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Wannier quantization of a superlattice subband under an electric field

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Abstract. Wavefunctions of electronic Wannier–Stark states in a superlattice are calculated with a finite Kronig–Penney model. Overlap integrals between electron and heavy-hole wavefunctions centred in the same well layer, and in first- and second-neighbour wells are calculated as functions of the applied field. The results show good agreement with experimental results on photoluminescence. The problem is also treated by a one-band approximation method, which gives a closed expression for the wavefunction of the Wannier–Stark states; this is compared with the results of accurate calculations with the Kronig–Penney model.

1. Introduction

Wannier [1] predicted long ago that the quasicontinuous energy bands, when subject to an applied electric field, will split up into discrete localized states which have become known as Wannier–Stark states. During the subsequent years there have been many theoretical investigations of the problem, concerned, however, mainly with the validity of Wannier's arguments. Recently, several theoretical [2–4] and experimental [5, 6] investigations, exploiting the favourable conditions afforded by superlattices (large period and small subband width), have clearly demonstrated the effect of Wannier–Stark states as predicted by Wannier. Therefore, for further investigation of the Wannier–Stark states, it will be of interest to develop convenient and effective methods for carrying out realistic calculations of the Wannier–Stark states.

In this paper we shall first carry out, by an expansion method, theoretical calculations for a finite Kronig–Penney model on which is superposed the potential of an applied electric field, focusing on the variation in the Wannier–Stark localization with increasing electric field. Our calculation results are quantitatively compared with the results of the photoluminescence (PL) experiment [5] for intermediate and high fields. Bastard and co-workers [2, 3] found that the simplest semiclassical treatment reproduced the Wannier–Stark localization remarkably well. We had proposed a more elaborate one-band approximation method in connection with Landau levels in a superlattice band in a parallel magnetic field with good results [7]. We shall show that this method leads simply to a closed expression for the Wannier–Stark localized wave function in terms of the

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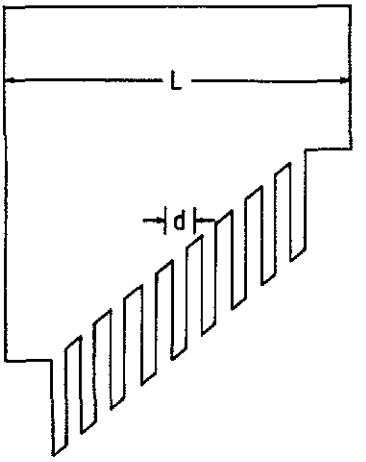

Figure 1. Finite Kronig–Penney model used in this paper.

band dispersion function $E(k)$, which has been found to reproduce closely the accurately calculated wavefunction.

2. Finite Kronig–Penney model for superlattices under an electric field

We shall use a Kronig–Penney model consisting of a finite number of quantum wells limited by infinite-potential walls as illustrated in figure 1 to simulate a superlattice under an applied electric field. The two barriers at the edge are wide enough (e.g. 100 Å) so that the wavefunctions of the bound states in the quantum wells are actually zero at the infinite-potential walls. We can use a series of sine functions as the basic functions for expanding the wavefunctions of the superlattice:

$$\psi(z) = \sqrt{\frac{2}{L}} \sum_n C_n \sin\left(\frac{n\pi z}{L}\right) \tag{1}$$

where L is the total width between the infinite walls; the origin of the z coordinate is taken at the left infinite wall. Inserting the wavefunction into the equation

$$-(1/2m^*)(\mathrm{d}^2\psi/\mathrm{d}z^2) + [V(z) + eFz]\psi = E\psi \tag{2}$$

where m^* is the effective mass (here we assume that the effective masses in the well and barrier materials are equal) and $V(z)$ is the finite Kronig–Penney potential in our model (figure 1) under zero field, we obtain the secular equation for the expansion coefficients C_n in (1). The Hamiltonian matrix elements of $V(z)$ and eFz are very simple with our use of the sine functions.

For direct comparison with the available experimental results [5], we have taken in our calculation the same parameters for the $GaAs/Al_{0.35}Ga_{0.65}As$ superlattice as in [5], namely the band offsets for the conduction and valence bands are 0.26 eV and 0.175 eV, the effective masses for electrons are $0.067m_0$ and $0.1m_0$, the effective masses for heavy holes are $0.4m_0$ and $0.4m_0$, and the widths for the well and the barrier are 30 Å and 35 Å. An average electronic effective mass of $0.085m_0$ is used in our calculation. The finite length of our model for the superlattice will interfere with the Wannier–Stark localization

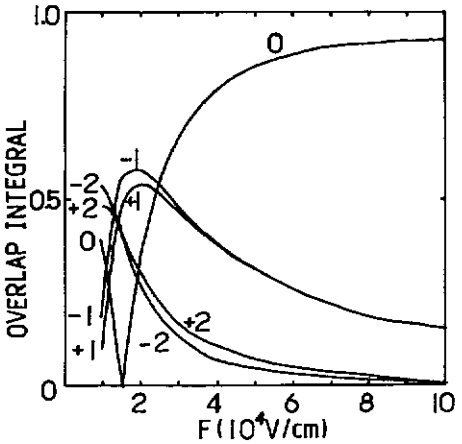

Figure 2. Overlap integrals of the electron and heavy-hole wavefunctions localized in the same well layer (denoted by 0) and in first- and second-neighbour wells (denoted by ±1, ±2) as functions of external electric field.

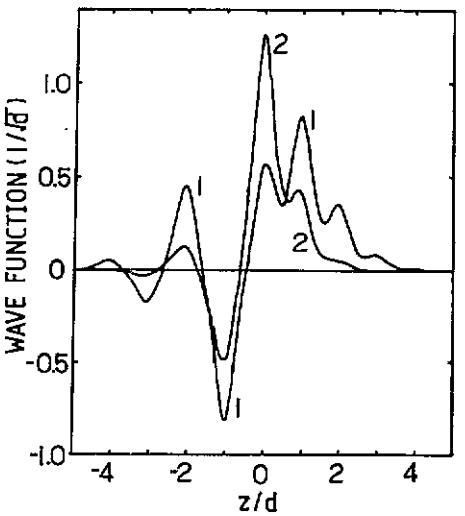

Figure 3. Electronic wavefunctions (in units of $1/\sqrt{d}$) for the electric field 2×10^4 V cm^{-1} (curve 1) and 5×10^4 V cm^{-1} (curve 2).

below a certain threshold electric field. We find that with an electric field F larger than 10^4 V cm^{-1}, the eigen-energies conform to the Wannier–Stark ladder $E = E_0 + eFnd$, where E_0 is the eigen-energy in a single quantum well. We have calculated the overlap integrals between electron and heavy-hole wavefunctions, which are localized around the same well layer, or first- and second-neighbour wells as functions of the external field F. The results are shown in figure 2, where 0, ±1, ±2 designate the relative dispositions of the localization sites for the electron and hole. In figure 2 we can distinguish two regions of the electric field: intermediate (1.5×10^4 V cm$^{-1} < F < 5 \times 10^4$ V cm^{-1}), and high ($F > 5 \times 10^4$ V cm^{-1}), just as in [5] (the low-electric-field region cannot be covered properly by our finite model (figure 1)). In the high-electric-field region, the Wannier wavefunctions are largely localized in one well; the overlap integral 0 is largest and approaches unity when the electric field increases, while the overlap integrals ±1 and ±2 decrease towards zero. In the intermediate-electric-field region, the case is more complex. When the electric field decreases, the overlap integral 0 decreases and the overlap integrals ±1 and ±2 increase. At a critical field (2.5×10^4 V cm^{-1} in our case) the overlap integral 0 becomes smaller than the overlap integral ±1, and at an electric field of 1.5×10^4 V cm^{-1} the overlap integral 0 equals zero. These results are completely in agreement with the PL experimental results (figure 2 in [5]). From figure 2 in [5] we see that the −1 PL peak is larger than the 0 peak at a bias voltage of +0.4 V (corresponding to an electric field of 2.4×10^4 V cm^{-1}), and the −1 peak becomes smaller than the 0 peak at a bias voltage of 0 V ($F = 3.2 \times 10^4$ V cm^{-1}). The electric field value at which the −1 and 0 peaks are equal is in agreement with the theoretical value (2.5×10^4 V cm^{-1}). At a bias voltage of +0.8 V ($F = 1.6 \times 10^4$ V cm^{-1}) the 0 PL peak disappears, which is also in agreement with the theoretical value (1.5×10^4 V cm^{-1}). This result is also in agreement with the result of the one-band tight-

binding model discussed by Bleuse *et al* [2]. According to that model the wavefunction value of the νth state in the nth well is given by $J_{n-\nu}(W/2eFd)$ ($J_{n-\nu}(x)$ is the Bessel function of order $n-\nu$). In our case, $n-\nu=0$, the band width $W=45$ meV and $d=65$ Å; thus for $F=1.5\times10^4$ V cm^{-1} we obtain $W/2eFd=2.3$, which is nearly the zero point of $J_0(x)$.

In figure 3 are shown the wavefunctions calculated with two electric fields (2×10^4 and 5×10^4 V cm^{-1}). From the figure we see that with a field of 2×10^4 V cm^{-1} the magnitude of the wavefunction in the centre well is smaller than that in the nearest-neighbour wells, resulting in -1 peaks larger than the 0 peak. In the case with a field of 5×10^4 V cm^{-1} the magnitude of the wavefunction in the centre well is much larger than that in the neighbouring wells, and the localization is obvious. It is also to be noted that the wavefunction is not symmetrical with respect to the origin: on the left-hand side (lower potential) the wavefunction is oscillatory, taking up positive and negative values at successive wells, while on the right-hand side (higher potential) the wavefunction is always positive with maxima at the successive wells.

3. One-band model of the Wannier–Stark ladder and corresponding wavefunction

In the above, we have treated the Wannier–Stark states by direct quantum mechanical calculation with a limited Kronig–Penney model on which is superposed the applied potential. As the Wannier–Stark problem is essentially the problem of quantization of an energy band in the presence of an applied field, it is thus of interest to explore effective methods to treat the problem on the basis of a superlattice energy band as given (e.g. that derived with a Kronig–Penney model). We have already developed such a method in connection with calculating Landau levels formed in a superlattice energy band in a parallel magnetic field with good results [7]. The method is a one-band approximation method. It is a formal generalization of the usual effective-mass theory, namely, for a given energy band, the envelope function is assumed to be governed by an effective Hamiltonian

$$H=E(k)+eFz \tag{3}$$

where $E(k)$ is the band dispersion function in the k_z direction, k is the operator $(1/\mathrm{i})(\mathrm{d}/\mathrm{d}z)$. For solving the problem we transform the Schrödinger equation into momentum representation by

$$z=\mathrm{i}\hbar\,\mathrm{d}/\mathrm{d}p. \tag{4}$$

The corresponding Schrödinger equation is

$$[eF\mathrm{i}\hbar\,\mathrm{d}/\mathrm{d}p+E(p/\hbar)]\psi(p)=E\psi(p). \tag{5}$$

The solution of (5) is easily obtained:

$$\psi(p)=C\exp\left\{-\mathrm{i}\frac{1}{eF}\int\left[E-E\left(\frac{p}{\hbar}\right)\right]\mathrm{d}\left(\frac{p}{\hbar}\right)\right\} \tag{6}$$

where C is a normalization constant. Owing to the nature of $E(k)$, k is in the nature of

a cyclic variable; thus $\psi(p)$ must be a periodic function in momentum space with period $\hbar(2\pi/d)$, which demands that

$$\frac{1}{eF}\int_{-\pi/d}^{\pi/d}[E - E(k)]\,\mathrm{d}k = 2\pi n \tag{7}$$

where $k = p/\hbar$. In this scheme, equation (7) provides the quantization condition for the eigen-energy, from which we obtain

$$E = eFnd + \frac{d}{2\pi}\int_{-\pi/d}^{\pi/d} E(k)\,\mathrm{d}k. \tag{8}$$

Equation (8) is just the Wannier–Stark ladder formula first derived by Wannier [1]. The second term in (8) is the average energy of the energy band.

The energy band $E(k)$ can be simulated by a series in cosine functions [7]:

$$E(k) = \sum_{n=0}^{N} \lambda_n \cos(nkd). \tag{9}$$

Then the eigen-energy in (8) is

$$E = eFnd + \lambda_0. \tag{10}$$

The normalization constant $C = \sqrt{d}$ in wavefunction (6) is obtained from the normalization condition

$$\frac{1}{2\pi}\int_{-\pi/d}^{\pi/d} |\psi(p)|^2\,\mathrm{d}\left(\frac{p}{\hbar}\right) = 1. \tag{11}$$

With the eigen-energy (10) we transform the wavefunction $\psi(p)$ (6) into the coordinate representation,

$$\psi(z) = \frac{\sqrt{d}}{2\pi}\int \mathrm{d}\left(\frac{p}{\hbar}\right)\varphi_k(z)\exp\left\{-\mathrm{i}\frac{1}{eF}\int_0^p\left[E - E\left(\frac{p'}{\hbar}\right)\right]\mathrm{d}\left(\frac{p'}{\hbar}\right)\right\}$$

$$= \frac{\sqrt{d}}{2\pi}\int_{-\pi/d}^{\pi/d}\mathrm{d}k\,U_k(z')\exp\left[\mathrm{i}\left(z'k + \frac{1}{eFd}\sum_{n=1}^{N}\frac{\lambda_n}{n}\sin(ndk)\right)\right] \tag{12}$$

where $z' = z - nd$, $\varphi_k(z)$ is the Bloch function with wavevector k in the single band;

$$\varphi_k(z) = \exp(\mathrm{i}kz)\,U_k(z). \tag{13}$$

Equation (12) gives a general formula of the wavefunction for any form of band energy $E(k)$. If we take only two terms in the band energy expansion (9),

$$E(k) \simeq \lambda_0 + \lambda_1\cos(kd), \tag{14}$$

and let $z'/d = n - \nu$ (i.e. the coordinate at the centre of wells), $U_k(z') = U_0[(n-\nu)d]$ = constant, from (12) we obtain

$$\psi(z) = \frac{1}{\sqrt{d}}\frac{1}{\pi}\int_0^{\pi}\cos\left((n-\nu)\xi + \frac{\lambda_1}{eFd}\sin\xi\right)\mathrm{d}\xi\,U_0 = \frac{1}{\sqrt{d}}J_{n-\nu}\left(\frac{\lambda_1}{eFd}\right)U_0 \tag{15}$$

which is just the result obtained by Bastard and co-workers [2, 3] with the one-band tight-binding model.

Table 1. Wave-function values (in units of $1/\sqrt{d}$) at well centres calculated from equation (2) (in the first rows), and from equation (12) (in the second rows), for electric fields 2×10^4, 5×10^4 and 1×10^5 V cm^{-1}.

F	$\psi(p)$ (units of $(1/\sqrt{d})$ for the following z/d-values								
(V cm^{-1})	−4	−3	−2	−1	0	1	2	3	4
2×10^4	0.050	−0.173	0.450	−0·813	0.572	0.828	0.352	0.083	0.012
	0.056	−0.175	0.450	−0.807	0.562	0.821	0.349	0.082	0.013
5×10^4	0.005	−0.026	0.120	−0.485	1.266	0.419	0.052	0.004	0.000
	0.006	−0.026	0.121	−0.488	1.256	0.416	0.052	0.003	0.000
1×10^5	0.016	−0.023	0.048	−0.265	1.375	0.193	0.009	0.001	0.000
	0.002	−0.009	0.048	−0.279	1.374	0.193	0.011	−0.001	0.000

We compared the wavefunctions for the superlattice in the electric field region of 2×10^4–1×10^5 V cm^{-1} calculated from equation (12) and directly from equation (2). The wavefunction values at well centres calculated by the two methods for three electric fields are given in table 1. From the table we see that the agreement is very good.

In summary, with a finite Kronig–Penney model on which is superposed an applied electric potential we have investigated the Wannier–Stark localization process for intermediate to high electric fields. We calculated the overlap integrals of the electron and heavy-hole wavefunctions localized around the same well layer or around first- and second-neighbour wells, and the results are in agreement with the PL experimental results. We derived by a one-band approximation method general formulae for the eigen-energy and wavefunction of the superlattice under an electric field. They can be reduced to the results of Bastard and co-workers as a special case. It has been verified that the wavefunction is completely in agreement with the accurately calculated wavefunction for the case of modelling the superlattice with a Kronig–Penney model.

Acknowledgment

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