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# Sensitivity of wave-function envelopes upon interface position: Semiconductor-insulator boundary

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Exact wave functions for a particle in a quantum well with infinite conduction-band offset are calculated for a well material described by the Kronig-Penney model. The exact wave-function envelopes are extremely sensitive to the position of the interfaces within certain "boundary-sensitive domains." At certain "critical positions" for the interface within these domains the envelopes fulfill zero-slope boundary conditions. In the $n$th band there are normally $n$ well defined boundary-sensitive domains. However, for narrow-gap materials the boundary-sensitive domains become wider and may fill the entire unit cell. In each band, effective-mass theory reproduces adequately the low-lying energy eigenvalues but not the wave-function envelopes, and may give misleading results for oscillator strengths.

## I. INTRODUCTION

With the invention of special growth techniques such as molecular-beam epitaxy and metalorganic chemical vapor deposition, semiconductors with tailor-made properties can be fabricated. These structures show unusual quantum effects not seen in bulk semiconductors. The freedom of choosing the compositional structures opens up possibilities of making composite materials with quantum confinement in one (quantum well), two (quantum wires), and three dimensions (quantum dots). In addition to the many possible applications of these structures, they also offer new and challenging problems from the point of view of pure physics.[1]

Theoretically, one is interested in solutions of the Schrödinger equation for the composite structure. But the lack of translational invariance along the growth direction seriously complicates matters. The most common procedure is to solve the Schrödinger equation in each constituent material, and then match the solutions at the interfaces. This would be straightforward if one had the exact solution at hand. Since this is hardly ever the case one must be careful when employing some approximate solution scheme.

One such popular method for determining electronic states in a semiconductor is the envelope-function method.[2] This is a generalization to composite structures of the well-known effective-mass approximation in bulk.[3] In the envelope-function approach the bulk effective-mass equation is solved in each constituent material and the envelopes are matched at the interfaces. Since the effective masses that enter into the effective-mass equation now become position dependent, the problem of *how* to connect the envelopes at the interface arises.[4] A second problem is *where* the envelopes should be matched.

The interface in real materials is not completely abrupt and it would seem more sensible to speak of an interface region. However, to avoid this complication the interface is commonly modeled as perfect, i.e., abrupt. But even in this idealized picture there is room for ambiguity as to where the interface should be located.[5] Are the exact energy eigenvalues and wave functions sensitive to this ambiguity? This is the main problem that we address in the present article. We choose a simple quantum-well setup for the analysis, with the barrier assumed to be an insulator. This leads to complete confinement of the electrons in the well material. A second question is how well effective-mass theory can handle this situation which effectively corresponds to an infinite potential-energy discontinuity.

Through an exact model calculation we show below that the ambiguity in the position of the interface hardly affects the energy levels for the present model, but that it has a dramatic effect on the wave functions. The most striking feature of the wave-function dependence upon the interface position is the existence of certain "boundary-sensitive domains," narrow regions of interface positions in which small displacements of the interface leads to rapid changes in the wave-function envelopes. This is important for physical properties that depend explicitly on the wave function (or its envelope). As an important case in point we study the interface-position dependence of optical transitions in a quantum well.

As a simple and exactly soluble model we take the well material to be a one-dimensional Kronig-Penney material consisting of periodic $\delta$ wells. Closed-form expressions for energy levels and wave functions for the confined electron are then easily obtained. In Fig. 1, we show an example of an exact wave function for the confined electron. Obviously, the envelope of this wave function does *not* vanish at the boundaries, as simple effective-mass theory would predict, but rather satisfies zero-slope conditions. As will be discussed below, the reason is that for this case the interface is located in the middle of one of the boundary-sensitive domains referred to above.

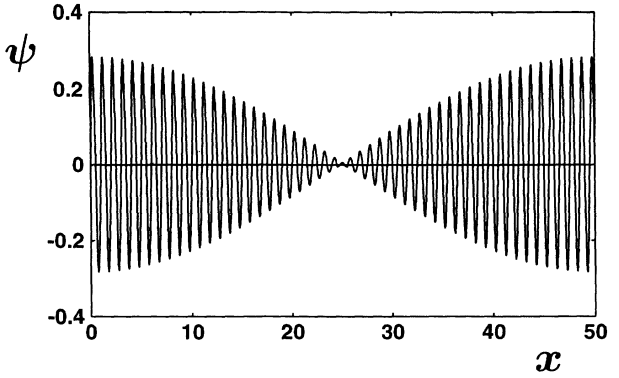

FIG. 1. An exact energy eigenfunction for an electron confined in a quantum well. The lattice constant is used as the unit of length.

In Sec. II, the model is presented and solved exactly for energy levels, wave functions, and boundary-sensitive domains. The results for this simple model motivate and guide the following discussion, in which we generalize some of our results to arbitrary periodic potentials in one dimension.

In Sec. III, we compare our exact results with the predictions of the effective-mass approximation. Intraband and interband optical absorption spectra for the quantum well are discussed in Sec. IV, with emphasis on the interface-position dependence. A discussion is given in Sec. V and a short summary is left for Sec. VI.

## II. EXACT SOLUTION OF THE QUANTUM-WELL PROBLEM

### A. Model

We let the well material be a one-dimensional Kronig-Penney material. An electron in a Kronig-Penney lattice with lattice constant $a$ and $\delta$ functions at

$$x_\nu = (\nu - \tfrac{1}{2})a, \qquad \nu = \text{integer}, \tag{1}$$

has a Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{\hbar^2 \alpha}{ma}\sum_\nu \delta(x - x_\nu). \tag{2}$$

Here $m$ is the free electron mass and $\alpha$ is a dimensionless potential-strength parameter, here assumed positive. The properties of the Kronig-Penney lattice are well known, and merely summarized here.[6] For positive energies,

$$E \equiv \frac{\hbar^2 q^2}{2ma^2} \geq 0, \tag{3}$$

it is seen from the dispersion relation

$$\cos(ka) = \cos q - \alpha q^{-1} \sin q \tag{4}$$

that the band structure has band minima

$$E_n^c = \frac{\hbar^2}{2ma^2} n^2 \pi^2 \tag{5}$$

for

$$q_c = n\pi, \qquad n = 1, 2, 3, \ldots . \tag{6}$$

Expanding the dispersion relation (4) around the positive-energy band minima to second order in the wave vector $k$, we obtain the effective mass

$$m^* = m\frac{\alpha}{n^2\pi^2} \tag{7}$$

at the $n$th band minimum. In addition to these bands there also exists a lowest (zeroth) band with a band minimum at negative energy. Throughout this article, however, we assume for simplicity *positive* energies. The dispersion relation shows, moreover, that band minima occur for $k = 0$ in the even bands and for $k = \pm\pi/a$ in the odd bands.

In the exact solution of the quantum-well problem we will also need the transfer matrix $T$ for the Kronig-Penney material. $T$ connects the wave function and its derivative across a $\delta$ well from $x_\nu - \frac{1}{2}a = \nu a$ to $x_\nu + \frac{1}{2}a = \nu a + a$:

$$\begin{bmatrix} \psi(\nu a + a) \\ a\psi'(\nu a + a) \end{bmatrix} = T \begin{bmatrix} \psi(\nu a) \\ a\psi'(\nu a) \end{bmatrix} . \tag{8}$$

We have used $a\psi'$ as the lower component in the state vector so that the transfer matrix is dimensionless. For the Kronig-Penney lattice the transfer matrix has the simple form[7]

$$T = \begin{bmatrix} \cos q - \alpha q^{-1} \sin q & q^{-1}\sin q - \alpha q^{-2}(1 - \cos q) \\ -q \sin q - \alpha(1 + \cos q) & \cos q - \alpha q^{-1} \sin q \end{bmatrix} . \tag{9}$$

The barrier material in our quantum-well model is taken as an insulator. Focusing upon energy levels close to the conduction band in the well material, we expect to be deep down in the energy gap in the insulator. The wave function will then decay so rapidly in this region that we approximate the insulator with a hard wall. The matching conditions on the exact wave functions at the semiconductor-insulator interface are, therefore, equivalent to the requirement that the wave function should vanish at the interface. To be specific we consider a quantum well of thickness $L$, consisting of $N$ unit cells. It might seem natural to choose the interfaces at $x = 0$ and $x = Na$, but we will be more general and allow the interfaces to be at $x = \varepsilon a$ and $x = Na + \varepsilon a$, with $-1/2 \leq \varepsilon \leq 1/2$, thus keeping the width of the well fixed at the value $L = Na$. In Fig. 1, we used the natural choice $\varepsilon = 0$.

In terms of the state vector introduced in (8), the matching conditions on the exact wave function are now

$$X_\varepsilon \equiv \begin{bmatrix} \psi(\varepsilon a) \\ a\psi'(\varepsilon a) \end{bmatrix} = \text{const} \begin{bmatrix} 0 \\ 1 \end{bmatrix} ,$$

and

$$X_{N+\varepsilon} = \text{const} \begin{bmatrix} 0 \\ 1 \end{bmatrix} . \tag{10}$$

### B. Energy levels

The energy levels in the quantum well are now readily determined by combining the transfer matrix (9) and the boundary conditions (10). Take first $\varepsilon = 0$. Transforming the wave function and its derivative across the well, we have

$$X_N = T^N X_0 . \tag{11}$$

Since the boundary conditions require the upper component of both state vectors $X_0$ and $X_N$ to vanish, the energies are given by the condition

$$(T^N)_{12} = 0 . \tag{12}$$

One can easily exponentiate the transfer matrix by first diagonalizing it. To prepare for this we introduce a convenient parametrization of the diagonal elements ($T_{11} = T_{22}$) in the transfer matrix via

$$T_{11} = \cos q - \alpha q^{-1} \sin q = \eta \cos U , \tag{13}$$

where the variable $\eta$ takes care of the sign of the diagonal element: $\eta = \text{sgn}(T_{11}) = \pm 1$. Since the dispersion relation (4) can be written $\cos(ka) = T_{11}$ and energy bands in the bulk material correspond to real $k$, it is seen that $U$ is real for energies in the bulk band range and purely imaginary in the bulk gaps. The transfer matrix is then diagonalized,

$$T = S \begin{bmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{bmatrix} S^{-1} , \tag{14}$$

with

$$S = \begin{bmatrix} T_{12} & T_{12} \\ i\eta \sin U & -i\eta \sin U \end{bmatrix} . \tag{15}$$

Using the fact that $\lambda_\pm = \eta e^{\pm iU}$, we arrive at the following form of the transfer matrix raised to an arbitrary power $s$

$$T^s = \eta^s \begin{bmatrix} \cos(sU) & \eta T_{12} \sin(sU)/\sin U \\ -\eta T_{12}^{-1} \sin(sU) \sin U & \cos(sU) \end{bmatrix} . \tag{16}$$

The condition $(T^N)_{12} = 0$ then reads[8]

$$NU = r\pi , \qquad r = \text{positive integer} , \tag{17}$$

so the energy levels in the box is determined by the equation

$$\cos q - \frac{\alpha}{q} \sin q = \eta \cos\left(\frac{r\pi}{N}\right) , \qquad r = 1, 2, \ldots, [N/2] , \tag{18}$$

where $q$ is related to the energy via Eq. (3) and $[x]$ denotes the integer part of $x$. The restriction on the number of $r$ values in Eq. (18) avoids double counting.

This was for $\varepsilon = 0$. However, for $\varepsilon \neq 0$ the same condition applies. This can be shown as follows. The boundary conditions are now that $X_\varepsilon$ and $X_{N+\varepsilon}$ have a vanishing upper component. These state vectors are related through

$$X_{N+\varepsilon} = T_\varepsilon T^N T_{-\varepsilon} X_\varepsilon , \tag{19}$$

where the transfer matrices $T_{\pm\varepsilon}$ connect state vectors over a distance $\pm\varepsilon a$. Multiplying both sides of (19) by $T_{-\varepsilon}$ we arrive after some algebra at the same condition, Eq. (12) as before. Keeping the width of the well fixed, the interface position has, therefore, *no effect* on the energy levels (except levels associated with band edges). We note that all the allowed energy levels in the quantum well lie at energies corresponding to *bands* in the bulk material.

The comparison with effective-mass results is postponed to Sec. III.

### C. Wave functions

We now turn to the wave functions in the well. In the intervals between the $\delta$ wells the wave functions satisfy the free-particle Schrödinger equation. Let us enumerate these intervals such that interval $\nu$ corresponds to $x_\nu < x < x_{\nu+1}$. Here $\nu = 1, 2, \ldots, N$, with the adjustment that $x_{N+1} = Na + \varepsilon a$. In addition there is an interval between the hard wall at $x = \varepsilon a$ and the first $\delta$ well at $x = \frac{1}{2}a$. In this zeroth interval the solution of the Schrödinger equation that fulfills the boundary condition at the wall is

$$\psi_\varepsilon(x) = A_\varepsilon \sin[q(x - \varepsilon a)/a] , \tag{20}$$

where $A_\varepsilon$ is a constant.

In interval number $\nu$ the general solution has the form

$$\psi_\nu(x) = A_\nu \sin[q(x - \nu a)/a] + B_\nu \cos[q(x - \nu a)/a] . \tag{21}$$

The constants $A_\nu$ and $B_\nu$ of neighboring intervals are related through the transfer matrix $T$. Since $\psi_\nu(\nu a) = B_\nu$ and $a\psi'_\nu(\nu a) = qA_\nu$ we have

$$\begin{bmatrix} B_{\nu+1} \\ qA_{\nu+1} \end{bmatrix} = T \begin{bmatrix} B_\nu \\ qA_\nu \end{bmatrix} . \tag{22}$$

Use of the boundary conditions from Eq. (20), $A_0 = A_\varepsilon \cos(q\varepsilon)$ and $B_0 = -A_\varepsilon \sin(q\varepsilon)$, and of the exponentiated transfer matrix (16), yields explicit expressions for $A_\nu$ and $B_\nu$:

$$
\begin{aligned}
A_\nu &= A_\varepsilon \eta^\nu [\eta \sin(\nu U)\sin(q\varepsilon)\sin U/(qT_{12}) \\
&\quad + \cos(\nu U)\cos(q\varepsilon)] , \\
B_\nu &= A_\varepsilon \eta^\nu [\eta \sin(\nu U)\cos(q\varepsilon) q T_{12}/\sin U \\
&\quad - \cos(\nu U)\sin(q\varepsilon)] .
\end{aligned}
\tag{23}
$$

The remaining constant $A_\varepsilon$ is determined by the normalization

$$
1 = \int_{\varepsilon a}^{Na+\varepsilon a} dx\, |\psi(x)|^2 , \tag{24}
$$

which gives

$$
\begin{aligned}
|A_\varepsilon|^{-2} = \frac{Na}{4}\Big\{ & 1 - q^{-1}\sin q \cos(2q\varepsilon) \\
& + [1 - q^{-1}\sin q] T_{12}^{-2} q^{-2} \sin^2(q\varepsilon)\sin^2 U \\
& + [1 + q^{-1}\sin q] q^2 T_{12}^2 \cos^2(q\varepsilon)/\sin^2 U \Big\} .
\end{aligned}
\tag{25}
$$

The phase of $A_\varepsilon$ is without significance and we take $A_\varepsilon$ real. With the exact solution at hand, we can now study the effect of varying the interface position simply by plotting the wave functions for different $\varepsilon$ values. Figures 2 and 3 show the wave function for the lowest energy state above the first conduction-band edge, i.e., $r = 1$ and $n = 1$. We have chosen four different interface positions, corresponding to $\varepsilon = 0$, $\frac{1}{6}$, $\frac{1}{3}$, and $\frac{1}{2}$ . The two figures represent, respectively, narrow-gap and wide-gap situations (corresponding to shallow and deep $\delta$ wells, respectively).

We see from the figures that the narrow-gap results are not sensitive to the interface position, as the wave function in this case hardly feels the periodic potential anyway. We note, however, that the exact envelope is fairly constant throughout the well and does *not* vanish at the interface, as one would expect from a simple (one-band) effective-mass point of view. We will return to this phenomenon in Sec. V.

The wide-gap results of Fig. 3 show, on the other hand, that the envelope for $\varepsilon = 1/2$ differs qualitatively from the other three envelopes. Furthermore, there must be a rather abrupt change in the envelope as $\varepsilon$ approaches 1/2. This is confirmed in Fig. 4 where we again plot the wave function in the strong $\delta$-potential limit, this time taking $\varepsilon = \frac{120}{250}$, $\frac{121}{250}$, $\frac{122}{250}$, and $\frac{123}{250}$. In this narrow range of interface positions the envelope changes character dramatically. We will denote an interval of interface position of this nature a *boundary-sensitive domain.*

So far we have merely presented evidence for one such boundary-sensitive domain for the first band. In the following section we look more closely at the number and positions of such domains.

### D. Critical interface positions and boundary-sensitive domains

To investigate the envelope, we rewrite the exact wave function, Eq. (21), in terms of an amplitude and a phase:

$$
\psi_\nu(x) = F_\nu \sin[q(x - \nu a)/a + \phi_\nu] . \tag{26}
$$

The amplitude $F_\nu$ and the phase $\phi_\nu$ are determined from

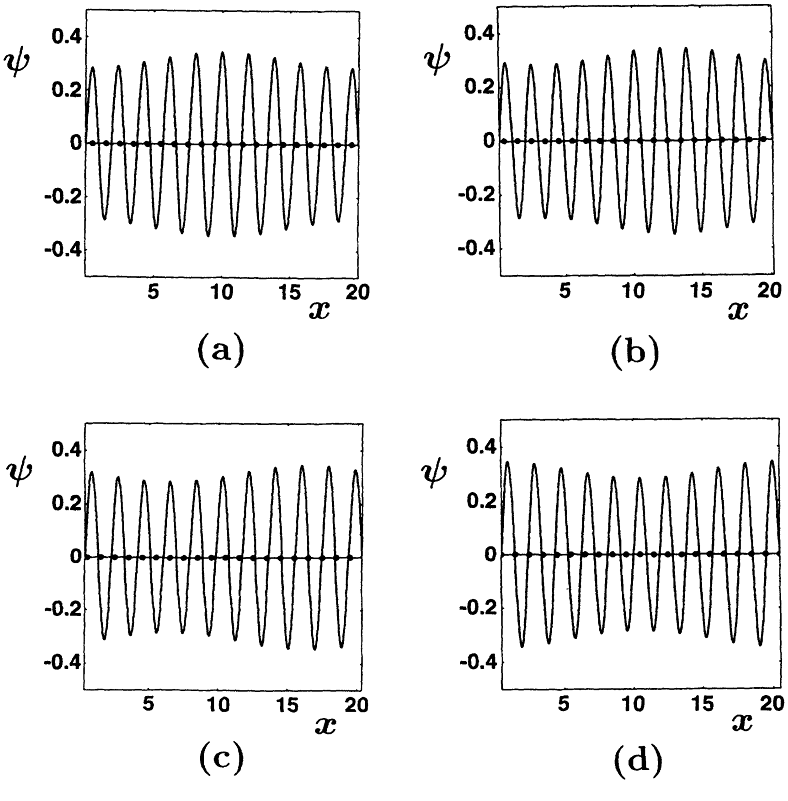

FIG. 2. The wave function inside the well in the weak potential limit, $\alpha = 0.1$, for four different interface positions. The well is $N = 20$ unit cells wide, and the positions of the $\delta$ wells are marked with black dots. (a) $\varepsilon = 0$, (b) $\varepsilon = 1/6$, (c) $\varepsilon = 1/3$, and (d) $\varepsilon = 1/2$. The first band is chosen and the lattice constant is used as the unit of length.

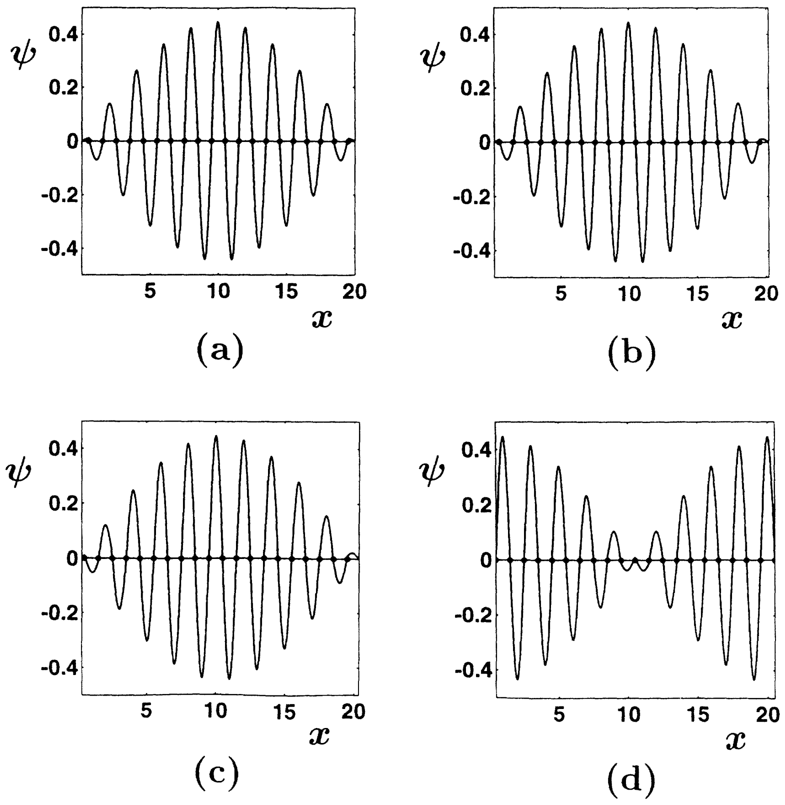

FIG. 3. The wave function inside the well in the strong potential limit, $\alpha = 10$, for four different interface positions. The well is $N = 20$ unit cells wide, and the positions of the $\delta$ wells are marked with black dots. (a) $\varepsilon = 0$, (b) $\varepsilon = 1/6$, (c) $\varepsilon = 1/3$, and (d) $\varepsilon = 1/2$. The first band is chosen and the lattice constant is used as the unit of length.

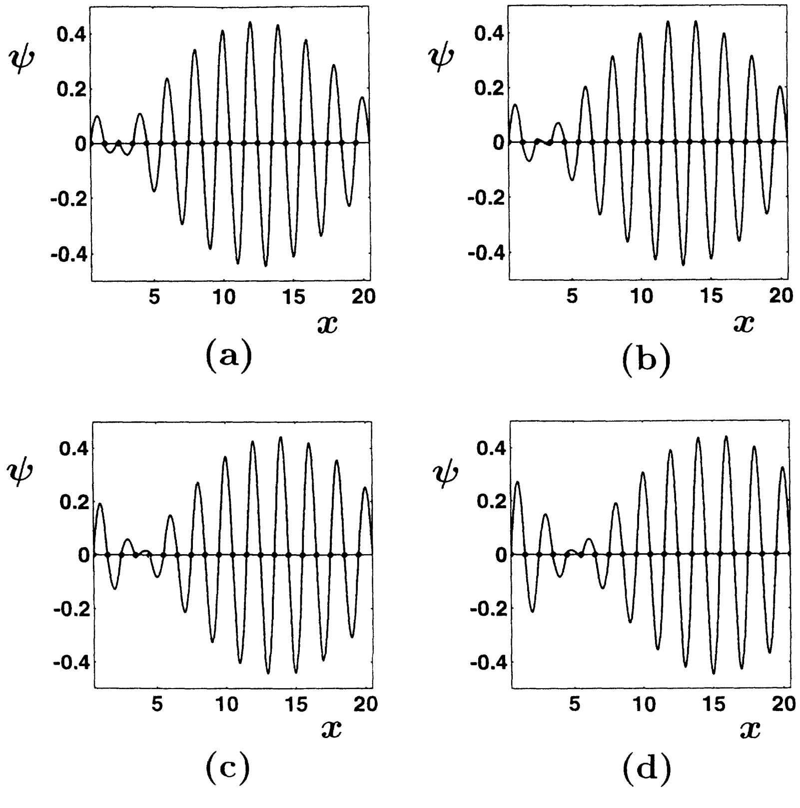

FIG. 4. Same as Fig. 3, but now with the interface positions (a) $\varepsilon = 120/250$, (b) $\varepsilon = 121/250$, (c) $\varepsilon = 122/250$, and (d) $\varepsilon = 123/250$.

the interval constants $A_\nu$ and $B_\nu$ through the relations

$$F_\nu^2 = A_\nu^2 + B_\nu^2\ , \quad \text{and} \quad \tan\phi_\nu = B_\nu/A_\nu\ . \tag{27}$$

The variation of the amplitude $F_\nu$ with the interval position $\nu$ characterizes the envelope of the complete wave function.

Insertion of the explicit form (23) for $A_\nu$ and $B_\nu$ determines the envelope $F_\nu$, and in the general case this is best done numerically. Our objective is different. We aim at *explicit* relations between position and width of the boundary-sensitive domains and the material parameters. Such explicit results can be obtained for energies close to the bulk band minima in the Kronig-Penney lattice. Moreover, this is the energy range in which the effective-mass approximation is expected to be valid (See Sec. III). At the band minima the variable $U$, defined by Eq. (13), vanishes. To be near the band minimum corresponds to $U = \pi r/N \ll 1$, i.e., the excitation number $r$ within the band should be small compared to the number of unit cells in the well.

Near the band minima in the bulk material, expansion of the off-diagonal transfer-matrix element $T_{12}$ to the lowest nonvanishing order in $U$ gives

$$T_{12} = \begin{cases} -\dfrac{2\alpha}{n^2\pi^2}\ , & \text{odd } n \\ \dfrac{1}{2\alpha}U^2\ , & \text{even } n\ . \end{cases} \tag{28}$$

Similarly we can expand the envelope $F_\nu$ to second order in $U$, with all other parameters fixed. Up to a $\nu$-independent proportionality constant we find in the odd bands

$$\begin{aligned} F_\nu^2 &\propto \cos^2(q_c\varepsilon)\sin^2(\nu U) + \frac{n\pi\sin(2q_c\varepsilon)}{4\alpha}U\sin(2\nu U) \\ &+\frac{n^2\pi^2}{4\alpha^2}U^2\cos^2(\nu U), \end{aligned} \tag{29}$$

and to the same order in $U$ we find in the even bands

$$\begin{aligned} F_\nu^2 &\propto \sin^2(q_c\varepsilon)\sin^2(\nu U) + \frac{n\pi\sin(2q_c\varepsilon)}{4\alpha}U\sin(2\nu U) \\ &+\frac{n^2\pi^2}{4\alpha^2}U^2\cos^2(\nu U). \end{aligned} \tag{30}$$

Now we clearly see the origin of the boundary-sensitive domains. For sufficiently small $U$, the envelope is given by the zeroth-order expansion in $U$,

$$F_\nu \propto \begin{cases} \cos(q_c\varepsilon)\sin(\nu U)\ , & \text{odd } n \\ \sin(q_c\varepsilon)\sin(\nu U)\ , & \text{even } n\ , \end{cases} \tag{31}$$

*except* for those interface positions ($\varepsilon$ values) for which the first factor vanishes. That happens precisely for

$$q_c\varepsilon_s = \begin{cases} (s+\frac{1}{2})\pi\ , & \text{integer } s \ \ \text{(odd bands)} \\ s\pi\ , & \text{integer } s \ \ \text{(even bands)}\ , \end{cases} \tag{32}$$

and by (29) and (30) the envelopes then have *maxima* at the interfaces; $F_\nu \sim \cos(\nu u)$ in both even and odd bands. Since $q_c = n\pi$ at the band minima, these *critical positions* of the interface are given by

$$\varepsilon_s = \begin{cases} (s+\frac{1}{2})/n\ , & s = 0,\pm1,\pm2,\ldots,\pm(n-1)/2 \\ & \text{(odd bands)} \\ s/n\ , & s = 0,\pm1,\pm2,\ldots,\pm(n-2)/2, n/2 \\ & \text{(even bands)}\ . \end{cases} \tag{33}$$

Because $|\varepsilon_s| \leq 1/2$ we note that there are $n$ critical interface positions for the $n$th band. Furthermore, we see that the natural choice $\varepsilon = 0$ corresponds to critical positions in the even bands.

To study the sensitivity of the wave-function envelope upon changes in the interface position, we introduce a *boundary-sensitive domain* $(\varepsilon_s - \Delta, \varepsilon_s + \Delta)$ around each critical (dimensionless) position $\varepsilon_s$. We define $\Delta$ such that at the domain boundaries $(\varepsilon_s \pm \Delta)a$ the envelope has, to lowest order, changed from the $\cos(\nu U)$ form at the critical position to

$$F_\nu \propto \sin(\nu U) \pm \cos(\nu U), \tag{34}$$

in some sense "halfway" to the normal form $\sin(\nu U)$.

We find that to lowest order in $U$ the domain width, for both even and odd bands, is given by

$$\Delta = \frac{\pi r}{2\alpha N} = \frac{r}{2\pi n^2 N}\,\frac{m}{m^*}\ . \tag{35}$$

The wave-function envelopes seen for the shallow and deep $\delta$ wells in Figs. 2 and 3, respectively, are now easy to interpret. For the first band we have a boundary-sensitive domain near the critical position $\varepsilon_0 = 1/2$. Since the corresponding width is inversely proportional to the $\delta$-well strength, the boundary-sensitive domains will fill the whole unit cell. In this extreme situation the wave-function envelopes do not really depend sensitively on the interface position, but possess nevertheless zero-gradient boundary conditions, at least approximately. This is seen in Fig. 2. The strong-potential situation in Figs. 3 and 4, where $\alpha = 10$ and $N = 20$, should, according to the present analysis, have a boundary-sensitive domain stretching out to $\varepsilon = 1/2 - \Delta \simeq 0.4921$. This agrees precisely with Fig. 4, since the value $\varepsilon = 123/250 = 0.492$ is just outside the domain.

## III. COMPARISON WITH THE EFFECTIVE-MASS APPROXIMATION

In the effective-mass approximation (EMA) the properties of the periodic potential are contained in the band-edge energy and the corresponding effective mass.[3] For our quantum-well problem the effective-mass wave functions $\phi(x)$ for electron states close to the band minima satisfy

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}\phi(x) = (E - E_n^c)\phi(x) \tag{36}$$

with boundary conditions $\phi(0) = \phi(L) = 0$. The solution to this textbook problem is

$$E = E_n^c + \frac{\hbar^2\pi^2}{2m^*L^2}r^2\ , \quad r = 1,2,3,\ldots, \tag{37}$$

and the corresponding wave functions are

$$\phi(x) = \sqrt{2/L}\sin(\pi r x/L). \tag{38}$$

Can we expect the EMA to give an adequate description of our quantum-well problem? *A priori* this might be doubtful, since usually EMA is associated with slowly varying perturbations of a periodic crystal, and the hard walls of the present problem can hardly fit that description.

In any case, the effective-mass approximation can only give an adequate description of states energetically close to the bulk band edges. For comparison we, therefore, extract values of the exact energy levels, determined in the previous section, near the conduction-band minimum. Combining Eqs. (3), (5), and (18) we find that

$$E = E_n^c + \frac{\hbar^2}{2ma^2}\frac{n^2\pi^2}{\alpha}U^2 + \cdots = E_n^c + \frac{\hbar^2\pi^2}{2m^*L^2}r^2 + \cdots, \qquad r = 1,2,3,\ldots \tag{39}$$

where we have used the result for the effective mass $m^*/m = \alpha/n^2\pi^2$ from Eq. (7). To this order the exact energy levels coincide with the effective-mass result (37). Thus the effective-mass energy levels are asymptotically exact when we are close to a band edge.

The EMA *wave function*, however, does not enjoy a similar status, in the sense that the envelopes of the exact wave functions are not well approximated by the effective-mass wave functions (38). In Sec. V we comment upon this in a more general setting.

## IV. SENSITIVITY OF OPTICAL ABSORPTION

In this section, we discuss a measurable quantity that depends on the interface positions, viz. the oscillator strength for optical transitions in the quantum well.

The oscillator strength $f$ characterizing the optical transition from the initial state $\psi_i$ to the final state $\psi_f$ is given by[9]

$$f = \frac{2}{m(E_f - E_i)}\left|\int \psi_f^*(x)\, p_x\, \psi_i(x)\, dx\right|^2 \equiv \frac{2}{m(E_f - E_i)}\left|P_{if}\right|^2 \tag{40}$$

assuming the light to be linearly polarized in the $x$ direction. The magnitude of the momentum matrix element $P_{if}$, which can be evaluated straightforwardly using the exact wave functions of Sec. II C, depends strongly on the interface position. This is illustrated by Fig. 5, which shows how the oscillator strength varies with the interface position for an intraband transition [Fig. 5(a)] and for an interband transition [Fig. 5(b)].

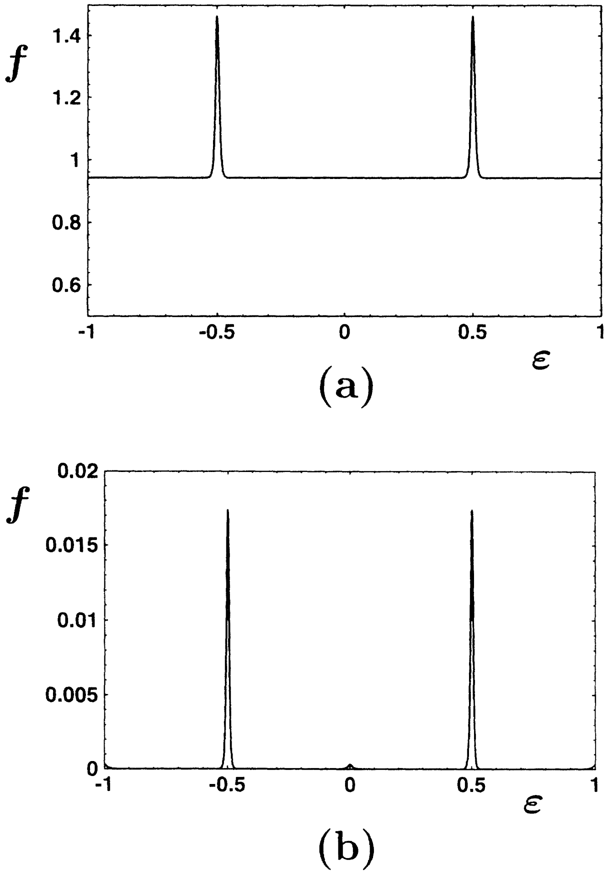

FIG. 5. Oscillator strengths for (a) intraband absorption in the first band between the $r_i = 1$ and $r_f = 2$ states, and for (b) interband absorption from the first to the second band between the $r_i = r_f = 1$ states. In both cases $N = 15$ and $\alpha = 10$.

Figure 5(a) corresponds to an intraband transition within the first band for a case with a single boundary-sensitive domain near $\varepsilon_0 = 1/2$ according to Eq. (33). In the intraband transition the initial and final states have boundary-sensitive domains around the same critical interface position, but with different widths. The peak seen in Fig. 5(a) for $\varepsilon = 1/2$, therefore, corresponds to both the initial and final state associated with the boundary-sensitive domain. The height of the peak, relative to the value outside the domain, can be shown to be

$$\frac{1}{4}\left(\frac{r_f}{r_i} + \frac{r_i}{r_f}\right)^2, \tag{41}$$

where $r_i$ and $r_f$ are the excitation numbers of the states involved. This factor can, of course, be large. The width of the peak is of the same order as the width of the smallest boundary-sensitive domain, here $2\Delta \simeq 0.0209$.

In the standard effective-mass description[2] the oscillator strength for an intraband transition is given by the wave-function envelopes $F_i(x)$ and $F_f(x)$:

$$f = \frac{2}{m(E_f - E_i)}\frac{m}{m^*}\left|\int_0^L F_f^*(x)\, p_x\, F_i(x)\, dx\right|^2, \tag{42}$$

a quantity that is independent of the interface position. For states close to the bulk band edge, the oscillator strength calculated with the effective-mass functions $\phi(x)$, Eq. (38), taken as envelopes, agrees well with exact values *outside* the boundary-sensitive domains. It is interesting to note that the enhancement factor (41) for the oscillator strengths associated with a boundary-sensitive domain can be recovered from the effective-mass expression (42) if the envelopes of the exact wave functions are used instead of the effective-mass functions (38).

Figure 5(b) shows the oscillator strength for an interband transition between states in the first and second band. The initial and the final state have the same excitation number, i.e., $r_i = r_f = 1$. The first band has merely one critical interface position, viz. for $\varepsilon_0 = 1/2$, whereas the second band has critical positions for $\varepsilon_0 = 0$ and $\varepsilon_1 = 1/2$. The oscillator strength has peaks for these interface positions. It can be shown that the height of the peak at $\varepsilon = 0$ is proportional to $1/L^2$ while the peak at $\varepsilon = 1/2$ is proportional to $1/L$, where $L$ is the width of the quantum well. So for large well widths, the interband transitions for which both the initial and final states are associated with boundary-sensitive domains will have the largest oscillator strengths.

For interband transitions in an infinitely deep quantum well, the oscillator strength in standard effective-mass theory[2] is proportional to $\int F_f^*(x)F_i(x)dx$. That the exact results in Fig. 5(b) cannot be described in this way, be it in terms of the effective-mass functions (38) or the exact envelopes, is not surprising, since for this interband transition the initial and final states correspond to band minima at *different* points in the Brillouin zone.

## V. DISCUSSION

An envelope constitutes a useful characterization of the wave function when it is a relatively slowly varying modulation $F(x)$ of a rapidly varying function $u(x)$, so that correction terms (in which the gradient of $F(x)$ enters) are very small:

$$\psi(x) = F(x)\, u(x) + \mathcal{O}\left(\frac{dF(x)}{dx}\right). \tag{43}$$

The enforcement of a boundary condition $\psi(x_0) = 0$ at $x_0 = 0$ requires $F(x_0) = 0$ if $u(x_0) \neq 0$. This is the normal situation. However, if $u(x_0) = 0$ then it is not necessary that the envelope vanishes at the boundary. On the contrary, the next-to-leading-order term in (43), proportional to the gradient of the envelope, gives $F'(x_0) = 0$. This is the basic mechanism behind the existence of critical interface positions.

A relevant example is the usual envelope-function expansion[10]

$$\psi(x) = \phi_n(x)u_{n0}(x) - i\hbar\frac{d\phi_n(x)}{dx}\frac{1}{m} \times \sum_{l\neq n}\frac{p_{ln}}{E_{n0}-E_{l0}}u_{l0}(x) + \cdots, \tag{44}$$

where the momentum matrix element $p_{ln}$ near a band edge at the zone center ($k = 0$), is given as the integral over a unit cell,

$$p_{ln} = \int_0^a u_{l0}^*(x)\left(-i\hbar\frac{d}{dx}\right)u_{n0}(x)\,dx. \tag{45}$$

The critical interface positions correspond in this case to the solutions of $u_{n0}(x) = 0$, and since for any periodic potential the Bloch function has $n$ zeroes in the $n$th band, there are $n$ critical interface positions for which the envelope of the exact wave function fulfills zero-gradient boundary conditions at the interface. From this argument one can also draw the conclusion that the existence of the boundary-sensitive domains is independent of the number of unit cells in the well, and hence the boundary-sensitive domains persist even when the well width is increased to infinity, as might not have been expected at first.

So far we have only considered parallel displacements of the two interfaces, and one might wonder whether other types of interface displacements would introduce any new features. We have, therefore, also considered displacements that change the width of the well. The new feature that appears is, of course, that the energy levels change, and may cross the bulk band-edge energies. In this respect the boundary-sensitive domains play a new role. The energy levels vary especially rapidly, and cross the band edges, when the interfaces are in boundary-sensitive domains. However, with respect to the wave-function envelopes, no essentially new features appear.

An infinitely high confining barrier is clearly an approximation of the physical situation and it is natural to reflect on what happens to the boundary-sensitive domains when the conduction-band offset is finite. Then there always will be an evanescent wave in the barrier material. Will boundary-sensitive domains still exist? The answer is yes.

Assume first that the insulator material is modeled by a very large, but finite offset. (The crudest approximation would be a *constant* potenial, but that is not necessary.) It is intuitively clear, and can be shown by explicit examples, that energies and interior wave functions are closely approximated by the infinite-offset results.

Second, assume the insulator to be modeled with a moderate offset, so that the bound-state energies are near the middle of an insulator band gap. The wave functions are still sensitive to the interface position, but the location of the critical interface positions are shifted. The simplest way to see this is as follows. For a given offset one can always find a position of the interface within the unit cell such that the energy of the state involved is the same as with infinite offset. This is so because at this energy the bound-state condition in the insulator fixes the ratio $\psi/\psi'$ at the insulator boundary. Since an infinite-offset eigenfunction possesses all values of $\psi/\psi'$ within a unit cell, one can simply position the boundary suitably in the unit cell so that the evanescent wave joins this interior wave function smoothly. This means that by some choice of the interface position, eigenfunctions with (almost) zero-slope envelopes at the interface still exist.

If the semiconductor is a periodic superlattice rather than a homogeneous material, the possibility of boundary sensitivity on a mesoscopic scale, rather than on a molecular level, is possible. (A quantum-well of superlattices is an example of such a material.[11]) In this case, the position of the interface within the superlattice unit cell can be varied *experimentally* by changing the number of layers in the two ultimate semiconductor regions. It would be interesting if corresponding phenomena occur on this mesoscopic scale.

Wave-function envelopes with zero-slope conditions at an infinite-potential barrier do also occur in Sham and Nakayama's version of effective-mass theory.[12] In their treatment evanescent waves apparently play a crucial role, and since they are absent in the one-dimensional situation it is not clear to us that the effects have the same origin.

Another setting with zero-slope wave-function envelopes at interfaces is confinement of a particle in a quantum well when the barrier effective mass is very large.[13] This is, however, a different physical phenomenon.

## VI. SUMMARY

In this article, we have studied the sensitivity of the exact wave-function envelopes at semiconductor-insulator interfaces. Using the Kronig-Penney model as a starting point we are led to the following conclusions for a general periodic potential in one dimension.

(i) In the $n$th band there exist $n$ critical interface positions for which the envelope satisfies zero-slope boundary conditions.

(ii) These $n$ critical positions are the $n$ zeroes of the Bloch function in the unit cell at the interface.

(iii) In a wide-gap situation the zero-slope boundary condition is exceptional, in the sense that the relative measure of the boundary-sensitive domains around the critical positions is small.

(iv) In a narrow-gap situation (weak periodic potential), however, the boundary-sensitive domains around the critical interface positions are wide and cover the whole unit cell, so the exact wave-function envelopes always fulfill zero-slope boundary conditions, at least approximately.

(v) In a theoretical treatment of physical properties like oscillator strengths the precise localization of the interface may be crucial.

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