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STARK LADDERS IN SEMICONDUCTOR STRUCTURES

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STARK LADDERS IN SEMICONDUCTOR STRUCTURES

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Abstract

The problem of band electrons in semiconductors under the influence of an electric field is investigated with the interband coupling being taken into account. Exact solutions for the energy spectrum and the wave functions in the three-dimensional case are obtained by using perturbation theory, by which it is shown that the energy spectrum not only involves a linear term of the applied electric field, i.e., the Stark ladder, but contains the reciprocal of the applied electric field to all orders. This means that the Stark regime will appear sharp for large values of the external electric field in semiconductors. Only in the approximation of the zero order of the perturbation theory, can the exact Wannier-Stark localization hold.

The Wannier-Stark localization for band electrons moving under the influence of lattice potentials and electric fields has been extensively discussed in the literature.[1-4] To such a problem, the analytic solutions for the case of one-band approximation were presented decades ago,[2,3,5] 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. Fukuyama, Bari and Fogedby[6] then studied the problem of a two-band tight-binding system and concluded that the two Stark ladders existed, each one being associated with one of the bands, and they are in some way coupled together. But, the precise details of the coupling were not discovered. Of late, this two-band tight-binding model has been solved analytically by means of the perturbation theory with the help of $SU(2)$ symmetry.[7] More recently, removing the tight-binding confinement, this method has been extended to the two-band approximation for the one-dimensional case quite generally, and the exact solutions for the energy spectrum and the wave function have been obtained under

the assumption of weak interband coupling. However, it is found that the energy spectrum not only involves a linear term in the applied electric field, i.e., the Stark ladder, but contains the reciprocal of the applied electric field to all orders. This means that the Stark regime would appear sharp for greater values of the external field.[8] For the case of N-band approximation ($N \geq 3$), it was also shown that the energy spectrum was that of interspaced Stark ladders,[9] but the precise details of the energy structure were not given owing to the interband coupling.

In this paper, we investigate the three-dimensional Wannier-Stark localization in semiconductors with taking into account the interband coupling by using our previous techniques. The Schrödinger equation for an electron in a periodic potential $V(\mathbf{r})$ and a constant electric field $\mathbf{E}_0$ is

$$\left(\frac{p^2}{2m} + V(\mathbf{r}) - e\mathbf{E}_0 \cdot \mathbf{r}\right)\Psi(\mathbf{r}) = \epsilon\Psi(\mathbf{r}) \tag{1}$$

For convenience, we will assume that the electric field is in the x direction. By expressing the eigenvector $\Psi(\mathbf{r})$ as a linear superposition of Bloch functions $\psi_{n\mathbf{k}}(\mathbf{r})$, i.e., $\Psi(\mathbf{r}) = \sum_{n\mathbf{k}} B_n(\mathbf{k})\psi_{n\mathbf{k}}(\mathbf{r})$, one obtains the following equation for the amplitudes $B_n(\mathbf{k})$ in the $n\mathbf{k}$ representation[10,11]

$$[\varepsilon_n(\mathbf{k}) - \epsilon - eE_0X_{nn}(\mathbf{k}) - eE_0 i\frac{\partial}{\partial k_x}]B_n(\mathbf{k}) - \sum_{m\neq n} eE_0X_{nm}(\mathbf{k})B_m(\mathbf{k}) = 0 \tag{2}$$

where $\varepsilon_n(\mathbf{k})$ is the energy corresponding to the Bloch function and

$$X_{nm}(\mathbf{k}) = \frac{(2\pi)^3}{\Omega}\int d^3\mathbf{r}u^*_{n\mathbf{k}}(\mathbf{r})i\frac{\partial}{\partial k_x}u_{m\mathbf{k}}(\mathbf{r}) \tag{3}$$

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

$$b_n(\mathbf{k}) = B_n(\mathbf{k})\exp\{\frac{-i}{eE_0}\int_0^{k_x} dk'_x[\epsilon - \varepsilon_n(\mathbf{k}') + eE_0X_{nn}(\mathbf{k}')]\} \tag{4}$$

$$\begin{aligned}\theta_{nm}(\mathbf{k}) &= \frac{1}{eE_0}\{\alpha_{nm}(\mathbf{k}) + \int_0^{k_x} dk'_x[\varepsilon_n(\mathbf{k}') - \varepsilon_m(\mathbf{k}') \\ &\quad -eE_0X_{nn}(\mathbf{k}') + eE_0X_{mm}(\mathbf{k}')]\}\end{aligned} \tag{5}$$

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

$$X_{nm}(\mathbf{k}) = \mid X_{nm}(\mathbf{k}) \mid \exp[i\alpha_{nm}(\mathbf{k})/eE_0], \qquad (n \neq m) \tag{6}$$

and considering the case of two-band approximation, Eq.(2) becomes

$$i\frac{\partial}{\partial k_x}b_0(\mathbf{k}) + \mid X_{01}(\mathbf{k}) \mid \exp[i\theta_{01}(\mathbf{k})]b_1(\mathbf{k}) = 0 \tag{7}$$

$$i\frac{\partial}{\partial k_x}b_1(\mathbf{k}) + \mid X_{01}(\mathbf{k}) \mid \exp[-i\theta_{01}(\mathbf{k})]b_0(\mathbf{k}) = 0 \tag{8}$$

Setting

$$R(\mathbf{k}) = \begin{pmatrix} b_0(\mathbf{k}) \\ b_1(\mathbf{k}) \end{pmatrix}, \qquad S(\mathbf{k}) = X(\mathbf{k})\sigma_x + Y(\mathbf{k})\sigma_y \tag{9}$$

$$X(\mathbf{k}) = -\mid X_{01}(\mathbf{k}) \mid \cos[\theta_{01}(\mathbf{k})], \quad Y(\mathbf{k}) = -\mid X_{01}(\mathbf{k}) \mid \sin[\theta_{01}(\mathbf{k})] \tag{10}$$

where σ_x and σ_y are the Pauli matrices, Eqs.(7) and (8) can be rewritten together as

$$R(\mathbf{k}) = R(\mathbf{k}_0) - i\int_{k_{0x}}^{k_x} dk_{x1} S(\mathbf{k}_1) R(\mathbf{k}_1) \tag{11}$$

Noticing that from (9) and (10), we have $\mid S(\mathbf{k}) \mid = \mid X_{01}(\mathbf{k}) \mid$. Therefore, if the interband coupling is small, Eq.(11) can be solved by using perturbation theory, *i.e.*,

$$R(\mathbf{k}) = \sum_{m=0}^{\infty} U^{(m)}(\mathbf{k}, \mathbf{k}_0) R(\mathbf{k}_0) \tag{12}$$

where

$$\begin{aligned} U^{(m)}(\mathbf{k}, \mathbf{k}_0) = (-i)^m \left(\prod_{l=1}^{m} \int_{k_{0x}}^{k_x} dk_{xl} \right) \theta(k_{x1} - k_{x2}) \theta(k_{x2} - k_{x3}) \\ \ldots \theta(k_{x(m-1)} - k_{xm}) S(\mathbf{k}_1) S(\mathbf{k}_2) \ldots S(\mathbf{k}_m) \end{aligned} \tag{13}$$

with $\theta(k_x) = 1$ for $k_x > 0$ and 0 otherwise. The function $B_n(\mathbf{k})$ is assumed to be periodic, i.e., $B_n(\mathbf{k}) = B_n(\mathbf{k} + \mathbf{G})$, where $\mathbf{G}$ is the primitive reciprocal-lattice vector. For simplicity, we assume that the field is in the direction of the reciprocal-lattice vector. This leads to the Stark-ladder energy structures

$$\begin{aligned} \epsilon \equiv \epsilon_n^{\pm} = \frac{2\pi n e E_0}{G} + \frac{1}{2G} \int_{-G/2}^{G/2} dk_x [\varepsilon_0(\mathbf{k}) + \varepsilon_1(\mathbf{k}) - eE_0 X_{00}(\mathbf{k}) \\ -eE_0 X_{11}(\mathbf{k})] \pm \frac{eE_0}{G} \phi(G/2, -G/2), \quad (n = integer) \end{aligned} \tag{14}$$

where

$$\begin{aligned} \phi(G/2, -G/2) = \cos^{-1}\{\cos\frac{(\alpha - \beta)}{2} \sum_{m=0}^{\infty} U_x^{(2m)}(G/2, -G/2) \\ - \sin\frac{(\alpha - \beta)}{2} \sum_{m=0}^{\infty} U_y^{(2m)}(G/2, -G/2)\} \end{aligned} \tag{15}$$

$$\alpha = \frac{-1}{eE_0} \int_{-G/2}^{G/2} dk_x [\varepsilon_0(\mathbf{k}) - eE_0 X_{00}(\mathbf{k})] \tag{16}$$

$$\beta = \frac{-1}{eE_0} \int_{-G/2}^{G/2} dk_x [\varepsilon_1(\mathbf{k}) - eE_0 X_{11}(\mathbf{k})] \tag{17}$$

$$\begin{aligned} U_{x(y)}^{(2m)}(G/2, -G/2) = (-1)^m \left(\prod_{l=1}^{2m} \int_{-G/2}^{G/2} dk_{xl} \right) \theta(k_{x1} - k_{x2}) \theta(k_{x2} - k_{x3}) \\ \ldots \theta(k_{x(2m-1)} - k_{x2m}) X(Y)(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_{2m}) \end{aligned} \tag{18}$$

with $X(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_m)$ and $Y(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_m)$ satisfying following recurrence formulas

$$\begin{aligned} X(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_m) = X(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_{m-1}) X(\mathbf{k}_m) \\ + Y(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_{m-1}) Y(\mathbf{k}_m), \quad (m \geq 2) \end{aligned} \tag{19}$$

$$\begin{aligned} Y(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_m) = X(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_{m-1}) Y(\mathbf{k}_m) \\ - Y(\mathbf{k}_1 \mathbf{k}_2 \ldots \mathbf{k}_{m-1}) X(\mathbf{k}_m), \quad (m \geq 2) \end{aligned} \tag{20}$$

The amplitudes $B_0(\mathbf{k}_0)$ and $B_1(\mathbf{k}_0)$ have also been obtained which we have not given here for saving space.

Now, let us turn to the validity of the perturbation condition. As examples, we consider the case of common semiconductors in which the interband coupling between the valence and the conduction bands is[12]

$$|X_{01}(\mathbf{k})| = \frac{E_g^{3/2} k_x}{2\sqrt{\mu}(E_g^2 + k^2 E_g/\mu) k} \tag{21}$$

where E_g and μ are, respectively, the band gap and the reduced effective mass for the pair of bands. Direct calculation from this result shows that $|U^{(1)}(\mathbf{k}, \mathbf{k}_0)| < \pi/4$. Hence, at least, our results can be applied to semiconductors.

It is worthy to note that the character of the spectrum in the three-dimensional case is same with that of the one-dimensional case, i.e., the spectrum not only involves a linear term in the applied electric field, but contains the reciprocal of the applied electric field to all orders. This implies that the Stark regime will appear sharp for great values of the external electric field. Such conclusion is qualitatively consistent with Movaghar's theoretical analyses[13] and is in agreement with many experimental results.[14-18] Only in the approximation of the zero order of the perturbation theory, can the exact Wannier-Stark localization hold. In this case, the spectrum becomes

$$\begin{aligned} \epsilon \equiv \epsilon_n^{\pm} = \frac{2\pi n e E_0}{G} + \frac{1}{2G} \int_{-G/2}^{G/2} dk_x [\varepsilon_0(\mathbf{k}) + \varepsilon_1(\mathbf{k}) - eE_0 X_{00}(\mathbf{k}) \\ -eE_0 X_{11}(\mathbf{k})] \pm \frac{eE_0}{2G}(\alpha - \beta) \end{aligned} \tag{22}$$

It should also be emphasized is that also same with that of the one-dimensional case, the perturbation condition in the three-dimensional case has still nothing to do with the external electric field. This is very interesting.

In conclusion, we should like to indicate that since the exact results for the energy spectrum and the wave functions in the three-dimensional case have been obtained with interband coupling being taken into account, to calculate other physical quantities of the system discussed in this paper up to any order of the perturbation theory is, in principle, straightforward.

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