Tamm minibands in superlattices

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The properties of Tamm minibands in superlattices are analyzed in a simple, exactly solvable one-dimensional model.

Interface states, i.e., states which are spatially localized at the boundaries of various layers, in semiconductor superlattices have been discussed in the literature for a long time now (Refs. 1–3; see also Ref. 4). It is exceedingly difficult to analyze the properties of interface states theoretically, since the complex band structure must be known (interface states are Tamm levels with an imaginary quasimomentum[5]).

We would like to propose a simple, exactly solvable model of a superlattice, formed by one-dimensional Kronig-Penney lattices with δ-function potentials. In this model, the minibands of the states localized at interfaces arise from an interaction of Tamm states at neighboring interfaces. In the case of inverted bands, such minibands arise at an arbitrary overlap of the lattice band gaps, in precise agreement with the results of Refs. 2 and 6. In the case of an overlap of uninverted bands, Tamm minibands arise to the extent that the Bloch functions of the band edges differ, and they vanish with increasing energy separation of the corresponding bands. It is extremely important to note that Tamm minibands can be described very accurately in the envelope approximation if the exact Bloch functions of the band edges in the layers in contact are used in the derivation of the boundary conditions. Under the boundary conditions that are ordinarily used,[7] which are found from the constant-flux condition in the effective-mass approximation, the discontinuity in the Bloch (envelope) functions is ignored, with the result that the Tamm minibands are lost (the sole exception to this statement is the case of inverted bands[2,6]).

The δ-functions are used in order to simplify the problem to the extent possible (the results found are also valid when there are square barriers of finite size). To the surprise of the author, he was not able to find a discussion of this simple but exceedingly instructive model in the literature. A similar model was studied in Ref. 8, but only in application to isolated interfaces. Interest in models of this sort has recently increased[9,10] because of the remarkable study by Ohno *et al.*,[11] who first observed Tamm states experimentally, in a model system consisting of a set of quantum wells and a barrier.

We consider a one-dimensional model of a superlattice consisting of N_a and N_b alternating "atomic" layers of "substances" A and B, with the potential

$$V(x) = \begin{cases} p_a\delta(\{x\}), & 0 \le x \le N_a \\ V_b + p_b\delta(\{x\}), & N_a < x < N_a + N_b \end{cases} . \qquad (1)$$

Here $\{x\}$ is the fractional part of x, and we have described only one period of the

superlattice, $D = N_a + N_b$. The "interatomic" distances in substances A and B are assumed for simplicity to be the same, equal to 1; we also assume $\hbar = m = 1$. The parameter V_b makes it possible to shift (along the energy scale) the spectra of A and B with respect to each other and to model various versions of the band overlap.

The spectrum of allowed states $E = E(k)$ in the Kronig-Penney problem with δ-function potentials of a common type is, as we know, found from the equation

$$\cos k = \cos \xi + \frac{p}{\xi} \sin \xi, \tag{2}$$

$[\xi = \sqrt{2(E - V)}]$. This spectrum is an alternation of allowed and forbidden bands. If $p > 0$, the points $\xi = \pi n$, $n = 1,2,...$, are the lower boundaries of the forbidden bands (gaps) (for $p < 0$ they are the upper boundaries; it thus becomes possible to model interfaces with an inversion of bands if $p_a p_b < 0$). We will refer to such band gaps as "$n\pi$ gaps."

An eigensolution of the Schrödinger equation with potential (1) corresponding to the energy E, in the interval $0 < x < D$, is

$$\Psi(x) = \begin{cases} A_0 e^{-i\xi_a\{x\}} + B_0 e^{i\xi_a\{x\}}, & 0 < x < 1 \\ \cdots & \cdots \\ A_{D-1} e^{-i\xi_b\{x\}} + B_{D-1} e^{i\xi_b\{x\}}, & D-1 < x < D \end{cases}. \tag{3}$$

Here

$$\begin{pmatrix} A_m \\ B_m \end{pmatrix} = T_m \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \tag{4}$$

and the transition matrix T_m is the product of m transition matrices t_{aa}, t_{ab}, t_{bb}, and t_{ba} between neighboring "atomic" layers. Explicit expressions for these transition matrices can easily be calculated as functions of the parameters $\xi_{a,b}$ and $p_{a,b}$.

Solutions along the entire x axis are found from the Bloch condition

$$\Psi(x + D) = e^{iKD}\Psi(x). \tag{5}$$

The dispersion relation $E = E(K)$ for a superlattice is given by an equation like (2):

$$\cos K = \frac{1}{2}\mathrm{Tr}[t_{ab}(t_{bb})^{N_b - 1} t_{ba}(t_{aa})^{N_a - 1}]. \tag{6}$$

Figure 1 shows some typical spectra and eigenfunctions (for $K = 0$) calculated from (6) and (3) for $N_a = N_b = 15$, $p_a = -1$, and $p_b = -3$. The value of V_b has been chosen in such a way that the lower boundaries of the 2π gaps of lattices A and B coincide exactly. [The energies in Fig. 1 are reckoned from specifically this value; the levels $\epsilon_{v(c)a}$ and $\epsilon_{v(c)b}$ shown by the dashed lines in Fig. 1 are the lower (upper) boundaries of the 2π gaps of A and B, respectively.] We see that the two minibands near coincident edges of the "valence" bands are interface minibands. They arise because of an interaction between Tamm states localized at neighboring interfaces.

Tamm states at isolated interfaces were recently studied on the basis of a similar

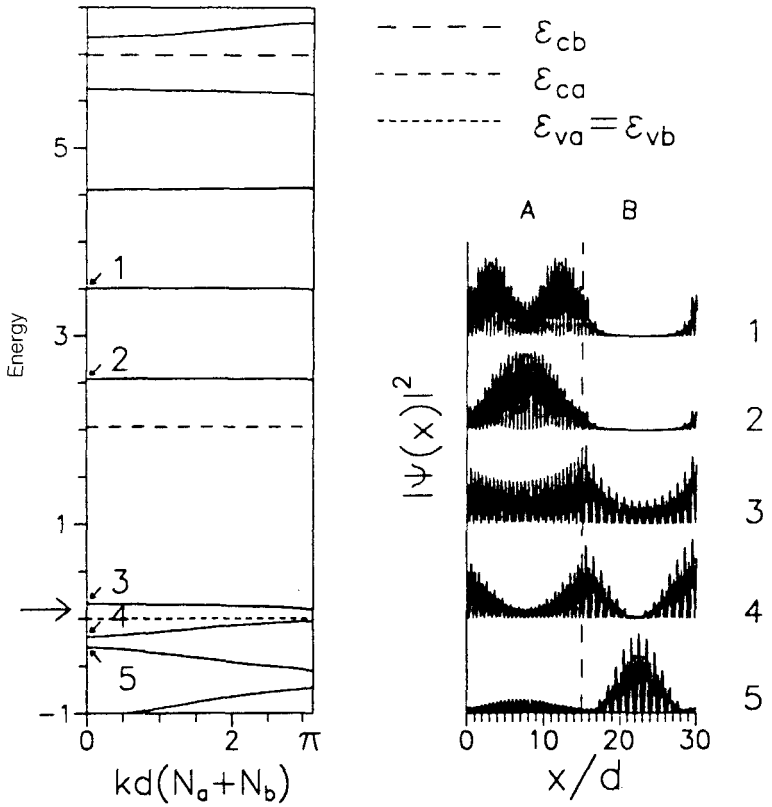

FIG. 1. Energy spectrum (at the left) and square of the modulus of the wave function of the superlattice for $N_a = N_b = 15$, $p_a = -1$, and $p_b = -3$. The values of E and $K = 0$, for which the calculations of $|\Psi|^2$ were carried out, are shown by the sloping arrows in the left-hand part of the figure. The horizontal arrow shows the position of the Tamm level of an isolated interface.

model by Trezeciakowski.[8] It is not difficult to show that the energy of a Tamm state for an isolated interface can be found from the equation (for the case of an overlap of $2n\pi$ gaps)

$$\frac{\xi_a}{\sin \xi_a}\sinh\kappa_a + \frac{\xi_b}{\sin \xi_b}\sinh\kappa_b = p_b - p_a, \tag{7}$$

where $\kappa = |\mathrm{Im}k|$ is the imaginary quasimomentum [a solution of Eq. (2) inside the gap]. If, for example, $p_b < p_a < 0$, a Tamm state arises near the lower boundaries of the 2π gaps if the latter coincide, and it vanishes with increasing distance between the bands. In the situation shown in Fig. 1, a Tamm level with the position shown by the horizontal arrow would exist in the case of an isolated interface. The interaction between states at neighboring interfaces in the superlattice leads (by virtue of their weak localization) to a lifting of the degeneracy and to a splitting of the levels into two Tamm minibands. If, as is typical of the 1D situation, there is no degeneracy of the

seed lattice spectra, this is a completely general topological property. In the 3D case, the situation may become much more complicated.

Note the following interesting circumstance. Although the lower Tamm miniband in Fig. 1 lies entirely in a region of allowed energies for both substances, the wave functions are nevertheless localized at the interfaces. If the degree of localization of the upper miniband corresponds to $\kappa_{a,b}$, that of the lower miniband is determined by an interference and depends on $N_{a,b}$.

If $p_a p_b < 0$, the inverted bands join with each other, and a Tamm state lies at the center of the overlapping gaps. This situation has been analyzed in detail in the literature.[2,6] Again in a superlattice, the interaction between interfaces leads to the formation of a pair of Tamm minibands. Figure 2 shows a typical example of the spectra and of the corresponding wave functions.

Going back to the situation in Fig. 1 (i.e., $p_a p_b > 0$), we note that states which are not interface states are absolutely typical of this joining of bands. The four minibands lying above the Tamm bands (in the "conduction band" of the narrower-gap sub-

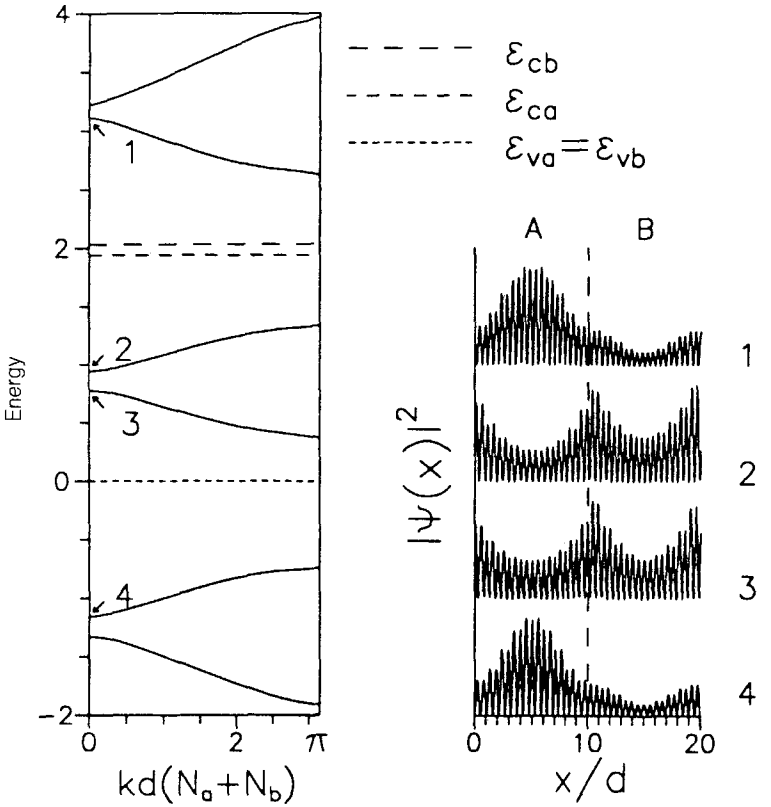

FIG. 2. Spectrum (at the left) and square of the modulus of the wave function of the superlattice for $N_a = N_b = 10$, $p_a = 1$, and $p_b = -1$.

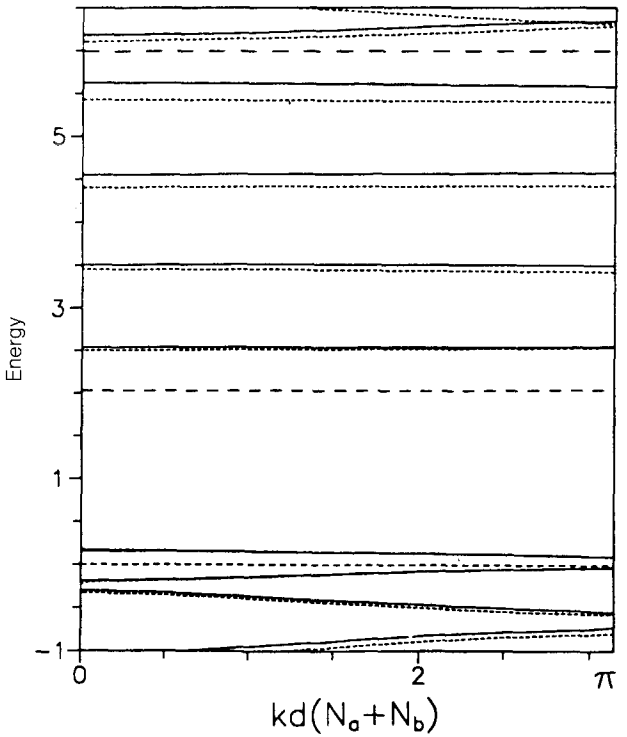

FIG. 3. Solid lines—Exact spectrum of the superlattice; dotted lines—spectrum calculated in the envelope approximation, with the exact form of the envelope Bloch functions, for $N_a = N_b = 15$, $p_a = -1$, and $p_b = -3$. The accuracy of this approximation is particularly high in the case of Tamm minibands.

stance, A) are essentially localized in the corresponding quantum wells. States below the Tamm bands are ordinary delocalized Bloch solutions (in substance B, the width of the gap is greater, and the holes are heavier, so they are localized predominantly there). States of this sort are usually found in the envelope approximation. Interface states do not arise, however, if boundary conditions in the effective-mass approximation are used.[7] If the exact form of the edge Bloch functions (i.e., envelope functions in the envelope method) is used, one can find an extremely good description of the exact spectrum, including the Tamm minibands. The situation is illustrated by Fig. 3, which shows, along with the exact spectrum corresponding to Fig. 1 (the solid lines), a spectrum calculated in the envelope approximation (dotted lines) with the help of the first-order (Cane) kp perturbation theory and the exact form of the Bloch functions of the band edges, (3).

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