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General solutions for a charged particle in a uniform electric field with alternating intersite interactions

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Received 22 October 1991

Abstract. A model Hamiltonian for a charged particle in a uniform electric field with alternating intersite interactions is studied in detail. For the case of weakly alternating intersite interactions, general solutions are obtained for the energy spectrum and the eigenvectors by using the perturbation theory developed in our previous papers, by which it is shown quite rigorously that the energy spectrum is that of two interspaced Stark ladders.

1. Introduction

In a one-dimensional lattice, the Hamiltonian for 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 the nearest-neighbour intersite overlap integrals can be generally written as

$$H = \sum_{m} V_m(|m\rangle\langle m+1| + |m+1\rangle\langle m|) - \mathscr{C}\sum_{m} m|m\rangle\langle m|$$
(1.1)

where $|m\rangle$ represents a Wannier state localized on lattice site m, V_m is the nearestneighbour intersite overlap integral between sites m and m + 1, and $\mathscr{C} = eE_0a$, where e, E_0 and a, respectively, are the charge on the particle, the external electric field and the lattice spacing. Here, V_m has been assumed to be real for simplicity, and the off-diagonal elements of the position operator in the Wannier basis have been neglected. In general, according to a practical crystal, the transfer energy V_m is a function of site m, which, however, often makes it impossible to seek exact solutions for the purpose of analytic discussions. Therefore, in order to obtain exact solutions, research workers usually pay attention to prefect crystals where V_m can be treated as a constant, and the problem can be exactly solved [1-3]. Recently, Kovanis and Kenkre [4] have studied a model in which the transfer energy V_m alternates between the values V_1 and V_2 . In the absence of an electric field, they obtained the exact probability self-propagators. In the present work, following the Kovanis-Kenkre model, we investigate the case when a uniform electric field is present.

If we write the difference $V_1 - V_2$ (assuming $V_1 > V_2 > 0$) as 2Δ and the average $(V_1 + V_2)/2$ as V, the Hamiltonian (1.1) becomes

m

$$H = \sum_{m} \left[V + \Delta(-1)^{m} \right] (|m\rangle\langle m+1| + |m+1\rangle\langle m|) - \mathscr{E} \sum_{m} m|m\rangle\langle m| \equiv H_{0} + H_{e}$$
(1.2)

$$H_0 = \sum \left[V + \Delta(-1)^m \right] \left(|m\rangle \langle m+1| + |m+1\rangle \langle m| \right)$$
(1.3)

$$H_{\rm e} = -\mathscr{E}\sum_{m} m |m\rangle \langle m| \tag{1.4}$$

where H_0 is the field-free Hamiltonian. Such a system is relevant to a variety of fields including electron states in superlattices [5, 6], and the localized properties of excitations in ferroelectric materials [7–9].

We note that usually, in practical crystals, $(V_1 - V_2)/(V_1 + V_2) \ll 1$, i.e. $\Delta/V \ll 1$. In fact, we often encounter this. Therefore, in the following, we study only this situation. We find that in this case the problem can be exactly solved by using the perturbation theory (PT) developed in our previous papers [10-12]. To do this, we first focus on seeking the explicit solutions for the field-free system in k-space (section 2). Then, by expressing the eigenvectors in (1.2) as a linear superposition of the field-free eigenvectors, the exact results are obtained for the energy spectrum and the eigenvectors by using PT (section 3). Finally, the concluding remarks are given in section 4.

2. Explicit solutions for H₀ in k-space

Following our previous paper [10], we express the eigenvector $|\varphi\rangle$ of H_0 as a linear superposition of Wannier states $|m\rangle$:

$$|\varphi\rangle = \sum_{m} C_{m} |m\rangle.$$
(2.1)

Here the amplitudes C_m satisfy

$$\varepsilon_0 C_{2m} = (V + \Delta) C_{2m+1} + (V - \Delta) C_{2m-1}$$
(2.2)

$$\varepsilon_0 C_{2m+1} = (V + \Delta) C_{2m} + (V - \Delta) C_{2m+2}$$
(2.3)

where ε_0 is the energy belonging to H_0 . These equations can be diagonalized by setting $C_{2m} = f(k) \exp(ikm)$ $C_{2m+1} = g(k) \exp(ikm)$ $0 \le k \le 2\pi$ (2.4) where k is the (dimensionless) wavevector. We get

$$\varepsilon_0 f(k) - 2g(k) \exp(-ik/2) [V \cos(k/2) + i\Delta \sin(k/2)] = 0$$
(2.5)

$$\varepsilon_0 g(k) - 2f(k) \exp(ik/2) [V \cos(k/2) - i\Delta \sin(k/2)] = 0.$$
(2.6)

The eigenvalue equation determined by equations (2.5) and (2.6) is

$$\varepsilon_0^2 - 4\{[V\cos(k/2)]^2 + [\Delta\sin(k/2)]^2\} = 0$$
(2.7)

with solutions

$$\varepsilon_0^{\pm}(k) = \pm 2\{[V\cos(k/2)]^2 + [\Delta\sin(k/2)]^2\}^{1/2}.$$
(2.8)

Thus, the eigenvectors of H_0 become

$$|\varphi(k)\rangle_{\pm} = \sum_{m} \exp(ikm) \left\{ f_{\pm}(k) | 2m \rangle + g_{\pm}(k) | 2m + 1 \rangle \right\}$$
(2.9)

with the relation

$$f_{\pm}(k) = \{2[V\cos(k/2) + i\Delta\sin(k/2)]/\varepsilon_0^{\pm}(k)\}\exp(-ik/2)g_{\pm}(k).$$
(2.10)

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

$$g_{\pm}(k) = 1/\sqrt{2}.$$
 (2.11)

From (2.8)–(2.11), it is easily shown that the following formulae are true:

$$|f_{\pm}(k)|^2 + |g_{\pm}(k)|^2 = 1 \qquad f_{\pm}^*(k)f_{\mp}(k) + g_{\pm}^*(k)g_{\mp}(k) = 0 \qquad (2.12)$$

$${}_{\pm}\langle\varphi(k)|\varphi(k')\rangle_{\pm} = \delta(k-k') \qquad {}_{\pm}\langle\varphi(k)|\varphi(k')\rangle_{\mp} = 0.$$
(2.13)

3. General solutions to *H* for the case $\Delta/V \ll 1$

Setting the eigenvector $|\psi\rangle$ of H to be of the form

$$|\psi\rangle = \int_{0}^{2\pi} \mathrm{d}k \left[a(k)|\varphi(k)\rangle_{+} + b(k)|\varphi(k)\rangle_{-}\right]$$
(3.1)

and using (1.2)–(1.4), we obtain the following equation for the amplitudes a(k) and b(k):

$$\varepsilon \int_{0}^{2\pi} dk \left[a(k) | \varphi(k) \rangle_{+} + b(k) | \varphi(k) \rangle_{-} \right] = \int_{0}^{2\pi} dk \left[\varepsilon_{0}^{+}(k) a(k) | \varphi(k) \rangle_{+} + \varepsilon_{0}^{-}(k) b(k) | \varphi(k) \rangle_{-} \right] - \mathscr{C} \int_{0}^{2\pi} dk \left(a(k) \sum_{m} m | m \rangle \langle m | \varphi(k) \rangle_{+} + b(k) \sum_{m} m | m \rangle \langle m | \varphi(k) \rangle_{-} \right)$$

$$(3.2)$$

where ε is the energy belonging to *H*. By multiplying both sides of equation (3.2) by $_{+}\langle \varphi(k) |$, and using (2.13) we have

$$\varepsilon a(k) = \varepsilon_0^+ a(k) - \mathscr{C} \int_0^{2\pi} \mathrm{d}k' \left(a(k') \sum_m m_+ \langle \varphi(k) | m \rangle \langle m | \varphi(k') \rangle_+ \right. \\ \left. + b(k') \sum_m m_+ \langle \varphi(k) | m \rangle \langle m | \varphi(k') \rangle_- \right) .$$
(3.3)

Substituting (2.9) into (3.3), we find (as shown in [10]) that

$$(d/dk)a(k) = i\{[\varepsilon + \mathcal{E} + \varepsilon_0^-(k)]/2\mathcal{E} + h(k)\}a(k) - ih(k)b(k)$$
(3.4)

with

$$h(k) = -V\Delta / [\varepsilon_0^-(k)]^2.$$
(3.5)

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

$$(\mathrm{d}/\mathrm{d}k)b(k) = \mathrm{i}\{[\varepsilon + \mathscr{C} - \varepsilon_0(k)]/2\mathscr{C} + h(k)\}b(k) - \mathrm{i}h(k)a(k). \tag{3.6}$$

By setting

 $a(k) = \exp\{i[\alpha(k) + \beta(k)]\}A(k) \qquad b(k) = \exp\{i[\alpha(k) - \beta(k)]\}B(k) \qquad (3.7)$ where

$$\alpha(k) = \frac{\varepsilon + \mathscr{C}}{2\mathscr{C}} k + \int_0^k \mathrm{d}k' \, h(k') \qquad \beta(k) = \frac{1}{2\mathscr{C}} \int_0^k \mathrm{d}k' \, \varepsilon_0(k') \qquad (3.8)$$

equations (3.4) and (3.6) reduce to

$$(d/dk)A(k) = -ih(k) \exp[-2i\beta(k)] B(k)$$
(3.9)

$$(d/dk)B(k) = -ih(k) \exp[2i\beta(k)] A(k).$$
(3.10)

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

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$$\frac{\mathrm{d}}{\mathrm{d}k} \binom{A(k)}{B(k)} = -\mathrm{i}h(k) \{\sigma_x \cos[2\beta(k)] + \sigma_y \sin[2\beta(k)]\} \binom{A(k)}{B(k)}$$
(3.11)

where σ_x and σ_y (as well as σ_z used below) are the Pauli matrices. By introducing

$$R(k) = \binom{A(k)}{B(k)} \tag{3.12}$$

$$G(k) = X(k)\sigma_x + Y(k)\sigma_y$$
(3.13)

$$X(k) = h(k) \cos[2\beta(k)] \qquad Y(k) = h(k) \sin[2\beta(k)]$$
(3.14)

equation (3.11) reduces to

$$(\mathbf{d}/\mathbf{d}k)R(k) = -\mathbf{i}G(k)R(k) \tag{3.15}$$

or equivalently

$$R(k) = R(0) - i \int_0^k dk_1 G(k_1) R(k_1).$$
(3.16)

From (3.13) and (3.14), using the well known properties of the Pauli matrices, we find that

$$|G(k)| = |h(k)|.$$
(3.17)

Substituting (2.8) and (3.5) into (3.17), we get

$$|G(k)| = [1/2\{1 + (\Delta/V)^2 + [1 - (\Delta/V)^2] \cos k\}](\Delta/V).$$
(3.18)

As indicated in section 1, what we are interested in is the case when $\Delta/V \leq 1$. From (3.18), this gives

$$\left| \int_{0}^{k} \mathrm{d}k_{1} G(k_{1}) R(k_{1}) \right| \leq |R(0)|.$$
(3.19)

Therefore, equation (3.16) can be solved using the PT. As the results, we obtain

$$R(k) = \sum_{m=0}^{\infty} U_{(k,0)}^{(m)} R(0)$$
(3.20)

where

$$U_{(k,0)}^{(0)} = 1 \tag{3.21}$$

$$U_{(k,0)}^{(m)} = (-i)^{m} \left(\prod_{l=1}^{m} \int_{0}^{k} dk_{l} \right) \theta(k_{1} - k_{2}) \theta(k_{2} - k_{3}) \dots \\ \times \theta(k_{m-1} - k_{m}) G(k_{1}) G(k_{2}) \dots G(k_{m})$$
(3.22)

$$\theta(k) = \begin{cases} 1 & k > 0 \\ 0 & k < 0 \end{cases}$$
(3.23)

It is easily shown that (the calculation method is presented in [10–12]) $G(k_1)G(k_2)\ldots G(k_m) =$

$$\begin{cases} X(k_1k_2\dots k_m) + iY(k_1k_2\dots k_m)\sigma_z & \text{if } m = 2l \\ X(k_1k_2\dots k_m)\sigma_x + Y(k_2k_2\dots k_m)\sigma_y & \text{if } m = 2l+1 \end{cases}$$
(3.24)

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$$X(k_1k_2...k_m) = X(k_1k_2...k_{m-1})X(k_m) + Y(k_1k_2...k_{m-1})Y(k_m) \qquad (m \ge 2)$$
(3.25)

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$$Y(k_1k_2...k_m) = X(k_1k_2...k_{m-1})Y(k_m) - Y(k_1k_2...k_{m-1})X(k_m) \qquad (m \ge 2).$$
(3.26)

Defining

$$U_{x(k,0)}^{(2m)} = (-1)^m \left(\prod_{l=1}^{2m} \int_0^k dk_l\right) \theta(k_1 - k_2) \theta(k_2 - k_3) \dots \times \theta(k_{2m-1} - k_{2m}) X(k_1 k_2 \dots k_{2m})$$
(3.27)

$$U_{y(k,0)}^{(2m)} = (-1)^m \left(\prod_{l=1}^{2m} \int_0^k \mathrm{d}k_l\right) \theta(k_1 - k_2) \theta(k_2 - k_3) \dots \times \theta(k_{2m-1} - k_{2m}) Y(k_1 k_2 \dots k_{2m})$$
(3.28)

$$U_{x(k,0)}^{(2m+1)} = (-1)^{m+1} \left(\prod_{l=1}^{2m+1} \int_0^k \mathrm{d}k_l \right) \theta(k_1 - k_2) \theta(k_2 - k_3) \dots$$

$$\times \theta(k_{2m} - k_{2m+1}) X(k_1 k_2 \dots k_{2m+1})$$
(3.29)

$$U_{y(k,0)}^{(2m+1)} = (-1)^{m+1} \left(\prod_{l=1}^{2m+1} \int_0^k \mathrm{d}k_l \right) \theta(k_1 - k_2) \theta(k_2 - k_3) \dots$$

$$\times \theta(k_{2m} - k_{2m+1})Y(k_1k_2 \dots k_{2m+1})$$
(3.30)

$$U_{x(k,0)}^{(0)} = 1 \qquad U_{y(k,0)}^{(0)} = 0 \tag{3.31}$$

we find that

$$\sum_{m=0}^{\infty} U_{(k,0)}^{(m)} = \sum_{m=0}^{\infty} U_{x(k,0)}^{(2m)} + i\sigma_z \sum_{m=0}^{\infty} U_{y(k,0)}^{(2m)} + i\sigma_x \sum_{m=0}^{\infty} U_{x(k,0)}^{(2m+1)} + i\sigma_y \sum_{m=0}^{\infty} U_{y(k,0)}^{(2m+1)}.$$
(3.32)

From (3.7), (3.8), (3.12) and (3.20), we have

$$\binom{a(k)}{b(k)} = \exp[i\alpha(k)] \binom{\exp[i\beta(k)] \quad 0}{0 \qquad \exp[-i\beta(k)]} \sum_{m=0}^{\infty} U^{(m)}_{(k,0)} R(0)$$
(3.33)

$$R(0) = \binom{A(0)}{B(0)} = \binom{a(0)}{b(0)}.$$
(3.34)

Note that, from (2.8)–(2.11), $\varepsilon_0^{\pm}(k+2\pi) = \varepsilon_0^{\pm}(k), f_{\pm}(k+2\pi) = f_{\pm}(k), g_{\pm}(k+2\pi) = f_{\pm}(k)$

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 $g_{\pm}(k)$, 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 $a(k) = _{+}\langle \varphi(k) | \psi \rangle$ and $b(k) = _{-}\langle \varphi(k) | \psi \rangle$. This leads to the following equation:

$$\binom{a(0)}{b(0)} = \exp[i\alpha(2\pi)] \binom{\exp[i\beta(2\pi)]}{0} \frac{0}{\exp[-i\beta(2\pi)]} \sum_{m=0}^{\infty} U^{(m)}_{(2\pi,0)} \binom{a(0)}{b(0)}.$$
 (3.35)

The eigenvalue equation determined by equation (3.35) is

$$\det\left\{\begin{pmatrix} \exp[i\beta(2\pi)] & 0\\ 0 & \exp[-i\beta(2\pi)] \end{pmatrix} \sum_{m=0}^{\infty} U_{(2\pi,0)}^{(m)} - \exp[-i\alpha(2\pi)] \right\} = 0$$
(3.36)

with solutions

$$\varepsilon_n^{\pm} = (2n - \frac{1}{2}) \mathscr{E} \pm (\mathscr{E}/\pi) \phi(2\pi, 0) \qquad (n \text{ integer})$$
(3.37)

where

$$\phi(2\pi,0) = \cos^{-1} \bigg(\cos[\beta(2\pi)] \sum_{m=0}^{\infty} U_{x(2\pi,0)}^{(2m)} - \sin[\beta(2\pi)] \sum_{m=0}^{\infty} U_{y(2\pi,0)}^{(2m)} \bigg).$$
(3.38)

Corresponding to ε_n^{\pm} , the solutions for $a_{\pm}(0)$ and $b_{\pm}(0)$ determined by both equation (3.35) and the normalization of the eigenvectors $|\psi\rangle_{\pm}$ are

$$a_{\pm}(0) = \frac{1}{2\sqrt{\pi}} \left\{ \left[\left(\sum_{m=0}^{\infty} U_{\chi(2\pi,0)}^{(2m+1)} \right)^2 + \left(\sum_{m=0}^{\infty} U_{y(2\pi,0)}^{(2m+1)} \right)^2 \right] / \left(1 - \cos[\alpha_{\pm}(2\pi) + \beta(2\pi)] \right] \right\} \\ \times \sum_{m=0}^{\infty} U_{\chi(2\pi,0)}^{(2m)} + \sin[\alpha_{\pm}(2\pi) + \beta(2\pi)] \sum_{m=0}^{\infty} U_{y(2\pi,0)}^{(2m)} \right)^{1/2}$$
(3.39)

$$b_{\pm}(0) = \left[\frac{1}{\left(\sum_{m=0}^{\infty} U_{y(2\pi,0)}^{(2m+1)} + i \sum_{m=0}^{\infty} U_{x(2\pi,0)}^{(2m+1)}\right)} \right] \left[\exp\{-i[\alpha_{\pm}(2\pi) + \beta(2\pi)] \right\} - \left(\sum_{m=0}^{\infty} U_{x(2\pi,0)}^{(2m)} + i \sum_{m=0}^{\infty} U_{y(2\pi,0)}^{(2m)}\right) \right] a_{\pm}(0)$$
(3.40)

where

$$\alpha_{\pm}(2\pi) = \frac{\varepsilon_n^{\pm} + \mathscr{C}}{\mathscr{C}} \pi + \int_0^{2\pi} \mathrm{d}k \, h(k). \tag{3.41}$$

From (3.1), (3.33) and (3.34), we obtain the final results for the eigenvectors

$$|\psi\rangle_{\pm} = \int_{0}^{2\pi} dk \left[a_{\pm}(k) |\varphi(k)\rangle_{\pm} + b_{\pm}(k) |\varphi(k)\rangle_{-} \right]$$
(3.42)

with

$$\binom{a_{\pm}(k)}{b_{\pm}(k)} = \exp[i\alpha_{\pm}(k)] \binom{\exp[i\beta(k)] \ 0}{0} \exp[-i\beta(k)] \sum_{m=0}^{\infty} U^{(m)}_{(k,0)} \binom{a_{\pm}(0)}{b_{\pm}(0)}$$
(3.43)

where

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$$\alpha_{\pm}(k) = \frac{\varepsilon_n^{\pm} + \mathscr{C}}{2\mathscr{C}} k + \int_0^k \mathrm{d}k' h(k'). \tag{3.44}$$

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

$${}_{\pm}\langle\psi|\psi\rangle_{\pm} = 1 \qquad {}_{\pm}\langle\psi|\psi\rangle_{\mp} = 0. \tag{3.45}$$

4. Concluding remarks

It is clearly seen from (3.37) that the energy spectrum for our model (1.2) is that of two interspaced Stark ladders, which is consistent with our previous results [10–12] on the existence of Wannier–Stark localization in solids for the case of a charged particle under the influence of a uniform electric field.

In principle, our results (3.37)–(3.45) can exactly hold for the case $\Delta/V \leq 1$. However, this means that one needs to use infinite integrals which, obviously, is impossible. Therefore, in practice, we have to make some approximations up to the required orders. For example, as the zero order of PT, we get from (3.31) and (3.38) that

$$\sum_{m=0}^{\infty} U_{x(2\pi,0)}^{(2m)} \simeq U_{x(2\pi,0)}^{(0)} = 1 \qquad \sum_{m=0}^{\infty} U_{y(2\pi,0)}^{(2m)} \simeq U_{y(2\pi,0)}^{(0)} = 0.$$
(4.1)

This leads to

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

where

$$\beta(2\pi) = \frac{1}{2\mathscr{C}} \int_0^{2\pi} \mathrm{d}k \, \varepsilon_0^-(k). \tag{4.3}$$

Substituting (2.8) into (4.3) and completing this integral yields

$$\beta(2\pi) = -4(V/\mathscr{E})E(\pi/2,\gamma) \tag{4.4}$$

where $E(\pi/2, \gamma)$ is the complete elliptic integral of the second kind [13], and γ is the modulus defined by

$$\gamma^2 = 1 - (\Delta/V)^2. \tag{4.5}$$

Substituting (4.2) and (4.4) into (3.37), we obtain the spectrum

$$\varepsilon_n^{\pm} = (2n - \frac{1}{2}) \mathscr{E} \pm (4V/\pi) E(\pi/2, \gamma).$$
 (4.6)

If we use the identity [14]

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

where F and Γ , respectively, are the hypergeometric function and the gamma function, the role of alternating intersite interactions in the spectrum can be explicitly found from (4.5)–(4.7), for which it should be noted that the enhancement of alternating intersite interactions (without destroying the PT requirement $\Delta/V \ll 1$) will give rise to an increase in the energy gap.

Another characteristic of our general results (3.37)-(3.45) is that, compared with Movaghar's [15] results where the Stark regime in semiconductor superlattice structures will appear for larger values of the external field E_0 , our conclusion about the existence

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of Wannier–Stark localization applies to quite a large range of the values of a (1–100 Å) and E_0 (0–10⁸ V m⁻¹), because there is no special confinement to these parameters in our model. In fact, the typical values above are in agreement with many experimental results [16–22].

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

Acknowledgments

It is a pleasure to thank Professor S G Chen, Professor X W Zhang and Professor W X Zhang for very illuminating discussions and helpful criticism.

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