of the self-trapped state, the self-trapped well and the energy of the electron, and the density of current carried by excitations are calculated. The relations between periodic solutions on a ring and soliton solutions on a chain are discussed.

1. Introduction

As is now known, a slowly moving electron (or hole) in a molecular-crystal medium may lower its energy by locally distorting the crystal lattice surrounding it [1]. Due to the electron–phonon interaction, such a lattice deformation can produce a potential well trapping the electron. This entity, the 'self-trapped' electron together with its induced lattice distortion, is commonly called the polaron, which has attracted much attention through the years [2]. The possibility of self-trapping in a one-dimensional electron–phonon system was first studied by Holstein [3]. Further research on polarons has been carried out by many authors [4]. In this paper, we consider the molecular-crystal model (MCM) with the dispersion term on a diatomic molecule ring. We find periodic solutions (cnoidal waves) for excitations in the model and show that periodic solutions tend to soliton solutions obtained in a previous paper [5] when the perimeter of the ring tends towards infinity. In addition, we also give the relative displacement of the self-trapped state, the self-trapped well and the energy of the electron, and the density of current carried by excitations.

In section 2 we will introduce the model and give the equations of motion, while in section 3 we obtain periodic solutions of the equations of motion and discuss their limits. Section 4 contains our conclusions.

2. The model and the equations of motion

The Lagrangian of the MCM with the dispersion term on a diatomic molecule ring can be written as

$$L = \int_0^l \mathrm{d}x \left[\frac{\rho}{2}\left(\frac{\partial u}{\partial t}\right)^2 - \frac{\rho(\omega_0^2+\omega_1^2)}{2}u^2 + \frac{\rho a^2\omega_1^2}{4}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{\mathrm{i}\hbar}{2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right) - \frac{\hbar^2}{2m}\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} + Au|\psi|^2\right] \tag{2.1}$$

where $u(x,t)$ is the relative displacement of atoms of the diatomic molecule at point x and time t, and $\psi(x,t)$ the wavefunction of electrons; ω_0 is the Einstein's frequency and ω_1 the dispersion frequency of the lattice optical vibrations; $\rho = M/a$ is the lattice density, M the molecular mass and a the lattice parameter; m is the effective mass for electrons in the conduction band, A the coupling constant, and l the perimeter of the ring. Obviously, $\psi(x,t)$ and $u(x,t)$ must satisfy the condition of periodicity

$$\psi(x,t) = \psi(x+l,t) \qquad u(x,t) = u(x+l,t). \tag{2.2}$$

The wavefunction ψ is normalized

$$\int_0^l |\psi(x,t)|^2\,\mathrm{d}x = 1. \tag{2.3}$$

The equations of motion for the Lagrangian (2.1) are

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - Au\psi \tag{2.4}$$

$$\frac{\partial^2 u}{\partial t^2} = -(\omega_0^2+\omega_1^2)u - \frac{a^2\omega_1^2}{2}\frac{\partial^2 u}{\partial x^2} + \frac{Aa}{M}|\psi|^2. \tag{2.5}$$

Equation (2.4) is the Schrödinger equation for an electron in a potential well given by

$$V(x,t) = -Au(x,t) \tag{2.6}$$

while equation (2.5) is an equation for an oscillator with frequency ω_0 affected by dispersion terms, which are ω_1^2-proportional, and an external field $|\psi|^2$.

We will look for solutions of the forms

$$\psi(x,t) = \phi(\eta)\exp\left[\mathrm{i}\left(kx - \frac{E}{\hbar}t\right)\right] \qquad u(x,t) = u(\eta) \tag{2.7}$$

for equations (2.4) and (2.5), where ϕ is a real function of $\eta = x - vt$. Substituting equation (2.7) in (2.4) and (2.5) and taking the adiabatic approximation, i.e. dropping the kinetic energy term of the lattice vibration, as the velocity v of the 'self-trapped' electron is very small, we get

$$\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} + Au\phi + \left(E - \frac{\hbar^2k^2}{2m}\right)\phi = 0 \tag{2.8}$$

$$(\omega_0^2+\omega_1^2)u = \frac{Aa}{M}\phi^2 - \frac{a^2\omega_1^2}{2}\frac{\mathrm{d}^2u}{\mathrm{d}\eta^2} \tag{2.9}$$

and

$$k = mv/\hbar \tag{2.10}$$

the wavenumber of the electron. It is interesting only for the narrow optical band case, i.e. $\omega_1 \ll \omega_0$. In this situation, an iterative solution of equation (2.9) is given by

$$u(\eta) = \frac{Aa}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)\phi^2(\eta) - \frac{Aa^3\omega_1^2}{2M\omega_0^4}\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} + \mathrm{O}\left[\left(\frac{\omega_1}{\omega_0}\right)^4\right]. \tag{2.11}$$

By combining equations (2.8) and (2.11), the equation for ϕ is obtained

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}\eta^2} - \frac{\gamma\phi}{2}\frac{\mathrm{d}^2\phi^2}{\mathrm{d}\eta^2} + 2\mu\phi^3 - \lambda\phi = 0 \tag{2.12}$$

where

$$\gamma = \frac{2mA^2a^3\omega_1^2}{\hbar^2M\omega_0^4} \qquad \mu = \frac{mA^2a}{\hbar^2M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \qquad \text{and} \qquad \lambda = k^2 - \frac{2mE}{\hbar^2}. \tag{2.13}$$

Equation (2.12) is a modified nonlinear Schrödinger equation. The γ-proportional term is the modification term.

The condition of periodicity (2.2) is changed accordingly into

$$\phi(\eta) = \phi(\eta + l) \qquad u(\eta) = u(\eta + l) \tag{2.14}$$

and

$$k = 2n\pi/l \qquad n = 0, \pm 1, \pm 2, \ldots \tag{2.15}$$

that is to say, the wavevector k, consequently, the velocity v of the electron from equation (2.10), is quantized

$$v = nh/ml \qquad n = 0, \pm 1, \pm 2, \ldots . \tag{2.16}$$

3. Periodic solutions and their limits

In order to obtain solutions of equation (2.12), we integrate (2.12) once to result in

$$(1 - \gamma\phi^2)\left(\frac{\mathrm{d}\phi}{\mathrm{d}\eta}\right)^2 = \mu(\phi_2^2 - \phi^2)(\phi^2 - \phi_1^2) \tag{3.1}$$

where

$$\phi_1^2 \leqslant \phi^2 \leqslant \phi_2^2 \qquad \phi_1^2 + \phi_2^2 = \frac{\lambda}{\mu} \qquad \phi_1^2\phi_2^2 = c \tag{3.2}$$

and c is an integration constant. There are two different sets of solutions of equation (2.12) depending on c being positive or negative.

3.1. The case of $c > 0$.

Integrating equation (3.1) once again, we arrive at the cnoidal wave solution†

$$\frac{1}{\sqrt{(1-\gamma\phi_1^2)\phi_2^2}}\,\mathrm{dn}^{-1}\left(\sqrt{\frac{\phi_2^{-2}-\gamma}{\phi^{-2}-\gamma}}, q\right) - \frac{\gamma}{\sqrt{(1-\gamma\phi_1^2)\phi_2^2}} \times\left[\left(\phi_2^2 - \frac{1}{\gamma}\right)\Pi(\delta, b, q) + \frac{1}{\gamma}F(\delta, q)\right] = \sqrt{\mu}(\eta - \eta_0) \tag{3.3}$$

where $\mathrm{dn}(x, q)$ is the Jacobian elliptic function of the third kind [6], $\Pi(\delta, b, q)$ and $F(\delta, q)$ are, respectively, the elliptic integrals of the third and the first kinds [6]

$$\Pi(\delta, b, q) = \int_0^\delta \frac{\mathrm{d}\theta}{(1 + b\sin^2\theta)\sqrt{1 - q^2\sin^2\theta}} \tag{3.4}$$

† Some details of obtaining equation (3.3) are given here. Equation (3.1) can be rewritten as

$$\frac{1}{\sqrt{(1-\gamma\phi^2)(\phi_2^2-\phi^2)(\phi^2-\phi_1^2)}}\,\mathrm{d}\phi - \frac{\gamma\phi^2}{\sqrt{(1-\gamma\phi^2)(\phi_2^2-\phi^2)(\phi^2-\phi_1^2)}}\,\mathrm{d}\phi = \sqrt{\mu}\,\mathrm{d}\eta.$$

Setting $y = \phi^{-2}$, the integration of the first term becomes

$$\frac{1}{2\sqrt{\phi_1^2\phi_2^2}}\int_{y_2}^{y}\frac{\mathrm{d}y}{\sqrt{-(y-y_1)(y-y_2)(y-y_3)}}$$

which gives the first term of equation (3.3) according to Greenhill in [6], where $y_1 = \phi_1^{-2}$, $y_2 = \phi_2^{-2}$, $y_3 = \gamma$.

The integration of the second term directly gives the second term of equation (3.3) according to Byrd and Friedman in [6].

$$F(\delta, q) = \int_0^\delta \frac{d\theta}{\sqrt{1 - q^2 \sin^2 \theta}} \tag{3.5}$$

$$q^2 = \frac{\phi_2^2 - \phi_1^2}{\phi_2^2(1 - \gamma\phi_1^2)} \qquad \delta = \arcsin\sqrt{\frac{(1 - \gamma\phi_1^2)(\phi_2^2 - \phi^2)}{(1 - \gamma\phi^2)(\phi_2^2 - \phi_1^2)}} \qquad b = \frac{\gamma(\phi_2^2 - \phi_1^2)}{1 - \gamma\phi_1^2} \tag{3.6}$$

while $\eta_0 = x_0 - vt_0$ is another integration constant which represents the location x_0 of some maximum of the cnoidal wave at time t_0. Parameter q is the modulus of the Jacobian elliptic function and the elliptic integrals given above, and $0 < q^2 < 1$.

When $\omega_1 \ll \omega_0$, from equation (2.13) one has $\gamma \ll 1$, so the second term on the left-hand side of (3.3), which is of the same order as γ, can be neglected. Then an approximate cnoidal wave solution of equation (2.12) can be obtained using (3.6), which is given by

$$\phi(\eta) = \left\{ \left(\frac{1}{\phi_2^2} - \gamma \right) \left[\mathrm{dn}\left(\frac{1}{q}\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0), q \right) \right]^{-2} + \gamma \right\}^{-1/2}. \tag{3.7}$$

The following results are based on equation (3.7). As the period of the Jacobian elliptic function $\mathrm{dn}(x, q)$ is $2K(q)$, where $K(q) = F(\pi/2, q)$, if taking $\delta = \pi/2$ in (3.5), is a complete elliptic integral of the first kind, the condition of periodicity (2.14) leads to

$$\frac{1}{q}\sqrt{\mu(\phi_2^2 - \phi_1^2)}l = 2n_1 K(q) \qquad n_1 = 1, 2, 3, \ldots \tag{3.8}$$

where n_1 is the number of periods of the cnoidal wave contained in the ring. It can be seen from equations (3.7) and (3.8) that the wavelength of the cnoidal wave may be read as l/n_1. In order to apply continuum limits, it is necessary that $l/n_1 \gg a$, therefore $n_1 \ll l/a = N$. The maximum of $\phi^2(\eta)$ is ϕ_2^2 at $\eta = \eta_0 + (n_2/n_1)l$, $n_2 = 1, 2, 3, \ldots, n_1$, and the minimum is ϕ_1^2 at $\eta = \eta_0 + ((n_2/n_1) + (1/2n_1))l$. As a result, using equation (3.8), the amplitude of the cnoidal wave (3.7) can be represented as

$$\phi_a^2 = \phi_{\max}^2 - \phi_{\min}^2 = \phi_2^2 - \phi_1^2 = Bq^2 \tag{3.9}$$

where

$$B = \frac{4n_1^2 K^2(q)}{\mu l^2}. \tag{3.10}$$

The normalization condition for $\phi(\eta)$ yields

$$2n_1[K(q) - (1 - \gamma\phi_2^2)\Pi(b_1, q)] = \frac{\gamma}{q}\sqrt{\mu(\phi_2^2 - \phi_1^2)} \tag{3.11}$$

with $b_1 = -b = -\gamma\phi_2^2 q^2$, where $\Pi(b_1, q) = \Pi(\pi/2, b_1, q)$, if replacing b by b_1 and taking $\delta = \pi/2$ in equation (3.4), is a complete elliptic integral of the third kind.

Introducing equation (3.7) in (2.11) and correcting to the first order in a and the second order in ω_1/ω_0, one can obtain the relative displacement of the self-trapped state

$$u(\eta) = \frac{Aa}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \left\{ \left(\frac{1}{\phi_2^2} - \gamma \right) \left[\mathrm{dn}\left(\frac{1}{q}\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0), q \right) \right]^{-2} + \gamma \right\}^{-1}. \tag{3.12}$$

From equation (2.6) the self-trapped potential well of the electron is given by

$$V(\eta) = -\frac{A^2 a}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \left\{ \left(\frac{1}{\phi_2^2} - \gamma \right) \left[\mathrm{dn}\left(\frac{1}{q}\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0), q \right) \right]^{-2} + \gamma \right\}^{-1}. \tag{3.13}$$

The density of current carried by the cnoidal wave can be obtained from equation (2.4)

$$j(\eta) = ev\phi^2(\eta) = ev\left\{\left(\frac{1}{\phi_2^2} - \gamma\right)\left[\mathrm{dn}\left(\frac{1}{q}\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0), q\right)\right]^{-2} + \gamma\right\}^{-1} \tag{3.14}$$

which is quantized as a result of quantization of v as shown in equation (2.16), where e is the charge of an electron.

From equations (3.9) and (3.12), we get the amplitude of the relative displacement of the self-trapped state

$$u_a = u_{\max} - u_{\min} = \frac{Aa}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)Bq^2. \tag{3.15}$$

The depth of the self-trapped potential well of the electron and the amplitude of the density of current carried by the cnoidal wave are expressed by the following expressions, respectively:

$$V_a = V_{\max} - V_{\min} = \frac{A^2a}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)Bq^2 \tag{3.16}$$

and

$$j_a = j_{\max} - j_{\min} = evBq^2. \tag{3.17}$$

Meanwhile ϕ_1^2 and ϕ_2^2 can be derived from equations (3.6) and (3.8)

$$\phi_{1,2}^2 = \frac{1}{2\gamma}[1 \pm \gamma Bq^2 - \sqrt{(1 + \gamma Bq^2)^2 - 4\gamma B}]. \tag{3.18}$$

Introducing equation (3.18) in (3.2) and combining equations (2.10) and (2.13) lead to the energy of the electron

$$E = \frac{1}{2}mv^2 - \frac{A^2a}{2M\omega_0^2\gamma}[1 - \sqrt{(1 + \gamma Bq^2)^2 - 4\gamma B}] \tag{3.19}$$

where the first term is the kinetic energy of the electron which is quantized as a result of quantization of v, and the second term is the potential energy of the electron in the potential well given by equation (3.13).

There are two limiting cases for the periodic solution (3.7). When $q \to 0$, the solution (3.7) becomes

$$\phi(\eta) = \sqrt{\frac{\lambda}{2\mu}} \tag{3.20}$$

which represents a plane wave. This is the case of a linear limit. Correspondingly, from equations (3.12)–(3.14), we have

$$u(\eta) = \frac{Aa}{M\omega_0^2 l}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \tag{3.21}$$

$$V(\eta) = -\frac{A^2a}{M\omega_0^2 l}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \tag{3.22}$$

and

$$j(\eta) = ev/l. \tag{3.23}$$

Here the normalization condition $l = 2\mu/\lambda$ is used. It is evident that $u_a = V_a = j_a = 0$. The corresponding energy of the electron is

$$E = \frac{1}{2}mv^2 - \frac{A^2a}{M\omega_0^2 l}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right). \tag{3.24}$$

It can be seen from equations (3.22) and (3.24) that the wavefunction (3.20) describes the situation that an electron moves in a constant potential.

When $q \to 1$, from equation (3.6) and (3.8), we arrive at $\phi_1 \to 0$ and $l \to \infty$, i.e. a ring being changed into a chain. As $q \to 1$, the Jacobian elliptic function $\mathrm{dn}(x, q) \to \mathrm{sech}\, x$, so the solution (3.7) is reduced to a soliton solution

$$\phi(\eta) = \left(\gamma \,\mathrm{cosech}^2 \frac{\sqrt{\mu\gamma}}{2n_1} \cosh^2 \frac{\eta - \eta_0}{L_s} + \gamma\right)^{-1/2} \tag{3.25}$$

with the width $L_s = \sqrt{\gamma/\mu}\coth(\sqrt{\mu\gamma}/2n_1)$. This is the case of the most nonlinear limit. The cnoidal waves are intermediary, being situated between plane waves and solitons. The peak of the soliton is $P_s = (1/\sqrt{\gamma})\tanh(\sqrt{\mu\gamma}/2n_1)$, while the energy of the soliton is

$$E = \frac{1}{2}mv^2 - \frac{A^2 a}{2M\omega_0^2\gamma}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)\tanh^2 \frac{\sqrt{\mu\gamma}}{2n_1}. \tag{3.26}$$

Hence, the larger the number n_1 of periods of the cnoidal wave contained in a ring, the wider the width of the corresponding soliton, the lower the peak, the higher the energy and the more unstable the corresponding soliton. This is why we usually take $n_1 = 1$ for polarons. When $n_1 = 1$, equations (3.25) and (3.26) are just the results of a previous paper [5] by the present authors and the corresponding $u(\eta)$, $V(\eta)$ and $j(\eta)$ can be attained from equations (3.12)–(3.14) with the limit $q \to 1$. While u_a and V_a respectively become

$$u_a = u_a^0\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)^2 \frac{1}{f^2(\alpha)} \qquad \text{and} \qquad V_a = V_a^0\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)^2 \frac{1}{f^2(\alpha)} \tag{3.27}$$

where

$$u_a^0 = \frac{mA^2a^2}{4\hbar^2 M^2\omega_0^4} \qquad \text{and} \qquad V_a^0 = \frac{mA^4a^2}{4\hbar^2 M^2\omega_0^4} \tag{3.28}$$

are, respectively, those in the usual MCM [3], and $f(\alpha) = \alpha\coth\alpha$ with $\alpha = \sqrt{\mu\gamma}/2$. j_a becomes

$$j_a = j_a^0\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)\frac{1}{f^2(\alpha)} \tag{3.29}$$

where

$$j_a^0 = \frac{evmA^2a^2}{4\hbar^2 M\omega_0^2}$$

is that in the usual MCM.

3.2. The case of $c < 0$

In this case, the cnoidal wave solution of equation (2.12) is

$$\frac{1}{\sqrt{\phi_2^2 - \phi_1^2}}\mathrm{cn}^{-1}\left(\sqrt{\frac{\phi_2^{-2} - \gamma}{\phi'^{-2} - \gamma}}, q\right) - \frac{\gamma}{\sqrt{\phi_2^2 - \phi_1^2}}\left[\left(\phi_2^2 - \frac{1}{\gamma}\right)\Pi(\delta', b', q') + \frac{1}{\gamma}F(\delta', q')\right]$$
$$= \sqrt{\mu}(\eta - \eta_0') \tag{3.30}$$

where $\mathrm{cn}(x, q')$ is the Jacobian elliptic function of the second kind [6], and

$$q'^2 = \frac{\phi_2^2(1 - \gamma\phi_1^2)}{\phi_2^2 - \phi_1^2} \qquad \delta' = \arcsin\sqrt{\frac{\phi_2^2 - \phi'^2}{\phi_2^2(1 - \gamma\phi'^2)}} \qquad b' = \gamma\phi_2^2. \tag{3.31}$$

The meanings of η_0' and q' are the same as those of η_0 and q as stated above. For the same reason for which equation (3.7) is derived from (3.3), we can arrive at another approximate cnoidal wave solution of (2.12)

$$\phi'(\eta) = \left\{\left(\frac{1}{\phi_2^2} - \gamma\right)[\mathrm{cn}(\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0'), q')]^{-2} + \gamma\right\}^{-1/2}. \tag{3.32}$$

As the period of $\mathrm{cn}^2(x, q')$ is $2K(q')$, the condition of periodicity (2.14) gives

$$\sqrt{\mu(\phi_2^2 - \phi_1^2)}l = 2n_1' K(q') \qquad n_1' = 1, 2, 3, \ldots \tag{3.33}$$

where n_1' is the number of periods of the cnoidal wave with wavelength l/n_1' contained in the ring. The maximum ϕ_2^2 of $\phi'^2(\eta)$ is located at $\eta = \eta_0' + (n_2'/n_1')l$, $n_2' = 1, 2, 3, \ldots, n_1'$, and the minimum zero of $\phi'^2(\eta)$ is at $\eta = \eta_0' + ((n_2'/n_1') + (1/2n_1'))l$. So the amplitude of the cnoidal wave (3.32) is

$$\phi_a'^2 = \phi_{\max}'^2 - \phi_{\min}'^2 = \phi_2^2. \tag{3.34}$$

The normalization condition for $\phi'(\eta)$ yields

$$2n_1'[K(q') - (1 - \gamma\phi_2^2)\Pi(b_1', q')] = \gamma\sqrt{\mu(\phi_2^2 - \phi_1^2)} \tag{3.35}$$

with $b_1' = -b' = -\gamma\phi_2^2$.

By a similar method used in the case of $c > 0$, we obtain the relative displacement of the self-trapped state

$$u'(\eta) = \frac{Aa}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)\left\{\left(\frac{1}{\phi_2^2} - \gamma\right)[\mathrm{cn}(\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0'), q')]^{-2} + \gamma\right\}^{-1} \tag{3.36}$$

the self-trapped potential well of the electron

$$V'(\eta) = -\frac{A^2 a}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right)\left\{\left(\frac{1}{\phi_2^2} - \gamma\right)[\mathrm{cn}(\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0'), q')]^{-2} + \gamma\right\}^{-1} \tag{3.37}$$

and the density of current carried by the cnoidal wave

$$j'(\eta) = ev\phi'^2(\eta) = ev\left\{\left(\frac{1}{\phi_2^2} - \gamma\right)\left[\mathrm{cn}(\sqrt{\mu(\phi_2^2 - \phi_1^2)}(\eta - \eta_0'), q')\right]^{-2} + \gamma\right\}^{-1} \tag{3.38}$$

which is also quantized like $j(\eta)$ of equation (3.14).

From equations (3.34), (3.36)–(3.38), one can respectively obtain the amplitude of the relative displacement of the self-trapped state, the depth of the self-trapped potential well of the electron and the amplitude of the density of current carried by the cnoidal wave

$$u_a' = \frac{Aa\phi_2^2}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \qquad V_a' = \frac{A^2 a\phi_2^2}{M\omega_0^2}\left(1 - \frac{\omega_1^2}{\omega_0^2}\right) \qquad \text{and} \qquad j_a' = ev\phi_2^2. \tag{3.39}$$

Meanwhile, from equations (3.31) and (3.33) ϕ_1^2 and ϕ_2^2 can be expressed as

$$\phi_{1,2}^2 = \frac{1}{2\gamma}[1 \mp \gamma B' - \sqrt{(1 + \gamma B')^2 - 4\gamma B' q'^2}] \tag{3.40}$$

where

$$B' = \frac{4n_1'^2 K^2(q')}{\mu l^2}. \tag{3.41}$$

From equations (2.10), (2.13), (3.2) and (3.40), the energy of the electron can be given by

$$E = \frac{1}{2}mv^2 - \frac{A^2 a}{2M\omega_0^2\gamma}[1 - \sqrt{(1+\gamma B')^2 - 4\gamma B' q'^2}] \tag{3.42}$$

whose two terms have the same meanings as those in equation (3.19).

There are also two limiting cases for the periodic solution (3.32), when $q' \to 0$, $\phi'(\eta) = 0$. This is an extremely trivial solution of equation (2.12) and is meaningless. In fact, when $q'^2 < \frac{1}{2}$, we can see from equation (3.42) that the potential energy of the electron is positive and thereby this kind of state of the electron is unstable.

When $q' \to 1$, $\phi_1 \to 0$ and $l \to \infty$. As $q' \to 1$, the Jacobian elliptic function $\mathrm{cn}(x, q') \to \mathrm{sech}\, x$. Apparently, the discussion for this limiting case is completely similar to that of the case for $c > 0$ and can lead to the same results.

On the other hand, when $\gamma \to 0$, we are able to verify that the periodic solutions (3.7) and (3.32) are equivalent to those of [7].

4. Conclusions

In summary, two different spatially periodic solutions for excitations in the MCM with the dispersion term on a diatomic molecule ring were found by use of the Jacobian elliptic functions of the second and the third kinds. The relative displacement of the self-trapped state, the self-trapped well and energy of the electron, and the density of current carried by excitations were also calculated. Two limits of periodic solutions were discussed. When the moduli of the Jacobian elliptic functions tend to zero, the periodic solution corresponding to $c > 0$ tends to the plane wave solution, and the other one corresponding to $c < 0$ tends to zero. In fact, when the square of the modulus of $\mathrm{cn}(x, q')$ is less than $\frac{1}{2}$, the periodic solution of $c < 0$ is unstable; this is because the potential energy of the electron becomes positive. When the moduli tend to one, both periodic solutions tend to the soliton solution. This is the case of $c = 0$. So the periodic solutions of the model are more universal than a soliton solution. Our results will be useful in the research of the mesoscopic phenomena of small size quantum systems when taking the influences of the Aharonov–Bohm potential into account. Applications of our results to the mesoscopic phenomena will be studied further in a forthcoming paper.

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