Exact solutions for a charged particle in a uniform electric field with alternating site energies: perturbation theory

1991 J. Phys.: Condens. Matter 3 6021

(http://iopscience.iop.org/0953-8984/3/32/009)

J. Phys.: Condens. Matter 3 (1991) 6021–6032. Printed in the UK

Exact solutions for a charged particle in a uniform electric field with alternating site energies: perturbation theory

Zhao Xian-Geng
Institute of Applied Physics and Computational Mathematics, PO Box 8009, Beijing 100088, People's Republic of China

Received 8 November 1990, in final form 29 April 1991

Abstract. The energy spectrum and the eigenvectors of a charged particle in a uniform electric field with alternating site energies are studied for infinite systems. For the case of large energy mismatch, exact solutions are presented by using perturbation theory, from which it is found that the spectrum is that of two interspaced Stark ladders. The character of these Stark ladders is that the difference of the ratio of the energy and the field between two energies on a same rung is an even number.

1. Introduction

This paper addresses the energy spectrum and the eigenvectors of a charged particle hopping on an infinite linear chain under the action of a uniform electric field in the direction of the chain, and with the approximation of nearest-neighbour intersite overlap integrals V. The character of this model is such that the site energies alternate between the values $\varepsilon \pm 2\Delta$ ($\Delta > 0$). Such a system is relevant to a variety of fields, including that of exciton states in molecular crystals [1, 2], electron localization in superlattices [3, 4], and the localized properties of excitations in ferroelectric materials [5–7]. The Hamiltonian considered here is thus

$$H = 2\Delta \sum_m (-1)^m |m\rangle\langle m| + V \sum_m (|m\rangle\langle m+1| + |m+1\rangle\langle m|) - eE_0 a \sum_m m|m\rangle\langle m| \tag{1.1}$$

where $|m\rangle$ represents a Wannier state localized on lattice site m, e is the charge on the particle, a is the lattice constant, and E_0 is the external electric field. Here, V has been assumed to be positive for simplicity, and the off-diagonal elements of the position operator $\hat{X}$ in the Wannier basis have been neglected, i.e., we have assumed that

$$\int_{-\infty}^{\infty} \mathrm{d}X \int_{-\infty}^{\infty} \mathrm{d}X' \, \langle m|X\rangle\langle X|eE_0\hat{X}|X'\rangle\langle X'|n\rangle = eE_0 am\delta_{m,n}. \tag{1.2}$$

Equation (1.1) can be rewritten as.

$$H = H_0 + H_e \tag{1.3}$$

$$H_0 = 2\Delta \sum_m (-1)^m |m\rangle\langle m| + V \sum_m (|m\rangle\langle m+1| + |m+1\rangle\langle m|) \tag{1.4}$$

$$H_e = -eE_0 a \sum_m m|m\rangle\langle m|. \tag{1.5}$$

Here, H_0 is the field-free Hamiltonian, whose probability self-propagators have been studied by Kovanis and Kenkre [8]. When the external field is present this model, in general, cannot be solved analytically. However, we find, for the case when the chain disturbance is large, i.e. for $\Delta \gg V$, the problem can be solved exactly by using perturbation theory (PT). In this paper, we only consider this case.

The rest of this paper is set out as follows. In section 2, we present our solutions to H_0 in k-space. Then, by expressing the eigenvectors to (1.3) as a linear superposition of the field-free eigenvectors, the exact results for the energy spectrum and the eigenvectors are obtained by using PT (section 3), from which it is found that the spectrum is that of two interspaced Stark ladders. Finally, concluding remarks are given in section 4.

2. Explicit solutions for the field-free system in k space

By expressing the eigenvector $|\varphi\rangle$ of H_0 as a linear superposition of Wannier states $|m\rangle$,

$$|\varphi\rangle = \sum_m C_m |m\rangle \tag{2.1}$$

one obtains the following equations for the amplitudes C_m as

$$\mathscr{E}_0 C_{2m} = 2\Delta C_{2m} + V(C_{2m+1} + C_{2m-1}) \tag{2.2}$$

$$\mathscr{E}_0 C_{2m+1} = -2\Delta C_{2m+1} + V(C_{2m+2} + C_{2m}) \tag{2.3}$$

where $\mathscr{E}_0$ is the energy belonging to H_0. These equations can be diagonalized by setting

$$C_{2m} = f(k)\,\mathrm{e}^{\mathrm{i}km} \qquad 0 \leqslant k < 2\pi \tag{2.4}$$

$$C_{2m+1} = g(k)\,\mathrm{e}^{\mathrm{i}km} \qquad 0 \leqslant k < 2\pi \tag{2.5}$$

where k is the (dimensionless) wavevector. We get

$$(\mathscr{E}_0 - 2\Delta)f(k) - 2V\,\mathrm{e}^{-\mathrm{i}(k/2)}\cos(k/2)g(k) = 0 \tag{2.6}$$

$$-2V\,\mathrm{e}^{\mathrm{i}(k/2)}\cos(k/2)f(k) + (\mathscr{E}_0 + 2\Delta)g(k) = 0. \tag{2.7}$$

The eigenvalue equation determined by (2.6) and (2.7) is

$$(\mathscr{E}_0 - 2\Delta)(\mathscr{E}_0 + 2\Delta) - (2V\cos(k/2))^2 = 0 \tag{2.8}$$

with solutions

$$\mathscr{E}_0^{\pm}(k) = \pm 2[\Delta^2 + (V\cos(k/2))^2]^{1/2}. \tag{2.9}$$

Thus, the eigenvectors of H_0 become

$$|\varphi(k)\rangle_{\pm} = \sum_{m=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}km}(f_{\pm}(k)|2m\rangle + g_{\pm}(k)|2m+1\rangle) \tag{2.10}$$

with the relation

$$f_\pm(k) = [2V\cos(k/2)\,\mathrm{e}^{-\mathrm{i}(k/2)}/(\mathscr{E}_0^\pm(k) - 2\Delta)]g_\pm(k). \tag{2.11}$$

$g_\pm(k)$ can be determined by the normalization of the eigenvectors $|\varphi(k)\rangle_\pm$, which gives

$$g_\pm(k) = \{1 + [2V\cos(k/2)/(\mathscr{E}_0^\pm(k) - 2\Delta)]^2\}^{-1/2}. \tag{2.12}$$

From (2.9)–(2.12), it is easily shown that the following formulae hold:

$$|f_\pm(k)|^2 + |g_\pm(k)|^2 = 1 \qquad f_\pm^*(k)f_\mp(k) + g_\pm^*(k)g_\mp(k) = 0 \tag{2.13}$$

$$_\pm\langle\varphi(k)|\varphi(k')\rangle_\pm = \delta(k-k') \qquad _\pm\langle\varphi(k)|\varphi(k')\rangle_\mp = 0. \tag{2.14}$$

3. Exact solutions of H for the case $\Delta \gg V$

Let eigenvector $|\psi\rangle$ of H be of the form

$$|\psi\rangle = \int_0^{2\pi} \mathrm{d}k\,(a(k)|\varphi(k)\rangle_+ + b(k)|\varphi(k)\rangle_-) \tag{3.1}$$

and using (1.3)–(1.5), we obtain the following equation for the amplitudes $a(k)$ and $b(k)$

$$\begin{aligned}\mathscr{E}\int_0^{2\pi} \mathrm{d}k\,(a(k)|\varphi(k)\rangle_+ + b(k)|\varphi(k)\rangle_-)\\ = \int_0^{2\pi}\mathrm{d}k\,(\mathscr{E}_0^+(k)a(k)|\varphi(k)\rangle_+ + \mathscr{E}_0^-(k)b(k)|\varphi(k)\rangle_-)\\ - eE_0a\int_0^{2\pi}\mathrm{d}k\left(a(k)\sum_m m|m\rangle\langle m|\varphi(k)\rangle_+ + b(k)\sum_m m|m\rangle\langle m|\varphi(k)\rangle_-\right)\end{aligned} \tag{3.2}$$

where $\mathscr{E}$ is the energy belonging to H. By multiplying $_+\langle\varphi(k)|$ on both sides of (3.2), and noticing that from (2.14), we have

$$\begin{aligned}\mathscr{E}a(k) = \mathscr{E}_0^+(k)a(k) - eE_0a\int_0^{2\pi}\mathrm{d}k'\,a(k')\sum_m m\,_+\langle\varphi(k)|m\rangle\langle m|\varphi(k')\rangle_+\\ - eE_0a\int_0^{2\pi}\mathrm{d}k'\,b(k')\sum_m m\,_+\langle\varphi(k)|m\rangle\langle m|\varphi(k')\rangle_-.\end{aligned} \tag{3.3}$$

Substituting (2.10) into (3.3), we find (see appendix A)

$$(\mathrm{d}/\mathrm{d}k)a(k) = \mathrm{i}[(\mathscr{E} + eaE_0 - \mathscr{E}_0^+(k))/2eaE_0]a(k) - G_{+-}(k)b(k) \tag{3.4}$$

with

$$G_{+-}(k) = g_+(k)g_-(k)\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k) - 2\Delta}\frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{2V\cos(k/2)}{\mathscr{E}_0^-(k) - 2\Delta}\right). \tag{3.5}$$

Similarly, by multiplying $_-\langle\varphi(k)|$ on both sides of (3.2), we get

$$(\mathrm{d}/\mathrm{d}k)b(k) = \mathrm{i}[(\mathscr{E} + eaE_0 - \mathscr{E}_0^-(k))/2eaE_0]b(k) + G_{+-}(k)a(k). \tag{3.6}$$

Noticing that from (2.9) $\mathscr{E}_0^+(k) = -\mathscr{E}_0^-(k)$, and by introducing

$$a(k) = \mathrm{e}^{\mathrm{i}(\alpha(k)+\beta(k))} A(k) \qquad b(k) = \mathrm{e}^{\mathrm{i}(\alpha(k)-\beta(k))} B(k) \tag{3.7}$$

where

$$\alpha(k) = \frac{\mathscr{E} + eaE_0}{2eaE_0} k \qquad \beta(k) = \frac{1}{2eaE_0} \int_0^k \mathrm{d}k' \, \mathscr{E}_0^-(k'). \tag{3.8}$$

Equations (3.4) and (3.6) reduce to

$$(\mathrm{d}/\mathrm{d}k)A(k) = -G_{+-}(k)\,\mathrm{e}^{-2\mathrm{i}\beta(k)}\,B(k) \tag{3.9}$$

$$(\mathrm{d}/\mathrm{d}k)B(k) = G_{+-}(k)\,\mathrm{e}^{2\mathrm{i}\beta(k)}\,A(k). \tag{3.10}$$

Equations (3.9) and (3.10) can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}k}\begin{pmatrix} A(k) \\ B(k) \end{pmatrix} = -\mathrm{i}G_{+-}(k)[-\sin(2\beta(k))\sigma_x + \cos(2\beta(k))\sigma_y]\begin{pmatrix} A(k) \\ B(k) \end{pmatrix} \tag{3.11}$$

where σ_x and σ_y (as well as σ_z, used below) are the Pauli matrices, whose explicit forms are [9]

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.12}$$

On introducing

$$R(k) = \begin{pmatrix} A(k) \\ B(k) \end{pmatrix} \tag{3.13}$$

$$S(k) = X(k)\sigma_x + Y(k)\sigma_y \tag{3.14}$$

$$X(k) = -G_{+-}(k)\sin(2\beta(k)) \qquad Y(k) = G_{+-}(k)\cos(2\beta(k)) \tag{3.15}$$

equation (3.11) reduces to

$$(\mathrm{d}/\mathrm{d}k)R(k) = -\mathrm{i}S(k)R(k) \tag{3.16}$$

or equivalently

$$R(k) = R(0) - \mathrm{i}\int_0^k \mathrm{d}k_1\, S(k_1)R(k_1). \tag{3.17}$$

Noticing that from (3.14) and (3.15), by using the well-known properties of the Pauli matrices, i.e., $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$, $\sigma_x\sigma_y = \mathrm{i}\sigma_z$, $\sigma_y\sigma_z = \mathrm{i}\sigma_x$ and $\sigma_z\sigma_x = \mathrm{i}\sigma_y$, we find

$$|S(k)| = (X^2(k) + Y^2(k))^{1/2} = |G_{+-}(k)|. \tag{3.18}$$

Substituting (2.9) and (2.12) into (3.5), we have

$$G_{+-}(k) = \left\{\left(\frac{V}{\Delta}\sin\frac{k}{2}\right)\Big/4\left[1 + \left(\frac{V}{\Delta}\cos\frac{k}{2}\right)^2\right]\right\} \times \left[\!\left[1 - \left(\frac{V}{\Delta}\cos\frac{k}{2}\right)^2 \Big/ \left[1 + \left(\frac{V}{\Delta}\cos\frac{k}{2}\right)^2\right]^{1/2} \left\{1 + \left[1 + \left(\frac{V}{\Delta}\cos\frac{k}{2}\right)^2\right]^{1/2}\right\}\right]\!\right]. \tag{3.19}$$

As indicated in section 1, we are interested in the case of $(V/\Delta) \ll 1$. This, because of (3.19), makes

$$\left| \int_0^k \mathrm{d}k_1\, S(k_1)R(k_1) \right| \ll |R(0)| \tag{3.20}$$

Therefore (3.17) can be solved by using PT. As a result, we obtain

$$R(k) = \sum_{m=0}^{\infty} U^{(m)}_{(k,0)} R(0) \tag{3.21}$$

where

$$U^{(0)}_{(k,0)} = 1 \tag{3.22}$$

$$U^{(m)}_{(k,0)} = (-\mathrm{i})^m \int_0^k \mathrm{d}k_1 \int_0^k \mathrm{d}k_2 \ldots \int_0^k \mathrm{d}k_m\, \theta(k_1 - k_2)\theta(k_2 - k_3) \times \ldots \theta(k_{m-1} - k_m) S(k_1)S(k_2)\ldots S(k_m) \tag{3.23}$$

$$\theta(k) = \begin{cases} 1 & k > 0 \\ 0 & k < 0. \end{cases} \tag{3.24}$$

It is easily shown that (see appendix B)

$$S(k_1)S(k_2)\ldots S(k_m) = \begin{cases} X(k_1k_2\ldots k_m) + \mathrm{i}Y(k_1k_2\ldots k_m)\sigma_z & \text{if } m = 2l \\ X(k_1k_2\ldots k_m)\sigma_x + Y(k_1k_2\ldots k_m)\sigma_y & \text{if } m = 2l+1 \end{cases} \tag{3.25}$$

$$X(k_1k_2\ldots k_m) = X(k_1k_2\ldots k_{m-1})X(k_m) + Y(k_1k_2\ldots k_{m-1})Y(k_m) \quad (m \geqslant 2) \tag{3.26}$$

$$Y(k_1k_2\ldots k_m) = X(k_1k_2\ldots k_{m-1})Y(k_m) - Y(k_1k_2\ldots k_{m-1})X(k_m) \quad (m \geqslant 2). \tag{3.27}$$

Defining

$$U_x^{(2m)}(k,0) = (-1)^m \int_0^k \mathrm{d}k_1 \int_0^k \mathrm{d}k_2 \ldots \int_0^k \mathrm{d}k_{2m}\, \theta(k_1 - k_2)\theta(k_2 - k_3) \times \ldots \theta(k_{2m-1} - k_{2m}) X(k_1k_2\ldots k_{2m}) \tag{3.28}$$

$$U_y^{(2m)}(k,0) = (-1)^m \int_0^k \mathrm{d}k_1 \int_0^k \mathrm{d}k_2 \ldots \int_0^k \mathrm{d}k_{2m}\, \theta(k_1 - k_2)\theta(k_2 - k_3) \times \ldots \theta(k_{2m-1} - k_{2m}) Y(k_1k_2\ldots k_{2m}) \tag{3.29}$$

$$U_x^{(2m+1)}(k,0) = (-1)^{m+1} \int_0^k \mathrm{d}k_1 \int_0^k \mathrm{d}k_2 \ldots \int_0^k \mathrm{d}k_{2m+1}\, \theta(k_1 - k_2)\theta(k_2 - k_3) \times \ldots \theta(k_{2m} - k_{2m+1}) X(k_1k_2\ldots k_{2m+1}) \tag{3.30}$$

$$U_y^{(2m+1)}(k,0) = (-1)^{m+1} \int_0^k \mathrm{d}k_1 \int_0^k \mathrm{d}k_2 \ldots \int_0^k \mathrm{d}k_{2m+1}\, \theta(k_1 - k_2)\theta(k_2 - k_3) \times \ldots \theta(k_{2m} - k_{2m+1}) Y(k_1k_2\ldots k_{2m+1}) \tag{3.31}$$

$$U_x^{(0)}(k,0) = 1 \qquad U_y^{(0)}(k,0) = 0 \tag{3.32}$$

we find

$$\sum_{m=0}^{\infty} U^{(m)}(k,0) = \sum_{m=0}^{\infty} U_x^{(2m)}(k,0) + \mathrm{i}\sigma_z \sum_{m=0}^{\infty} U_y^{(2m)}(k,0) + \mathrm{i}\sigma_x \sum_{m=0}^{\infty} U_x^{(2m+1)}(k,0) + \mathrm{i}\sigma_y \sum_{m=0}^{\infty} U_y^{(2m+1)}(k,0). \tag{3.33}$$

From (3.7), (3.8), (3.13) and (3.21), we have

$$\begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \mathrm{e}^{\mathrm{i}\alpha(k)} \begin{pmatrix} \mathrm{e}^{\mathrm{i}\beta(k)} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\beta(k)} \end{pmatrix} \sum_{m=0}^{\infty} U^{(m)}(k,0) R(0) \tag{3.34}$$

$$R(0) = \begin{pmatrix} A(0) \\ B(0) \end{pmatrix} = \begin{pmatrix} a(0) \\ b(0) \end{pmatrix}. \tag{3.35}$$

Note that from (2.9)–(2.12), $\mathscr{E}_0^{\pm}(k+2\pi) = \mathscr{E}_0^{\pm}(k)$, $f_{\pm}(k+2\pi) = f_{\pm}(k)$, $g_{\pm}(k+2\pi) = g_{\pm}(k)$ and $|\varphi(k+2\pi)\rangle_{\pm} = |\varphi(k)\rangle_{\pm}$. Thus, we have $a(0) = a(2\pi)$ and $b(0) = b(2\pi)$ because of $a(k) = {}_{+}\langle\varphi(k)|\psi\rangle$ and $b(k) = {}_{-}\langle\varphi(k)|\psi\rangle$. This leads to the following equation:

$$\begin{pmatrix} a(0) \\ b(0) \end{pmatrix} = \mathrm{e}^{\mathrm{i}\alpha(2\pi)} \begin{pmatrix} \mathrm{e}^{\mathrm{i}\beta(2\pi)} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\beta(2\pi)} \end{pmatrix} \sum_{m=0}^{\infty} U_{(2\pi,0)}^{(m)} \begin{pmatrix} a(0) \\ b(0) \end{pmatrix}. \tag{3.36}$$

The eigenvalue equation determined by (3.36) is

$$\det\left[\begin{pmatrix} \mathrm{e}^{\mathrm{i}\beta(2\pi)} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\beta(2\pi)} \end{pmatrix} \sum_{m=0}^{\infty} U_{(2\pi,0)}^{(m)} - \mathrm{e}^{-\mathrm{i}\alpha(2\pi)}\right] = 0 \tag{3.37}$$

with solutions (see appendix C)

$$\mathscr{E}_n^{\pm} = (2n-1)eaE_0 \pm (eaE_0/\pi)\phi(2\pi,0) \qquad (n = \text{integer}) \tag{3.38}$$

where

$$\phi(2\pi,0) = \cos^{-1}\left(\cos\beta(2\pi) \sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0) - \sin\beta(2\pi) \sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0)\right). \tag{3.39}$$

Corresponding to $\mathscr{E}_n^{\pm}$, the solutions for $a_{\pm}(0)$ and $b_{\pm}(0)$ determined by both (3.36) and the normalization of the eigenvectors $|\psi\rangle_{\pm}$ are

$$a_{\pm}(0) = \frac{1}{2\sqrt{\pi}}\left\{\left[\left(\sum_{m=0}^{\infty} U_x^{(2m+1)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m+1)}(2\pi,0)\right)^2\right] \times \left(1 - \cos(\alpha_{\pm}(2\pi)+\beta(2\pi)) \sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0) + \sin(\alpha_{\pm}(2\pi)+\beta(2\pi)) \sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0)\right)^{-1}\right\}^{1/2} \tag{3.40}$$

$$b_\pm(0) = \left(\sum_{m=0}^{\infty} U_y^{(2m+1)}(2\pi, 0) + \mathrm{i} \sum_{m=0}^{\infty} U_x^{(2m+1)}(2\pi, 0)\right)^{-1} \times \left[\mathrm{e}^{-\mathrm{i}(\alpha_\pm(2\pi)+\beta(2\pi))} - \left(\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi, 0) + \mathrm{i} \sum_{m=0}^{\infty} U_y^{(2m)}(2\pi, 0)\right)\right] a_\pm(0) \tag{3.41}$$

where

$$\alpha_\pm(2\pi) = [(\mathscr{E}_n^\pm + eaE_0)/eaE_0]\pi. \tag{3.42}$$

From (3.1), (3.4) and (3.35), we obtain the final results for the eigenvectors

$$|\psi\rangle_\pm = \int_0^{2\pi} \mathrm{d}k\, (a_\pm(k)|\varphi(k)\rangle_+ + b_\pm(k)|\varphi(k)\rangle_-) \tag{3.43}$$

with

$$\begin{pmatrix} a_\pm(k) \\ b_\pm(k) \end{pmatrix} = \mathrm{e}^{\mathrm{i}\alpha_\pm(k)} \begin{pmatrix} \mathrm{e}^{\mathrm{i}\beta(k)} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\beta(k)} \end{pmatrix} \sum_{m=0}^{\infty} U^{(m)}(k, 0) \begin{pmatrix} a_\pm(0) \\ b_\pm(0) \end{pmatrix} \tag{3.44}$$

where

$$\alpha_\pm(k) = [(\mathscr{E}_n^\pm + eaE_0)/2eaE_0]k. \tag{3.45}$$

It is straightforward to check the orthogonality conditions, i.e.,

$$_\pm\langle\psi|\psi\rangle_\pm = 1 \qquad _\pm\langle\psi|\psi\rangle_\mp = 0. \tag{3.46}$$

4. Concluding remarks

It can be clearly seen from (3.38) that the energy spectrum for our model (1.3) is that of two interspaced Stark ladders. This is consistent with many theoretical results about the existence of Wannier–Stark localization in solids for a charged particle under the influence of a uniform electric field [10–12].

What we find quite interesting is the fact that the value of $(\mathscr{E}_n^\pm - \mathscr{E}_{n'}^\mp)/eaE_0$ is an even number, i.e., $(\mathscr{E}_n^\pm - \mathscr{E}_{n'}^\mp)/eaE_0 = 2(n - n')$. In other words, the value of $(\mathscr{E}_n^\pm - \mathscr{E}_{n'}^\mp)/eaE_0$ cannot be an odd number. This forbidden effect is different from the two-band model of Fukuyama *et al* [13] where the value of $(\mathscr{E}_n^\pm - \mathscr{E}_{n'}^\pm)/eaE_0$ can be an even or an odd number.

In principle, our results (3.38)–(3.46) can hold exactly for the case of $(V/\Delta) \ll 1$. However, this means that one needs to do an infinite number of integrals, which, obviously, is impossible. Therefore, in practice, we have to make further approximations up to the required orders. For example, as the zero order of the PT, from (3.32) and (3.39) we get

$$\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi, 0) = U_x^{(0)}(2\pi, 0) = 1 \qquad \sum_{m=0}^{\infty} U_y^{(2m)}(2\pi, 0) = U_y^{(0)}(2\pi, 0) = 0. \tag{4.1}$$

This leads to

$$\phi(2\pi, 0) = \beta(2\pi) \tag{4.2}$$

where

$$\beta(2\pi) = \frac{1}{2eaE_0}\int_0^{2\pi} \mathrm{d}k\, \mathscr{E}_0^-(k). \tag{4.3}$$

Substituting (2.9) into (4.3) and completing this integral yields

$$\beta(2\pi) = -(4/eaE_0)(\Delta^2 + V^2)^{1/2}\mathrm{E}(\pi/2, \gamma) \tag{4.4}$$

where $\mathrm{E}(\pi/2, \gamma)$ is the complete elliptic integral of the second kind [14], and γ is the modulus defined through

$$\gamma^2 = V^2/(\Delta^2 + V^2). \tag{4.5}$$

Substituting (4.2) and (4.4) into (3.38), we obtain the spectrum

$$\mathscr{E}_n^{\pm} = (2n-1)eaE_0 \pm (4/\pi)(\Delta^2 + V^2)^{1/2}\,\mathrm{E}(\pi/2, \gamma). \tag{4.6}$$

If we use the identity [15]

$$\mathrm{E}\left(\frac{\pi}{2}, \gamma\right) = \frac{\pi}{2}\mathrm{F}(-\tfrac{1}{2}, \tfrac{1}{2}; 1; \gamma^2) = \frac{\pi}{2}\frac{\Gamma(1)}{\Gamma(-\frac{1}{2})\Gamma(\frac{1}{2})}\sum_{m=0}^{\infty}\frac{\Gamma(m-\frac{1}{2})\Gamma(m+\frac{1}{2})}{\Gamma(m+1)}\frac{\gamma^{2m}}{m!} \tag{4.7}$$

where F and Γ are, respectively, the hypergeometric function and the gamma function, the role of alternating site energies in the spectrum can be explicitly found from (4.5)–(4.7), whose notable character is the fact that the enhancement of chain disturbance will give rise to an increase in the energy gap.

Another character for our general results (3.38)–(3.46) is that, compared to Movaghar's results [16] where the Stark regime, in semiconductor superlattice structures, will appear for greater values of the external field E_0, our conclusion about the existence of Wannier–Stark localization can occur for a quite large range of the values of a (1–100 Å) and E_0 (0–10^8 V m^{-1}), because there is no special confinement to these parameters in our model. In fact, the above typical values are in agreement with many experimental results [13, 17–23].

Finally, we should like to indicate that since the eigenvectors for our model have been obtained here, it is possible to calculate other physical quantities up to any order of PT.

Acknowledgments

The author is grateful to Professors S G Chen, X W Zhang and W X Zhang for valuable conversations.

Appendix A

Substituting (2.10) into (3.3), we have

$$\begin{aligned}(\mathscr{E} - \mathscr{E}_0^{+}(k))a(k) = {}& -eaE_0\int_0^{2\pi} \mathrm{d}k'\, a(k') \\ & \times \sum_m \mathrm{e}^{\mathrm{i}(k'-k)m}[2mf_+^*(k)f_+(k') + (2m+1)g_+^*(k)g_+(k')] \\ & - eaE_0\int_0^{2\pi} \mathrm{d}k'\, b(k') \\ & \times \sum_m \mathrm{e}^{\mathrm{i}(k'-k)m}[2mf_+^*(k)f_-(k') + (2m+1)g_+^*(k)g_-(k')]\end{aligned}$$

$$= 2eaE_0\,\mathrm{i}\int_0^{2\pi} \mathrm{d}k'\, a(k')(f_+^*(k)f_+(k') + g_+^*(k)g_+(k'))\frac{\partial}{\partial k'}\sum_m \mathrm{e}^{\mathrm{i}(k'-k)m}$$

$$+ 2eaE_0\,\mathrm{i}\int_0^{2\pi} \mathrm{d}k'\, b(k')(f_+^*(k)f_-(k') + g_+^*(k)g_-(k'))\frac{\partial}{\partial k'}\sum_m \mathrm{e}^{\mathrm{i}(k'-k)m}$$

$$- eaE_0\int_0^{2\pi} \mathrm{d}k'\,(a(k')g_+^*(k)g_+(k') + b(k')g_+^*(k)g_-(k'))\sum_m \mathrm{e}^{\mathrm{i}(k'-k)m}$$

$$= 2eaE_0\,\mathrm{i}\int_0^{2\pi} \mathrm{d}k'\, a(k')(f_+^*(k)f_+(k') + g_+^*(k)g_+(k'))\frac{\partial}{\partial k'}\delta(k-k')$$

$$+ 2eaE_0\,\mathrm{i}\int_0^{2\pi} \mathrm{d}k'\, b(k')(f_+^*(k)f_-(k') + g_+^*(k)g_-(k'))\frac{\partial}{\partial k'}\delta(k-k')$$

$$- eaE_0\int_0^{2\pi} \mathrm{d}k'(a(k')g_+^*(k)g_+(k') + b(k')g_+^*(k)g_-(k'))\delta(k-k')$$

$$= 2eaE_0\,\mathrm{i}f_+^*(k)\int_0^{2\pi} \mathrm{d}k'(a(k')f_+(k') + b(k')f_-(k'))\frac{\partial}{\partial k'}\delta(k-k')$$

$$+ 2eaE_0\,\mathrm{i}g_+^*(k)\int_0^{2\pi} \mathrm{d}k'(a(k')g_+(k') + b(k')g_-(k'))\frac{\partial}{\partial k'}\delta(k-k')$$

$$- eaE_0(a(k)|g_+(k)|^2 + b(k)g_+^*(k)g_-(k)). \tag{A1}$$

By successive integrations by parts for the first two integrals, and the use of the facts that $f_\pm(0) = f_\pm(2\pi)$, $g_\pm(0) = g_\pm(2\pi)$, $a(0) = a(2\pi)$ and $b(0) = b(2\pi)$, we find that

$$(\mathscr{E} - \mathscr{E}_0^+(k))a(k) = -2eaE_0\,\mathrm{i}[f_+^*(k)(\mathrm{d}/\mathrm{d}k)(a(k)f_+(k) + b(k)f_-(k))$$
$$+ g_+^*(k)(\mathrm{d}/\mathrm{d}k)(a(k)g_+(k) + b(k)g_-(k))]$$
$$- eaE_0(a(k)|g_+(k)|^2 + b(k)g_+^*(k)g_-(k)). \tag{A2}$$

Using (2.13), equation (A2) becomes

$$(\mathscr{E} - \mathscr{E}_0^+(k))a(k) = -2eaE_0\,\mathrm{i}(\mathrm{d}/\mathrm{d}k)a(k) - eaE_0(a(k)|g_+(k)|^2 + b(k)g_+^*(k)g_-(k))$$
$$- 2eaE_0\,\mathrm{i}a(k)[f_+^*(k)(\mathrm{d}/\mathrm{d}k)f_+(k) + g_+^*(k)(\mathrm{d}/\mathrm{d}k)g_+(k)]$$
$$- 2eaE_0\,\mathrm{i}b(k)[f_+^*(k)(\mathrm{d}/\mathrm{d}k)f_-(k) + g_+^*(k)(\mathrm{d}/\mathrm{d}k)g_-(k)]. \tag{A3}$$

Noticing that from (2.11) and (2.12), one has $g_\pm^*(k) = g_\pm(k)$ and

$$\frac{\mathrm{d}}{\mathrm{d}k}f_\pm(k) = -\frac{\mathrm{i}}{2}f_\pm(k) + \mathrm{e}^{-\mathrm{i}(k/2)}\frac{\mathrm{d}}{\mathrm{d}k}\left(\frac{2V\cos(k/2)}{\mathscr{E}_0^\pm(k) - 2\Delta}g_\pm(k)\right). \tag{A4}$$

Therefore (A3) reduces to

$$(\mathscr{E} - \mathscr{E}_0^+(k))a(k) = -2eaE_0\,\mathrm{i}(\mathrm{d}/\mathrm{d}k)a(k) - eaE_0(a(k)g_+^2(k) + b(k)g_+(k)g_-(k))$$
$$- eaE_0\left(a(k)|f_+(k)|^2 + b(k)\frac{(2V\cos(k/2))^2}{(\mathscr{E}_0^+(k) - 2\Delta)(\mathscr{E}_0^-(k) - 2\Delta)}g_+(k)g_-(k)\right)$$

$$- 2eaE_0\, \mathrm{i}a(k)\Big[\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta} g_+(k)\frac{\mathrm{d}}{\mathrm{d}k}\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta} g_+(k)\Big) + g_+(k)\frac{\mathrm{d}}{\mathrm{d}k} g_+(k)\Big] - 2eaE_0\, \mathrm{i}b(k)\Big[\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta} g_+(k)\frac{\mathrm{d}}{\mathrm{d}k} \times \Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^-(k)-2\Delta} g_-(k)\Big) + g_+(k)\frac{\mathrm{d}}{\mathrm{d}k} g_-(k)\Big]. \tag{A5}$$

Since from (2.9) and (2.12), we have

$$g_+^2(k)\Big[1+\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta}\Big)^2\Big]=1 \qquad \frac{(2V\cos(k/2)^2}{(\mathscr{E}_0^+(k)-2\Delta)(\mathscr{E}_0^-(k)-2\Delta)} = -1. \tag{A6}$$

Therefore, the last two terms of (A5) can be derived as

$$\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta} g_+(k)\frac{\mathrm{d}}{\mathrm{d}k}\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta} g_+(k)\Big) + g_+(k)\frac{\mathrm{d}}{\mathrm{d}k} g_+(k) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}k}\Big\{g_+^2(k)\Big[1+\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta}\Big)^2\Big]\Big\} = 0 \tag{A7}$$

$$\begin{aligned}\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta} g_+(k)\frac{\mathrm{d}}{\mathrm{d}k}\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^-(k)-2\Delta} g_-(k)\Big) + g_+(k)\frac{\mathrm{d}}{\mathrm{d}k} g_-(k) &= g_+(k)g_-(k)\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta}\frac{\mathrm{d}}{\mathrm{d}k}\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^-(k)-2\Delta}\Big)\\ &\quad + \frac{(2V\cos(k/2))^2}{(\mathscr{E}_0^+(k)-2\Delta)(\mathscr{E}_0^-(k)-2\Delta)} g_+(k)\frac{\mathrm{d}}{\mathrm{d}k}g_-(k) + g_+(k)\frac{\mathrm{d}}{\mathrm{d}k}g_-(k)\\ &= g_+(k)g_-(k)\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta}\frac{\mathrm{d}}{\mathrm{d}k}\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^-(k)-2\Delta}\Big).\end{aligned} \tag{A8}$$

Substituting (A6)–(A8) into (A5), and using (2.13) again, we find

$$(\mathscr{E}-\mathscr{E}_0^+(k))a(k) = -2eaE_0\,\mathrm{i}(\mathrm{d}/\mathrm{d}k)a(k) - eaE_0 a(k) - 2eaE_0\,\mathrm{i}b(k)g_+(k)g_-(k)\frac{2V\cos(k/2)}{\mathscr{E}_0^+(k)-2\Delta}\frac{\mathrm{d}}{\mathrm{d}k}\Big(\frac{2V\cos(k/2)}{\mathscr{E}_0^-(k)-2\Delta}\Big). \tag{A9}$$

By defining $G_{+-}(k)$ as given by (3.5), we finally obtain (3.4).

Appendix B

From (3.14) and by using the well-known properties of the Pauli matrices, i.e., $\sigma_x^2=\sigma_y^2=\sigma_z^2=1$, $\sigma_x\sigma_y=\mathrm{i}\sigma_z$, $\sigma_y\sigma_z=\mathrm{i}\sigma_x$ and $\sigma_z\sigma_x=\mathrm{i}\sigma_y$, we have

$$S(k_1)S(k_2) = X(k_1)X(k_2)+Y(k_1)Y(k_2)+\mathrm{i}(X(k_1)Y(k_2)-Y(k_1)X(k_2))\sigma_z \equiv X(k_1k_2)+\mathrm{i}Y(k_1k_2)\sigma_z \tag{B1}$$

with

$$X(k_1k_2) = X(k_1)X(k_2) + Y(k_1)Y(k_2) \tag{B2}$$

$$Y(k_1k_2) = X(k_1)Y(k_2) - Y(k_1)X(k_2) \tag{B3}$$

and

$$\begin{aligned} S(k_1)S(k_2)S(k_3) &= (X(k_1k_2)X(k_3) + Y(k_1k_2)Y(k_3))\sigma_x \\ &\quad + (X(k_1k_2)Y(k_3) - Y(k_1k_2)X(k_3))\sigma_y \\ &\equiv X(k_1k_2k_3)\sigma_x + Y(k_1k_2k_3)\sigma_y \end{aligned} \tag{B4}$$

with

$$X(k_1k_2k_3) = X(k_1k_2)X(k_3) + Y(k_1k_2)Y(k_3) \tag{B5}$$

$$Y(k_1k_2k_3) = X(k_1k_2)Y(k_3) - Y(k_1k_2)X(k_3). \tag{B6}$$

Similarly, by direct calculations, we arrive at (3.25)–(3.27).

Appendix C

Substituting (3.33) (taking $k = 2\pi$) into (3.37), we get

$$\begin{aligned} & e^{-2i\alpha(2\pi)} - 2e^{-i\alpha(2\pi)}\left(\cos\beta(2\pi)\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0) - \sin\beta(2\pi)\sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0)\right) \\ &\quad + \left(\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0)\right)^2 \\ &\quad + \left(\sum_{m=0}^{\infty} U_x^{(2m+1)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m+1)}(2\pi,0)\right)^2 = 0. \end{aligned} \tag{C1}$$

Note that from (3.36), we have

$$\begin{aligned} |a(0)|^2 + |b(0)|^2 &= (a^*(0)b^*(0))\begin{pmatrix} a(0) \\ b(0) \end{pmatrix} \\ &= (a^*(0)b^*(0))\left(\sum_{m=0}^{\infty} U^{(m)}(2\pi,0)\right)^+\left(\sum_{m=0}^{\infty} U^{(m)}(2\pi,0)\right)\begin{pmatrix} a(0) \\ b(0) \end{pmatrix}. \end{aligned} \tag{C2}$$

When using (3.33) again, equation (C2) becomes

$$\begin{aligned} |a(0)|^2 + |b(0)|^2 &= \left[\left(\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0)\right)^2 \right. \\ &\quad \left. + \left(\sum_{m=0}^{\infty} U_x^{(2m+1)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m+1)}(2\pi,0)\right)^2\right](|a(0)|^2 + |b(0)|^2). \end{aligned} \tag{C3}$$

This gives

$$\left(\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_x^{(2m+1)}(2\pi,0)\right)^2 + \left(\sum_{m=0}^{\infty} U_y^{(2m+1)}(2\pi,0)\right)^2 = 1. \tag{C4}$$

Substituting (C4) into (C1), and introducing

$$\cos\phi(2\pi,0) = \cos\beta(2\pi)\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi,0) - \sin\beta(2\pi)\sum_{m=0}^{\infty} U_y^{(2m)}(2\pi,0) \tag{C5}$$

we obtain

$$\exp[\mathrm{i}(\alpha(2\pi) \mp \phi(2\pi,0))] = 1. \tag{C6}$$

This leads to

$$\alpha_{\pm}(2\pi) = 2\pi n \pm \phi(2\pi,0) \qquad (n = \text{integer}) \tag{C7}$$

where $\alpha_{\pm}(2\pi)$ is given by (3.42). Substituting (3.42) into (C7), we arrive at the final results (3.38).

References

[1] Kenkre V M and Reineker P 1982 *Exciton Dynamics in Molecular Crystals and Aggregates* ed G Hohler (Berlin: Springer)
[2] Bílek O and Skala L 1986 *Phys. Lett.* **119A** 300
[3] Tsu R and Dohler G 1975 *Phys. Rev.* B **12** 680
[4] Robin P and Muller M W 1986 *Phys. Rev.* B **32** 5222
[5] Patel J S and Hanson D M 1982 *Chem. Phys. Lett.* **89** 473
[6] Patel J S and Hanson D M 1981 *J. Chem. Phys.* **75** 5203
[7] Hanson D M 1980 *Mol. Cryst. Liq. Cryst.* **57** 243
[8] Kovanis V I and Kenkre V M 1988 *Phys. Lett.* **130A** 147
[9] Merzbacher E 1970 *Quantum Mechanics* (New York: Wiley) p 270
[10] Wannier G H 1969 *Phys. Rev.* **181** 1364
[11] Emin D and Hart C F 1987 *Phys. Rev.* B **36** 7353
[12] Hart C F and Emin D 1988 *Phys. Rev.* B **37** 6100
[13] Fukuyama H, Bari R A and Fogedby H C 1973 *Phys. Rev.* B **8** 5579
[14] Byrd P F and Friedman M D 1971 *Handbook of Elliptic Integrals for Engineers and Scientists* (Berlin: Springer) p 10
[15] Abramowitz M and Stegun I A 1966 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards) chs 15, 17
[16] Movaghar B 1987 *Semicond. Sci. Technol.* **2** 185
[17] Maekawa S 1970 *Phys. Rev. Lett.* **24** 1175
[18] Koss R W and Lambert L N 1972 *Phys. Rev.* B **5** 1479
[19] Voisin P, Bleuse J, Bouche C, Gaillard S, Alibert C and Regreny A 1988 *Phys. Rev. Lett.* **61** 1639
[20] Agullo-Rueda F, Mendez E E and Hong J M 1988 *Phys. Rev.* B **38** 12720
[21] Mendez E E, Agullo-Rueda F and Hong J M 1988 *Phys. Rev. Lett.* **60** 2426
[22] Leavitt R P and Little J W 1990 *Phys. Rev.* B **41** 5174
[23] Whittaker D M, Skolnick M S, Smith G W and Whitehouse C R 1990 *Phys. Rev.* B **42** 3591