中山大学学报 (自然科学版)
第 37卷 第 6期 ACTA SCIENTIARUM NATURALIUM Vol. 37 No. 6
1998年 11月 UNIVERSITATIS SUNYATSENI Nov. 1998

Elliptic Function Waves on a Molecular-Crystal Ring*

Chen Yuan[1] Chen Hao[2]
(1) Department of Physics, Zhongshan University, Guangzhou 510275, China;
2) Department of Physics, South China Normal University)

Abstract An elliptic function wave solution of the molecular-crystal model with the dispersion term on a ring is found. In the limit that the perimeter of the ring tends to infinite, the elliptic function wave solution tends to an improved optical polaron solution of the model on a chain. The lattice displacement of the self-trapped state and the self-trapped well of the electron are calculated.

Keywords elliptic function wave, molecular-crystal model, elliptic function
Classificational number O 471.3

As is now known, an electron (or hole) in the crystal lattice may lower its energy by locally distorting the crystal lattice surrounding it. The self-trapped electron together with its reduced lattice distortion is called the polaron[1]. The possibility of self-trapping in a one dimensional electron-phonon system was first studied by Holstein[2]. Further research on polarons was made by many physicists[3]. In this letter, we consider the molecular-crystal model with the dispersion term on a ring. We find an elliptic function wave solution of the model and give out the lattice displacement of the self-trapped state and the self-trapped well of the electron. These results tends towards those obtained by us in a previous letter[4], when the perimeter of the ring tends towards infinite.

We start from Hamiltonian[5] describing the electrons interacting with lattice optical vibrations through the deformation potential in one dimemsion

$$H=-\frac{\hbar}{2m}\frac{\partial}{\partial x^2}+\sum_{n=1}^{N}V(x-R_n,u_n)+\sum_{n=1}^{N}\left(-\frac{\hbar^2}{2M}\frac{\partial}{\partial u_n^2}+\frac{M}{2}k_0^2u_n^2+\frac{M}{2}k_1^2u_nu_{n+1}\right) \tag{1}$$

where x and m are the electron coordinate and mass respectively; $R_n=na$, u_n and a denote the location and displacement of a molecule at the n-th site and the lattice spacing respectively; $V(x-R_n, u_n)$ is the interaction potential energy between an electron and a molecule; M is the reduced mass of a molecule; N is the number of molecules in the ring; k_0 is the Einstein's frequence, and the k_1^2-proportional term is the so called dispersion term.

Following Holstein[5], we assume the wavefunction Ψ of H is

$$\Psi=\sum_n a_n\Phi_n(x,u_n) \tag{2}$$

* 收稿日期: 1998-04-01 陈渊, 男, 29岁, 博士研究生

Here a_n, which depends on u_n and time t, is the probability amplitude of the electron at the n-th site. $\Omega(x, u_n)$, the local orbit of a molecule, satisfies the eigenequation

$$\left[-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}+V(x-R_n,u_n)\right]\Omega(x-R_n,u_n)=E(u_n)\Omega(x-R_n,u_n) \tag{3}$$

where eigenvalue $E(u_n)$ only depends on the displacement of the molecule at n-th site. Obviously a_n and u_n must satisfy the periodical boundary conditions

$$a_n=a_{n+N},u_n=u_{n+N} \tag{4}$$

Making use of the linear approximation, we has

$$E(u_n)=-Au_n \tag{5}$$

From Schrodinger equation $\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi=H\Psi$, and using the method of Ref. [4], we get following eigenfunction satisfied by a_n with eigenvalue $E(u_1,\cdots,u_N)$

$$\left[\frac{Mk_0^2}{2}\sum_m u_m^2+\frac{Mk_1^2}{2}\sum_m u_m u_{m+1}-Au_n\right]a_n-J(a_{n+1}+a_{a-1})=E(u^1,\cdots u_N)a_n \tag{6}$$

where J is the exchange integral. The normalization condition $\int|\Psi|^2\mathrm{d}x=\sum_{n=1}^{N}|a_n|^2=1$, and the minimal energy condition, $\partial E/\partial u_m=0$, lead to the minimal energy displacement $u_m^{(0)}$ to be

$$u_m^{(0)}=\frac{A}{Mk_0^2}|a_m^{(0)}|^2-\frac{k_1^2}{2k_0^2}(u_{m+1}^{(0)}+u_{m-1}^{(0)}) \tag{7}$$

It is interesting only for the narrow-band, i. e., $\omega_1\ll\omega_0$. In this case, the iterative solution of Eq. (7) is

$$u_m^{(0)}=\frac{A}{Mk_0^2}|a_m^{(0)}|^2-\frac{Ak_1^2}{2Mk_0^4}(a_{m+1}^{(0)}+a_{m-1}^{(0)})+O[(k_1/k_0)^4] \tag{8}$$

Assuming a_n is a smooth function of its lattice-site "argument" n, one can approximate

$$a_{n\pm1}^{(0)}\approx a_n^{(0)}\pm\frac{\mathrm{d}a_n^{(0)}}{\mathrm{d}n}+\frac{1}{2}\frac{\mathrm{d}^2a_n^{(0)}}{\mathrm{d}n^2} \tag{9}$$

Introducing Eqs. (8) and (9) in Eq. (6), We obtain the equation for $a_n^{(0)}$

$$[1-V|a_n^{(0)}|^2]\frac{\mathrm{d}^2a_n^{(0)}}{\mathrm{d}n^2}-Va_n^{(0)}\left[\frac{\mathrm{d}a_n^{(0)}}{\mathrm{d}n}\right]^2+2Ua_n^{(0)}|a_n^{(0)}|^2-Ta_n^{(0)}=0 \tag{10}$$

with

$$T=\frac{X}{J},\quad U=\frac{A^2}{2JMk_0^2}\left(1-\frac{k_1^2}{k_2^2}\right),\quad V=\frac{A^2k_1^2}{JMk_0^4} \tag{11}$$

$$X=\frac{Mk_0^2}{2}\sum_m u_m^{(0)2}+\frac{Mk_1^2}{2}\sum_m u_m^{(0)}u_{m+1}^{(0)}-E(u_1^{(0)},\cdots,u_N^{(0)})-2J \tag{12}$$

Equation (10) is a nonlinear equation, integrating once, we arrive at

$$(1-Va_n^{(0)2})\left[\frac{\mathrm{d}a_n^{(0)}}{\mathrm{d}n}\right]^2=U\left(q_2^2-a_n^{(0)2}\right)\left(a_n^{(0)2}-q_1^2\right) \tag{13}$$

where $q_1^2<a_n^{(0)2}<q_2^2$, $q_1^2+q_2^2=T/U$, $q_1^2q_2^2=c>0$, and c is an integration constant. Eq. (13) has the elliptic function wave solution

$$\frac{1}{\sqrt{c(q_2^2-V)}}\mathrm{dn}^{-1}\left(\sqrt{\frac{q_2^2-V}{a_n^{(0)2}-V}},k\right)-\frac{V}{\sqrt{(1-Vq_1^2)q_2^2}}\left[\left(q_2^2-\frac{1}{V}\right)\Pi(W,b,k)+\frac{1}{V}F(W,k)\right]=U(n-n_0) \tag{14}$$

where n_0 is another integration constant denoting the location of some maximum of the el-

liptic function wave. While $\mathrm{dn}(x,k)$ is the Jacobian elliptic function[6], $\Pi(W,b,k)$ and $F(W,k)$ are the elliptic integrals of the third and the first kinds[6], respectively

$$\Pi(W,b,k)=\int_0^W \frac{\mathrm{d}\theta}{(1+b\sin^2\theta)\sqrt{1-k^2\sin^2\theta}},\ F(W,k)=\int_0^W \frac{\mathrm{d}\theta}{\sqrt{1-k^2\sin^2\theta}},$$
$$k^2=\frac{q_2^2-q_1^2}{q_2^2(1-Vq_1^2)},\ W=\arcsin\sqrt{\frac{(1-Vq_1^2)(q_2^2-a_n^{(0)2})}{(1-Va_n^{(0)2})(q_2^2-q_1^2)}},\ b=\frac{V(q_2^2-q_1^2)}{1-Vq_1^2} \tag{15}$$

Parameter k is the modulus of the Jacobian elliptic function and the elliptic integrals given above and $0<k^2<1$. Since $k_1\ll k_0$, so $V\ll 1$. Then the second term on the left-hand side of Eq. (14), which is order of V, can be neglected and an approximative elliptic function wave solution of Eq. (13) is

$$a_n^{(0)}=\left\{\left(\frac{1}{q_2^2}-V\right)\mathrm{dn}^{-2}\left[\frac{1}{k}\sqrt{U(q_2^2-q_1^2)}(n-n_0),k\right]+V\right\}^{-1/2} \tag{16}$$

Our following results for the lattice displacement of the self-trapped state and the self-trapped well of the electron are based on Eq. (16). Substituting Eq. (16) into Eq. (8) and correcting to the second order in k_1/k_0, one can get the lattice displacement of the self-trapped state

$$u_n^{(0)}=\frac{A}{Mk_0^2}\left(1-\frac{k_1^2}{k_0^2}\right)\left\{\left(\frac{1}{q_2^2}-V\right)\mathrm{dn}^{-2}\left[\frac{1}{k}\sqrt{U(q_2^2-q_1^2)}(n-n_0),k\right]+V\right\}^{-1} \tag{17}$$

and the self-trapped potential well of the electron is given by

$$V(u_n^{(0)})=-\frac{A^2}{Mk_0^2}\left(1-\frac{k_1^2}{k_0^2}\right)\left\{\left(\frac{1}{q_2^2}-V\right)\mathrm{dn}^{-2}\left[\frac{1}{k}\sqrt{U(q_2^2-q_1^2)}(n-n_0),k\right]+V\right\}^{-1} \tag{18}$$

As the period of the Jacobian elliptic function $\mathrm{dn}(x,k)$ is $2K(k)$, where $K(k)=F(\pi/2,k)$, i.e., taking $W=\pi/2$ in Eq. (15), is the complete elliptic integral of the first kind, so the periodical boundary conditions (4) yield

$$\sqrt{U(q_2^2-q_1^2)}N=2m_1kK(k),\ m_1=1,2,3,\cdots \tag{19}$$

where m_1 is the number of the elliptic function waves contained on the ring. The normalization condition yields

$$2[K(k)-(1-Vq_1^2)\Pi(b',k)]=\frac{V}{k}\sqrt{U(q_2^2-q_1^2)} \tag{20}$$

with $b'=-b=-Vq_2^2k^2$, where $\Pi(b',k)=\Pi(\pi/2,b',k)$, i.e., replacing b by b' and taking $W=\pi/2$ in Eq. (15), is the complete elliptic integral of the third kind.

When the perimeter N of the ring tends to infinite, i.e. a ring becoming a chain, from Eqs. (15) and (19), one has $k\to 1$, $q_1\to 0$, and $\mathrm{dn}(x,k)\to\mathrm{sech}\,x$. Therefore Eq. (20) becomes $T=(U/V)\tanh^2(\sqrt{UV}/2m_1)$, and Eq. (16) is recovered to an improved optical polaron solution

$$a_n^{(0)}=\left(V\mathrm{cosech}^2\frac{\sqrt{UV}}{2m}\cosh^2\frac{n-n_0}{L_p}+V\right)^{-1/2} \tag{21}$$

with the width $L_p=a\sqrt{\frac{V}{U}}\coth\frac{\sqrt{UV}}{2m_1}$. When $m_1=1$, the solution (21) is most stable, and Eq. (20) coincides with the Eq. (21) of Ref. [4]. Corresponding $u_n^{(0)}$, $V(u_n^{(0)})$ can be resulted from Eqs. (17) and (18), while also coincide with the results of Ref. [4] when $m_1=1$. On the other hand, when $V\to 0$, we can show that the elliptic function wave solution (16) is equivalent to that of Ref. [7].

In summary, we consider the elliptic function wave solution of the molecular- crystal model with the dispersion term on a ring. Since the elliptic function wave solution tends to the improved optical polaron solution when a ring changes into a chain, so the elliptic function wave solution of the model is more general than the improved optical polaron solution and helpful in studying the small size quantum systems.

References

1 Castro Neto A H, Caldeira A O. Alternative approach to the dynamics of polarons in one dimension. Phys Rev (B), 1992, 46: 8858

2 Holstein T. Studies of polaron motion. Ⅰ. The molecular crystal model. Ann Phys, 1959, 8: 325

3 Campbell D K, Bishop A R, Fesser K. Polarons in quasi-one-dimensional systems. Phys Rev (B), 1982, 26: 6862

4 Chen H, Chen Y. On optical polarons in one dimensional molecular-crystal chains. Chin Phys Lett, 1996, 13: 617

5 Holstein T. Studies of polaron. Ⅱ. The "small" polaron. Ann Phys, 1959, 8: 343

6 Greenhill A G. The applications of elliptic functions. New York: Dover Pub, 1959. 30- 42

7 Smondyrev M A, Vansant P, Peeters F M, et al. Nonlinear schrodinger equation on a circle. Phys Rev (B), 1995, 52: 11231

分子晶体环上的椭圆函数波

陈　渊*　陈　浩

摘　要　得到了环上的有色散项的分子晶体模型的椭圆函数波解.当环的周长趋于无穷大时,模型的椭圆函数波解回复于一维链的改进光学极化子解.计算了模型中自陷态的晶格位移和电子的自陷阱.

关键词　椭圆函数波解,分子晶体模型,椭圆函数波

分类号　O 471.3

* 中山大学物理学系,广州 510275