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LETTER TO THE EDITOR

Stark ladders of the two-band approximation

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Abstract. The problem of Bloch electrons in infinite crystals under the influence of an electric field is investigated with the interband coupling being taken into account. Of special interest is the case of the two-band approximation. Exact solutions for the energy spectrum and the wave functions are obtained by using perturbation theory for the case of weak interband coupling, and it is shown that the energy spectrum is that of two interspaced Stark ladders. Since the spectrum contains, in addition to a linear term of the applied electric field, the reciprocal of the applied electric field to all orders, it implies that the Stark regime will appear sharp for greater values of the external field. For the zero-order case of the perturbation theory, the exact Wannier–Stark localization holds.

The character of the wave functions and the energy spectrum for Bloch electrons moving under the influence of an external electric field has been extensively discussed in the literature [1–3]. The analytic solutions to such a problem for the case of the one-band approximation were presented decades ago [2–4], from which it was found that the extended Bloch states would localize and the continuous energy bands would evolve into an evenly spaced Stark ladder. For the case of the N-band approximation ($N \geqslant 2$), it was also shown that the energy spectrum was that of interspaced Stark ladders [5]. However, owing to the interband coupling, the search for exact solutions is so difficult that the explicit expressions for the wave functions and the energy spectrum have not been obtained to date, not even if only the two-band approximation is involved. In this letter, we show that for the two-band approximation case, if the interband coupling is small, the problem can be solved exactly by using perturbation theory. As a result, it is found that in addition to a linear term due to the applied electric field, i.e., the Stark ladder, the spectrum also contains a reciprocal term due to the applied electric field to all orders. This means that the Stark regime will appear sharp for great values of the external field. Only for the zero-order case of the perturbation theory can the exact Stark ladder exist.

For simplicity, we consider the one-dimensional case. The Schrödinger equation for an electron in a periodic potential $V(x)$ and a constant electric field E_0 has the form

$$\left(\frac{p^2}{2m} + V(x) - eE_0x\right)\Psi(x) = \epsilon\Psi(x). \tag{1}$$

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By expressing the eigenvector $\Psi(x)$ as a linear superposition of Bloch functions $\psi_{nk}(x)$,

$$\Psi(x) = \sum_{nk} B_n(k)\psi_{nk}(x) \tag{2}$$

one obtains the following equation for the amplitudes $B_n(k)$ in the nk representation [6, 7]

$$\left(\epsilon_n(k) - \epsilon - eE_0X_{nn}(k) - eE_0\mathrm{i}\frac{\partial}{\partial k}\right) B_n(k) - \sum_{m\neq n} eE_0X_{nm}(k)B_m(k) = 0 \tag{3}$$

where $\epsilon_n(k)$ is the energy corresponding to the Bloch function and

$$X_{nm}(k) = \int \mathrm{d}x\, u^*_{nk}(x)\mathrm{i}\frac{\partial}{\partial k}u_{mk}(x) \tag{4}$$

with $u_{nk}(x)$ being the periodic part of the Bloch function. By introducing (for $E_0 \neq 0$)

$$b_n(k) = B_n(k)\exp\left(\frac{-\mathrm{i}}{eE_0}\int_0^k \mathrm{d}k'\,[\epsilon - \epsilon_n(k') + eE_0X_{nn}(k')]\right) \tag{5}$$

$$\theta_{nm}(k) = \frac{1}{eE_0}\left(\alpha_{nm}(k) + \int_0^k \mathrm{d}k'\,[\epsilon_n(k') - \epsilon_m(k') - eE_0X_{nn}(k') + eE_0X_{mm}(k')]\right) \tag{6}$$

with $\alpha_{nm}(k)$ satisfying

$$X_{nm}(k) = |X_{nm}(k)|\exp[\mathrm{i}\alpha_{nm}(k)/eE_0] \qquad (n \neq m) \tag{7}$$

equation (3) becomes

$$\mathrm{i}\frac{\partial}{\partial k}b_n(k) + \sum_{m\neq n}|X_{nm}(k)|\exp[\mathrm{i}\theta_{nm}(k)]b_m(k) = 0. \tag{8}$$

It is easy to show that

$$\alpha_{nm}(k) = -\alpha_{mn}(k) \qquad \theta_{nm}(k) = -\theta_{mn}(k). \tag{9}$$

Therefore, in the two-band approximation case, equation (8) reads

$$\mathrm{i}(\mathrm{d}/\mathrm{d}k)b_0(k) + |X_{01}(k)|\exp[\mathrm{i}\theta_{01}(k)]b_1(k) = 0 \tag{10}$$

$$\mathrm{i}(\mathrm{d}/\mathrm{d}k)b_1(k) + |X_{01}(k)|\exp[-\mathrm{i}\theta_{01}(k)]b_0(k) = 0. \tag{11}$$

Setting

$$R(k) = \begin{pmatrix} b_0(k) \\ b_1(k) \end{pmatrix} \tag{12}$$

$$S(k) = X(k)\sigma_x + Y(k)\sigma_y \tag{13}$$

$$X(k) = -|X_{01}(k)|\cos[\theta_{01}(k)] \qquad Y(k) = -|X_{01}(k)|\sin[\theta_{01}(k)] \tag{14}$$

where σ_x and σ_y are the Pauli matrices, equations (10) and (11) can be rewritten together as

$$R(k) = R(0) - \mathrm{i}\int_0^k \mathrm{d}k_1\, S(k_1)R(k_1). \tag{15}$$

Notice that from (13) and (14) we have $|S(k)| = |X_{01}(k)|$. Therefore, if the interband coupling is small, equation (15) can be solved by using perturbation theory, i.e.,

$$R(k) = \sum_{m=0}^{\infty} U^{(m)}(k,0)R(0) \tag{16}$$

where

$$U^{(m)}(k,0) = (-\mathrm{i})^m \left(\prod_{l=1}^{m}\int_0^k \mathrm{d}k_l\right)\theta(k_1-k_2)\theta(k_2-k_3)$$
$$\ldots\theta(k_{m-1}-k_m)S(k_1)S(k_2)\ldots S(k_m) \tag{17}$$

with $\theta(k) = 1$ for $k > 0$ and 0 otherwise. The function $B_n(k)$ is assumed to be periodic, i.e., $B_n(k) = B_n(k + 2\pi/a)$, where a is the lattice constant. Therefore, without loss of generality, $B_n(0) = B_n(2\pi/a)$. This leads to the energy

$$\epsilon \equiv \epsilon_n^{\pm} = neaE_0 + \frac{a}{4\pi}\int_0^{2\pi/a} \mathrm{d}k\,[\epsilon_0(k) + \epsilon_1(k) - eE_0X_{00}(k) - eE_0X_{11}(k)]$$
$$\pm \frac{eaE_0}{2\pi}\phi(2\pi/a,0) \qquad (n = \text{integer}) \tag{18}$$

where

$$\phi(2\pi/a,0) = \cos^{-1}\left(\cos\frac{(\alpha-\beta)}{2}\sum_{m=0}^{\infty} U_x^{(2m)}(2\pi/a,0)\right.$$
$$\left. - \sin\frac{(\alpha-\beta)}{2}\sum_{m=0}^{\infty} U_y^{(2m)}(2\pi/a,0)\right) \tag{19}$$

$$\alpha = \frac{-1}{eE_0}\int_0^{2\pi/a} \mathrm{d}k\,[\epsilon_0(k) - eE_0X_{00}(k)]$$
$$\beta = \frac{-1}{eE_0}\int_0^{2\pi/a} \mathrm{d}k\,[\epsilon_1(k) - eE_0X_{11}(k)] \tag{20}$$

$$U_x^{(2m)}(2\pi/a,0) = (-1)^m \left(\prod_{l=1}^{2m}\int_0^{2\pi/a} \mathrm{d}k_l\right)\theta(k_1-k_2)\theta(k_2-k_3)$$
$$\ldots\theta(k_{2m-1}-k_{2m})X(k_1k_2\ldots k_{2m}) \tag{21}$$

$$U_y^{(2m)}(2\pi/a,0) = (-1)^m \left(\prod_{l=1}^{2m}\int_0^{2\pi/a} \mathrm{d}k_l\right)\theta(k_1-k_2)\theta(k_2-k_3)$$
$$\ldots\theta(k_{2m-1}-k_{2m})Y(k_1k_2\ldots k_{2m}) \tag{22}$$

$$U_x^{(0)}(2\pi/a,0) = 1 \qquad U_y^{(0)}(2\pi/a,0) = 0 \tag{23}$$

with $X(k_1k_2\ldots k_m)$ and $Y(k_1k_2\ldots k_m)$ satisfying the following recurrence formulae

$$X(k_1k_2\ldots k_m) = X(k_1k_2\ldots k_{m-1})X(k_m) + Y(k_1k_2\ldots k_{m-1})Y(k_m) \qquad (m\geqslant 2) \tag{24}$$

$$Y(k_1k_2\ldots k_m) = X(k_1k_2\ldots k_{m-1})Y(k_m) - Y(k_1k_2\ldots k_{m-1})X(k_m) \qquad (m\geqslant 2). \tag{25}$$

The derivation of the above results ((18)–(25)) is rather tedious but straightforward. The amplitudes $B_0(0)$ and $B_1(0)$ have also been obtained but we will not give them here.

From the above investigation, some obvious characteristics can be seen clearly, which we present as follows.

(i) Our general solutions for the energy spectrum and the wave functions do hold exactly as long as the interband coupling is small, from which we find that the spectrum is that of two interspaced Stark ladders. This is in agreement with both the qualitative analyses [5] and the numerical calculations [8].

(ii) From definition (4), one can see that the interband coupling, which, in our arguments, is merely involved in the perturbation condition, has nothing to do with the external field. Therefore, our solutions for the two-band approximation are valid for a quite large range of $E_0(\leqslant 10^8\,\mathrm{V\,m^{-1}})$, since in our above analyses no special confinement of this parameter has been involved. This gives more freedom for our results to be applied in practice.

(iii) From (6), (14) and (18)–(25), we find that, compared to the well-known one-band approximation [2–4], the spectrum in the case of the two-band approximation not only involves a linear term in the applied electric field, but also contains the reciprocal of the applied electric field to all orders, which implies that the Stark regime will appear sharp for large values of the external electric field. This conclusion is qualitatively consistent with Movaghar's theoretical analyses [9] and is in agreement with many experimental results [10–14]. Of course, if we take the energy as that of the zero order of perturbation theory, the exact Wannier–Stark localization holds. In this case, the spectrum becomes

$$\epsilon_n^{\pm} = nea E_0 + \frac{a}{4\pi}\int_0^{2\pi/a}\mathrm{d}k\,[\epsilon_0(k)+\epsilon_1(k)-eE_0X_{00}(k)-eE_0X_{11}(k)]$$
$$\pm\frac{a}{4\pi}\int_0^{2\pi/a}\mathrm{d}k\,[\epsilon_1(k)-\epsilon_0(k)+eE_0X_{00}(k)-eE_0X_{11}(k)]. \tag{26}$$

In conclusion, we should like to indicate that since the exact results for the energy spectrum and the wave functions in the two-band approximation case have been obtained, the calculation of other physical quantities of the system discussed in this letter, up to any order of the perturbation theory, is, in principle, straightforward.

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