An alternative method for the exact calculation of Wannier–Stark localization in superlattices

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We present an alternative method for the exact calculations of the Wannier–Stark (WS) localization in a long periodic potential corresponding to a (50 Å/30 Å) GaAs/Ga0.7Al0.3As superlattice. We show that the electric field dependence of the electron wavefunction has unique localization dynamics. One interesting prediction is a small effect involving the change of the dipole field with increasing WS field. It is argued that this may give rise to parasitic effects in Bloch oscillations and, therefore, to noise in coherent terahertz emission.

Key words: Wannier–Stark, superlattices, quantum wells.

1. Introduction

The existence or otherwise of the Wannier–Stark (WS) localization and the Bloch oscillations have been two of the most controversial issues of solid-state physics [1, 2]. Earlier work on electron motion in periodic potentials in the presence of an external uniform electric field [3, 4] predicted charge oscillations, the so-called Bloch oscillations. These occur, in the absence of scattering, as a result of the increase, with time, in the wavevector and the energy of the electrons up to the first Brillouin zone boundary, and with the subsequent decrease in the second zone. Thus, periodic modulation of the electron energy and the resultant spatial oscillations with a frequency \( \nu = e F \Lambda / \hbar \) are expected. (Here \( e \) is the electronic charge, \( F \) in the applied field, \( \Lambda \) is the superlattice period and \( \hbar \) is the Plank’s constant.)

The observations of the WS ladder and the Bloch oscillations are not possible in bulk semiconductors at electric fields below the impact ionization threshold. This is because the lattice constant is too small and the oscillation period is much longer than typical scattering times. Therefore all the experiments on WS ladders involve superlattices, and involve the steady-state measurements of [5, 6]. These experiments clearly
demonstrate that the electric field induced localization of electron–hole pairs in the individual wells would otherwise be free to move in the superlattice through the minibands.

Bloch oscillations have been investigated in semiconductor superlattices with a number of inter- and intraband optical techniques. In the inter-band excitation experiments Bloch oscillations are, in principle, utilized as a source of tunable coherent terahertz emission [7]. This has been achieved by using coherent optical excitations of Bloch wavepackets in superlattices in the WS regime. Spatial charge oscillations are then measured by the time-resolved detection of the emitted electromagnetic dipole radiation, experiments indicate that the emission is super-radiant [7, 8]. Reciprocal experiments concerning the absorption of terahertz radiation by the miniband electron in GaAs/As superlattices show negative differential resistance (NDR) due to Bloch oscillations [7–9]. It has also been shown that stable Bloch oscillations can be generated electrically by using inter-band tunneling as injection mechanism and the coherency can be sustained over many periods of the SL [10, 11].

Recently a novel experimental technique that measures the displacement of the Bloch oscillating wavepacket with a spatial resolution of a few angstrom has been used to investigate the spatial amplitude of the oscillating wavepacket as a function of time [12]. In the experiments the dipole field created by oscillating Bloch wavepackets is determined by using the field shift of the WS ladder transitions as sensitive detector. Displacements are then derived, directly, from the shift without any adjustable parameters. The accuracy of the results is primarily determined by the sensitivity of the detector, i.e. the WS localization parameters. We believe, that our current attempt to carry out an exact calculation of the WS localization using a simpler alternative method is timely.

2. Theory

The concept of the WS ladder was introduced by Wannier [13–16] to explain the states of an electron in a periodic potential in a uniform external electric field. In the absence of an electric field all the electronic states are degenerate, therefore eigenstates of a periodic system form bands of delocalized states which extend over the entire solid. The application of an electric field lifts the degeneracy between the local electronic levels. As a result, electronic states become localized.

Since 1987, Emin and Hart [17] and others (Leo and MacKinnon [18, 19], Kleinman [20]) have discussed the possibility of the existence of an inter-band matrix element in a superlattice in a uniform external electric field as to remove the subbands, hence lift the degeneracy. As a result each quantum well in the periodic chain has its own eigenstates and the wavefunctions are well localized. If the energy difference of localized states between adjacent wells belonging to the same band index \( n \) is less than different \(|eF|\) inter-band coupling could not be zero. If however, this energy difference is \(|eF|\), the derivative of the matrix element with respect to \( k \) vector \( \frac{\partial}{\partial k} I(n, k; n', k') \) must be zero [21]. Here inter-band matrix element \( I \), is given by:

\[
I(n, k; n', k') = \int_0^A dx \cdot e^{i(k-k')x} \cdot u_{F,n,k}^*(x) \cdot u_{F,n',k}(x)
\]

where \( n \) is the band index and \( F \) is the electric field and thus \( u \) is the periodic part of Bloch function depending on external field \( F \).

In a previous publication we reported the vanishing inter-band matrix element by using a simple potential profile previously [22]. In this case each well thickness \( t_A \) is located over a \( dV \) increment in energy with respect to the adjacent one and the wells are separated from the barriers by thickness \( s \). In that study, a step-like increment in the potential simulates the effect of an external field applied along the growth direction.

In this study, we show the same simple method of WS localization. Following Emin and Hart [21], we
write the potential term of the Hamiltonian as,

\[ V_E(z) = \sum_{i=0}^{N-1} \{ eF(z - i\Lambda) \cdot S(z - i\Lambda) + V_0 S(z - i\Lambda - t_\Lambda) \} \cdot S[(i + 1)\Lambda - z] \]  \hspace{1cm} (2a) \\
\[ V_S(z) = eF \sum_{i=1}^{N} S(z - i\Lambda). \]  \hspace{1cm} (2b)

Here \( S \) is the step function, \( \Lambda \) is the superlattice (SL) period. The sum of \( V_E \) and \( V_S \) is the true potential profile of the SL in the homogeneous external electric field \( F \). Equation (2a) defines the field-dependent periodic structure as shown in Fig. 1C, which is the sum of the saw-tooth potential in Fig. 1A and the zero field periodic potential in Fig. 1B. Equation (2b) describes the step-like potential as shown in Fig. 1D.

Thus, the Hamiltonian of the system is given as,

\[ H = \frac{\dot{p}^2}{2m^*} + V_E(z) + V_S(z). \]  \hspace{1cm} (3)

This equation can be divided into two parts:

\[ H_E = \frac{\dot{p}^2}{2m^*} + V_E(z) \]  \hspace{1cm} (4)
which is the periodic part of the full Hamiltonian, and $V_S$ which is the step-like potential. The Schrödinger equation of the field-dependent periodic structure (see Fig. 1C) in terms of a dimensionless reduced coordinate $\tilde{z} = z/\Lambda$ becomes

$$\frac{\partial^2 \Psi_{\tilde{F},n,k}(\tilde{z})}{\partial \tilde{z}^2} = \left(\pi / \tilde{F}\right)^{2/3} \otimes \left[ \sum_{i=1}^{N-1} (\tilde{F}(\tilde{z} - i)S(\tilde{z} - i) + \tilde{V}_0S(\tilde{z} - i - \tilde{\epsilon}_F(n,k)))S(i + 1 - \tilde{z}) - \tilde{\epsilon}_F(n,k) \right] \Psi_{\tilde{F},n,k}(\tilde{z}) = 0 \quad (5)$$

where $\tilde{F} = eF/E_0$ ($E_0$ is the zero field ground-state energy, its normalized well width is 1 ($\Lambda/\Lambda$) and $\tilde{\epsilon}_F(n,k)$ is eigenenergy in the $n$th band which has wavevector $k$ in electric field $F$). $\tilde{V}_0$ is the normalized barrier height normalized with respect to $E_0$. The wavefunction can therefore be represented by Airy functions that are defined as:

$$\Psi_{n,k,F}(\tilde{z}) = [A_n \text{AiryAi}(U_{n,k,F}(\tilde{z})) + B_n \text{AiryBi}(U_{n,k,F}(\tilde{z}))]e^{i\tilde{z}} \quad (6a)$$

$$\Psi_{b,n,k,F}(\tilde{z}) = [C_n \text{AiryAi}(U_{n,k,F}(\tilde{z})) + D_n \text{AiryBi}(U_{n,k,F}(\tilde{z}))]e^{i\tilde{z}} \quad (6b)$$

in the well and barrier regions, respectively. Here:

$$U_{n,k,F}(\tilde{z}) = (\pi / \tilde{F})^{2/3} \sum_{i=0}^{N-1} (\tilde{F}(\tilde{z} - i)S(\tilde{z} - i) + \tilde{V}_0S(\tilde{z} - \tilde{\epsilon}_F(n,k)))S(i + 1 - \tilde{z}) - \tilde{\epsilon}_F(n,k) \quad (7a)$$

$$U_{b,n,k,F}(\tilde{z}) = (\pi / \tilde{F})^{2/3} \sum_{i=0}^{N-1} (\tilde{F}(\tilde{z} - i)S(\tilde{z} - i) + \tilde{V}_0S(\tilde{z} - i - \tilde{\epsilon}_F(n,k)))S(i + 1 - \tilde{z}) - \tilde{\epsilon}_F(n,k) \quad (7b)$$

In eqns (7a) and (7b), reduced well width ($\tilde{\epsilon}_F = \epsilon F/\Lambda$) is used.

In the numerical calculations we used $N = 21$ well/barriers with widths 50 Å and 30 Å respectively. For convenience, in the calculation $m^*_e$ is taken as a variable. (For the results presented in this paper $m^*_e = 0.45 m_e$ to correspond to heavy hole effective mass.) Figure 2A shows the first and second subband wavefunctions in the SL in the absence of the applied electric fields. It is evident from the figure that the wavefunctions have the typical characteristic of a short period SL as expected. In Fig. 2B and C the first two subband wavefunctions of field-dependent periodic potential are shown for applied electric fields of $F = 5 \times 10^4$ V cm$^{-1}$ and $F = 10^5$ V cm$^{-1}$ respectively. It is obvious that as the electric field is increased from zero the first subband wavefunction accumulates to the left-hand side of the quantum wells. This is due to the finite potential gradient arising from zero the first subband wavefunction of the external field, at the bottom of the wells. The second subband wavefunctions, however, move to the right-hand side of the quantum wells. This is because the barrier height as seen by the second subband electron is reduced by the external field and, therefore, the electron wavefunction penetrates further into the barriers. Eigenfunction of the total Hamiltonian must satisfy,

$$H\psi^m_{F}(\tilde{z}) = \tilde{\epsilon}_m\psi^m_{F}(\tilde{z}) \quad (8)$$

where $\tilde{\epsilon}_m$ is the reduced eigen energy of the real system, and $\psi^m_{F}(\tilde{z})$ is the superposition of the electric-field dependent Bloch functions, belonging to the $m$th eigenvalue and defined as;

$$\psi^m_{F}(\tilde{z}) = \sum_{n,k} A_m(n,k)\Psi_{n,k,F}(\tilde{z}). \quad (9)$$

One possible treatment of the field-dependent Bloch functions has been demonstrated by Emin and Hart [21] which involves the expansion of coefficients $A_m(n,k)$. However, we believe that a better solution would be the expansion for all the states in terms of field-dependent Wannier functions as they are peaked functions and therefore better suited to the solution of the localization problem as it is here.
Wannier function for nth band and at site \(p\) is expressed by field-dependent Bloch functions as

\[
W_n^\tilde{F}(\tilde{z} - p) = N^{-1/2} \sum_k e^{-ikp} \psi_{n,k;\tilde{F}}(\tilde{z}).
\] (10)

The wavefunction of the total Hamiltonian in eqn (9) can therefore be written as,

\[
\psi_m^\tilde{F}(\tilde{z}) = N^{-1/2} \sum_{n',k'} A_{m(n',k')} e^{ik'p'} W_{n'}^\tilde{F}(\tilde{z} - p').
\] (11)

If we write,

\[
\epsilon_{n',p'}^m = N^{-1/2} \sum_k A_{m(n',k')} e^{ik'p'}
\] (12)

eqn (11) is now independent of \(k\), i.e.

\[
\psi_m^\tilde{F}(\tilde{z}) = \sum_{n',p'} \epsilon_{n',p'}^m W_{n'}^\tilde{F}(\tilde{z} - p').
\] (13)

If we apply the full Hamiltonian \(H\) to eqn (13) and by multiplying \(W_{n'}^\tilde{F}(\tilde{z} - p)\) on the left-hand side and integrating over the full space, the following effective Schrödinger equation can be formed in Dirac repre-
sensation,
\[ \langle \tilde{F}; p, n|H_E + V_S(\tilde{z})|\tilde{F}, m \rangle = N^{-1} \sum_{p', k} C_{n', p'}^{m} e^{i(p' - p')\tilde{z}}(n, k) \]
\[ + N^{-1} \tilde{F} \sum_{n', p', k', k} C_{n', p'}^{m} e^{i(kp' - kp)\tilde{z}} \left( \langle \tilde{F}; n, k \left| \sum_{i=1}^{N} S(\tilde{z} - i) \right| \tilde{F}, n', k' \rangle \right) \]
\[ = \tilde{e}_{m} \sum_{n', p'} C_{n', p'}^{m} \delta_{p, p'} \delta_{n, n'}. \quad (14) \]

From [21], the inter-matrix element is
\[ \langle \tilde{F}; n, k \left| \sum_{i=1}^{N} S(\tilde{z} - i) \right| \tilde{F}, n', k' \rangle = I(n, k; n', k') \int \frac{d\tilde{z}}{i} \frac{\partial}{\partial \tilde{z}} (\delta_{kk'}) \quad (15) \]
where \( \langle \tilde{F}; n', k' \rangle \) is a field-dependent Bloch function. Equation (15) takes the form;
\[ \langle \tilde{F}; p, n|H|\tilde{F}, m \rangle = N^{-1} \sum_{p', k} C_{n', p'}^{m} e^{i(p' - p')\tilde{z}}(n, k) \]
\[ + \frac{\tilde{F}}{i} \sum_{n', p', k', k} C_{n', p'}^{m} e^{i(kp' - kp)\tilde{z}} I(n, k; n', k') \frac{\partial}{\partial k'} (\delta_{kk'}) \]
\[ = \tilde{e}_{m} \sum_{n', p'} C_{n', p'}^{m} \delta_{p, p'} \delta_{n, n'}. \quad (16) \]

where \( I(n, k; n', k') = \int_{0}^{\Lambda} d\tilde{z} e^{i(k' - k)\tilde{z}} u_{F,n,k}(\tilde{z}) u_{F,n,k}(\tilde{z}) \) is the periodic part of the Bloch function. Inter-band coupling in eqn (16) can be rewritten as
\[ -i \tilde{F} \sum_{n', p', k', k} C_{n', p'}^{m} \frac{\partial}{\partial k'} (e^{i(p - p')\tilde{z}} I(n, k; n', k') \delta_{kk'}) + i \tilde{F} \sum_{n', p', k', k} C_{n', p'}^{m} \delta_{kk'} \frac{\partial}{\partial k'} (e^{i(k' - k)\tilde{z}} I(n, k; n', k')) \]
\[ = \left\langle n, k \left| \tilde{F} \sum_{i=1}^{N} S(\tilde{z} - i) \right| n', k' \right\rangle. \quad (17) \]

The first term on the left-hand side in eqn (17) is
\[ -i \tilde{F} \sum_{n', p', k'} C_{n', p'}^{m} (i(p - p')) e^{i(p - p')k'} I(n, k'; n', k') - i \tilde{F} \sum_{n', p', k'} C_{n', p'}^{m} e^{i(p - p')k'} \frac{\partial}{\partial k'} I(n, k; n', k') \quad (18) \]
and the second term is
\[ i \tilde{F} \left\{ \sum_{n', p', k'} C_{n', p'}^{m} \left( -ip' e^{i(p - p'k') I(n, k'; n', k')} + e^{i(p - p'k') \frac{\partial}{\partial k'} I(n, k; n', k')} \right|_{k=k'} \right\}. \quad (19) \]

The sum of eqns (18) and (19) gives
\[ -i \tilde{F} \sum_{n', p', k'} C_{n', p'}^{m} e^{i(p - p')k'} \left( \frac{\partial}{\partial k'} I(n, k'; n', k') \right) + i \tilde{F} \sum_{n', p', k'} C_{n', p'}^{m} e^{i(p - p')k'} \left( \frac{\partial}{\partial k'} I(n, k; n', k') \right)_{k=k'} \]
\[ + \tilde{F} \sum_{p', k'} C_{n', p'}^{m} p \delta_{pp'} \delta_{kk'}. \quad (20) \]
Because of $I(n, k' ; n', k') = N^{-1} \delta_{n,n'} \delta_{k,k'}$ inter-band matrix element

$$
\left\langle n, k | \tilde{F} \sum_{i=1}^{N} S(\tilde{z} - i) | n', k' \right\rangle = \tilde{F} \sum_{n', p'} c_{n', p'}^m \delta_{n,n'} \delta_{p,p'} - \tilde{F} \sum_{n', p', k'} c_{n', p'}^m e^{i(p-p')k'} \frac{\partial}{\partial k} I(n, k ; n', k') \big|_{k=k'}.
$$

(21)

If we examine eqn (21), we see that the inter-band matrix elements can be given by a second-line term which contains the term $\partial I(n, k ; n', k') / \partial k$. This term indeed has a vanishing value as claimed in [21] because its derivative with respect to $k$ is zero (the function differentiated is a periodic function of $k$). Thus, the eigenvalue equation seen in eqn (14) now takes the form,

$$
\sum_{p', n} \left[ \frac{1}{N} \sum_{k} e^{ik(p-p')} \tilde{\epsilon}(n, k) \delta_{n,n'} - \tilde{\epsilon}_m \delta_{p,p'} \delta_{n,n'} + \tilde{F} p \delta_{n,n'} \delta_{p,p'} \right] c_{n', p'}^m = 0.
$$

(22)

Using numerical method, eqn (22) has been exactly solved and energy eigenvalues have been obtained. This also shows that the inter-band coupling of nondegenerate states remove. Furthermore this simple master equation shows that the first term in eqn (22) gives average subband energy for $p = p'$ (21 meV) in the first subband while the contribution is very small (0.001 meV) for $p \neq p'$ for practical parameters given in our article. As a result of eqn (22) we can also say that each well has its own localized state, that its energy shifts as an amount of an integer multiplier of the central localized energy resulting as a ladder-like energy spectrum.

3. Results and discussions

It is obvious from eqn (22) that for a given site index $p$ the energy of the localized state ($\tilde{\epsilon}_m$) is equal to the sum of $\tilde{F} p$ and the average subband energy $\tilde{\epsilon}(\tilde{F}, n)$, i.e.

$$
\tilde{\epsilon}_m = \tilde{\epsilon}(\tilde{F}, n) + \tilde{F} p
$$

(23)

where $\tilde{\epsilon}(\tilde{F}, n) = \left[ \frac{1}{N} \sum_{k} e^{ik(p-p')} \tilde{\epsilon}(n, k) \delta_{n,n'} \right]$ for $p = p'$ if $k'$'s are discrete and $\tilde{\epsilon}(\tilde{F}, n) = \Lambda/2\pi \int_0^{2\pi/\Lambda} dk e^{ik(p-p')} \tilde{\epsilon}(n, k)$ if $k'$'s are continuous and also for $p = p'$. Therefore, the eigenvalues have the ladder structure as expected (WS). Figure 3 shows the localized wavefunctions for the first subband at different electric field strength (1, 5, and $10 \times 10^4$ V cm$^{-1}$). Localized wavefunctions for three different electric fields are similar to those in [24] by using the Kane wavefunction of the lowest miniband for superlattice structure, consisting of 12-monolayers GaAs and 6-monolayers AlAs. In order to eliminate the edge effects we only look at the first five wells on all sides of the 11th edge which is marked as 0 in this figure. It is evident from the figure that for the center well and the adjacent well on the right-hand side, increasing the electric field results in an increase in the localization. The first adjacent wells on the left-hand side, however, show a decrease in localization with field. In a terahertz emission experiment this behavior would imply the growth of electric dipole field as expected. It is worth pointing out the remarkable sensitivity of the localization characteristics on the applied field. Furthermore, although it is a very small effect, for the third well on the left and the second well on the right of the center well the change in localization with applied electric field shows exactly the opposite behavior to those in the other wells. That is the localization increases in the third left-hand side well and decreases in the second right-hand side well. This small effect might give rise to parasitic effects and noise in experiments concerning field-dependent oscillations and terahertz emission as often observed at elevated temperatures [23].
4. Conclusion

A simple alternative and elegant method for the exact numerical calculation of WS localization parameters are presented. Our results give results similar to those by others [21] and predict, in principle, the experimental results involving the measurements of Bloch oscillations.

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