

EFFECTIVE-MASS APPROACHES FOR ONE-DIMENSIONAL QUANTUM
WELL STRUCTURES. COMPARISON WITH EXACT RESULTS (*)

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ABSTRACT

Exact k -space equations are employed to calculate the energy levels and envelope functions of several one-dimensional quantum well structures having both step and graded-potential profile. We consider finite as well as infinite structures and compare the obtained results with those given by standard effective-mass methods.

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1. INTRODUCTION

The effective-mass model has been widely used in the calculation of energy levels and envelope functions of MQW structures, particularly when a more complicated basis than a single square well is considered or an electric field is applied. Frequently, the transfer-matrix technique has been used in combination with the effective-mass equation to describe superlattices [1-10]. The application and validity of the effective-mass theory for studying semiconductor heterostructures have been greatly clarified by Burt's work [11-13], who has reviewed and justified previous semi-heuristic approaches putting them in a more general, rigorous framework. In [12], a one-dimensional lattice-matched periodic structure built on a fictitious crystal was used to illustrate several results of Burt's theory. The periodicity of such a superlattice allows to reduce the problem of calculating the energies and envelope functions to a matrix eigenvalue problem in k -space.

With the approach of [12], and once the one-dimensional atomic potential has been defined, "exact" results are obtained which can be compared with others given by standard methods. On the other hand, the structure actually described by the resulting equations in k -space is necessarily periodic. Therefore, when a finite structure with evanescent wavefunction at both ends is considered, care must be taken in defining the periodic cell. As will be evident below, this results in a significant increase of the size of the matrix to be diagonalized when the wavefunctions of the MQW are not well confined.

In this paper we employ the k -space equations to study two finite structures of single and double square quantum well, respectively. The case of a superlattice with a single square quantum well basis will also be considered. The results will be compared with those given by the effective-mass approach, which we shall implement by using the Yeh, Yariv and Hong method for the finite structures [14, 15] and the Kronig-

Penney method for the superlattice [6]. All these calculations are presented in Section 3. Then, in Section 4, the k -space method is suitably adapted to describe finite structures with graded-potential profile. The results are compared with those of the effective-mass approach, which in this case is solved by a standard finite-element technique [16]. All the methods used are previously summarized in Section 2, in which Burt's method is given a little more detailed description. Finally, the conclusions are presented in Section 5.

2. DESCRIPTION OF THE METHODS

In the envelope-function method of [11-13], the wavefunction is written as

$$\psi(z) = \sum_n F_n(z) U_n(z), \quad (1)$$

where $U_n(z)$ are a complete set of functions with the periodicity of the Bravais lattice, and $F_n(z)$ are envelope functions with a plane-wave expansion restricted to the first Brillouin zone. The functions $U_n(z)$ are the same throughout the entire structure, hence they cannot be eigenstates of all the local Hamiltonians, and in fact, do not need to. The wavefunctions (1) are the solutions of the stationary Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} \psi(z) + V(z) \psi(z) = E \psi(z), \quad (2)$$

with m the electron mass and $V(z)$ the atomic potential of the semiconductor structure.

In the k -space, the Schrödinger equation (2) reads [12]

$$\frac{\hbar^2 k^2}{2m} \tilde{F}_n(k) + \frac{\hbar}{m} \sum_{n'} k p_{nn'} \tilde{F}_{n'}(k) + \sum_{n'} \sum_{k'} \tilde{H}_{nn'}(k, k') \tilde{F}_{n'}(k') = E \tilde{F}_n(k), \quad (3)$$

with

$$p_{nn'} = \sum_G \hbar G (U^{-1})_{Gn} U_{n'G} \quad (4)$$

$$\tilde{H}_{nn'}(k, k') = T_{nn'} \delta_{kk'} + \tilde{V}_{nn'}(k, k') \quad (5)$$

$$T_{nn'} = \sum_G \frac{\hbar^2 G^2}{2m} (U^{-1})_{Gn} U_{n'G} \quad (6)$$

$$\tilde{V}_{nn'}(k, k') = \sum_{G, G'} (U^{-1})_{Gn} \tilde{V}_{G-G'-G_b}(k_b) U_{n'G} \quad (7)$$

U_{nG} , $\tilde{F}_n(k)$ and $\tilde{V}_G(k)$ are the Fourier expansion coefficients of $U_n(z)$ and $F_n(z)$ and $V(z)$, respectively:

$$U_n(z) = \sum_G U_{nG} \exp(i G z) \quad (8)$$

$$F_n(z) = \sum_k \tilde{F}_n(k) \exp(i k z) \quad (9)$$

$$V(z) = \sum_{k, G} \tilde{V}_G(k) \exp[i(k + G)z]. \quad (10)$$

In the definitions above, G are vectors of the reciprocal lattice [$G = l(2\pi/a)$, with l an integer and a the atomic spacing] while k denotes vectors inside the first Brillouin zone of the periodic heterostructure. G_b and k_b are two vectors chosen so that $k + k' = G_b + k_b$ in (7) [11]. The $U_n(z)$ are chosen to be eigenstates of the hamiltonian of a virtual crystal having a potential which is an average of the well and the barrier potentials.

Since the expansion of $F_n(z)$ is limited to the first Brillouin zone, it has a finite number of terms which we shall denote as N_B . On the contrary, the expansion of the atomic potential $V(z)$ has in general an infinite number of terms because of the sum in G . Of these G 's, we shall have to retain a finite number N_G such that the truncation error remains negligible. As we shall see below, the number of bands n also turns out to be equal to N_G .

The Kronig-Penney method (KP) based on the transfer-matrix technique was first described in [2] and extended in [6] to analyze the minibands of superlattices of arbitrary basis. We shall use this method for an infinite periodic structure with a single

square well basis in the one-band effective-mass approximation. In this case, the BenDaniel-Duke hamiltonian is used and the resulting equation is

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left[\frac{1}{m_c(z)} \frac{d}{dz} F_c(z) \right] + V_c(z) F_c(z) = E F_c(z), \quad (11)$$

where $F_c(z)$ is the envelope function for the conduction band, $V_c(z)$ is the potential defining the structure [not to be confused with the atomic potential of (10)], and $m_c(z)$ is the effective mass at z , which in this case is constant within each layer of the basis. This method uses a two-dimensional vector, $\Gamma(z) = [\Gamma_1(z) \ \Gamma_2(z)]$, containing the functions whose continuity is to be preserved at any point z , *i.e.* $\Gamma_1(z) = F_c$; $\Gamma_2(z) = (1/m_c) dF_c/dz$. The vectors at two different coordinates are related by a transfer-matrix: $\Gamma(z) = S(z, z') \Gamma(z')$. The method requires knowing two independent solutions of the differential equation (11) at each kind of layer (well and barrier), which in our case are simply sine and cosine functions. The band structure is obtained from a well-known dispersion relation [6].

While the KP method above will be used to study a infinitely periodic structure, we shall employ the Yeh, Yariv and Hong approach (YY) [14, 15] to analyze, in the single-band effective-mass approximation, a finite structure with evanescent wavenfunction at its ends. Essentially, the YY approach is similar to the KP approach when a square well basis is considered; the condition of evanescent wavefunction is obtained by setting to zero one of the elements of the matrix relating the initial and final $F_c(z)$ and $(1/m_c) dF_c/dz$ functions. The equation solved by this method is also equation (11). Further comments on this method will be made when its application is presented in Section 3.

Finally, for the graded profile structure analyzed in Section 4, a standard finite-element method will be used to solve equation (11).

3. APPLICATION TO SQUARE-WELL STRUCTURES

In this section we shall apply the "exact" method of (3) to compute the energy levels and envelope functions of several one-dimensional structures, all with step-profile potential, and compare the obtained results with those given by the effective-mass methods. We shall mainly focus on finite structures, although results of an infinite superlattice will also be given at the end of the section. The two finite structures considered will be a single and a double quantum well. The computational cost of the exact method increases significantly if a MQW structure with more wells is analyzed; however, the results for these two cases will suffice for our comparison purposes.

As said in the Introduction, the exact equations (3) necessarily describe a periodic structure. Nevertheless, in contrast to the effective-mass methods based on the transfer-matrix formalism, this numerical, exact approach automatically accounts for any possible form of the solutions; the resulting envelope functions, whether sinusoidal, exponential, or with any other shape, will all arise from their Fourier expansion as calculated from (3). Thus, in order to describe a single QW structure with decaying wavefunction in the barrier, we only need to let the length of the barrier be sufficiently large. Fig. 1(a) shows the single QW structure we wish to analyze and the periodic structure actually described by (3); the barrier is made long enough to consider there is no overlap between the wavefunctions of adjacent cells. The finite and periodic structures corresponding to a double quantum well are shown in Fig. 1(b), and the same caution applies.

We shall use the same potential as in [12]:

$$V(z) = V_{0i} + V_{1i} \cos\left(\frac{2\pi}{a}z\right), \quad (12)$$

where i denotes "well" or "barrier". We have taken $V_{0well} = 0.7460$ eV, $V_{1well} = 2.7512$ eV, $V_{0barrier} = 0$ eV, and $V_{1barrier} = 5.0596$ eV. This atomic potential is represented in Fig. 2 for the two cases. The virtual potential is chosen to be

$$V_{\text{virtual}}(z) = V_0 + V_1 \cos\left(\frac{2\pi}{a}z\right), \quad (13)$$

with $V_0 = (V_{0\text{well}} + 2V_{0\text{barrier}})/3$ and $V_1 = (V_{1\text{well}} + 2V_{1\text{barrier}})/3$. As mentioned in Section 2, $\psi(z) = U_n(z)\exp(ikz)$ are taken to be solutions of the Schrödinger equation (2) when the virtual crystal with the potential (13) is considered. Rather than (10), the expansion of (13) will read:

$$V_{\text{virtual}}(z) = \sum_G \tilde{V}_G \exp(iGz). \quad (14)$$

With all this, the Schrödinger equation in k -space for the virtual crystal is readily obtained as

$$\frac{\hbar^2}{2m}(k+G)^2 U_G + \sum_{G'} \tilde{V}_{G-G'} U_{G'} = E U_G. \quad (15)$$

For each k fixed, (15) gives a N_G equation system yielding N_G eigenvalues of E , that is, N_G bands, as stated above. We shall set $N_G = 11$, which keeps the truncation error negligible. The set of N_G basis functions $U_n(z)$ can be next obtained from (8).

On the other hand, the equation system (3), which describes the heterostructure, is of dimension $N_G \times N_B$. For the single QW structure, we take $L = L_w + 2L_{\text{end}} = Na = 40a$ [see Fig. 1(a)]. Since $k = l2\pi/(Na)$ (l integer), there are 40 k 's in the first Brillouin zone, *i.e.* $N_B = 40$. Therefore, the dimension of (3) is 440. For the two-well structure, we take $L = 2L_w + L_b + 2L_{\text{end}} = Na = 70a$ [see Fig. 1(b)], so the dimension is 770. There is the problem of assigning the $N_G \times N_B$ eigenvalues E of (3) to each pair of values n, k , particularly if the bands overlap. To accomplish this, one considers first an homogeneous structure made up of the material of the barrier only; the pertinent equation is formally identical to (15), and the assignment of eigenvalues is direct. Then, by inspecting the evolution of the solutions while gradually increasing the well-depth, the correspondence between the virtual crystal eigenstates and the superlattice eigenstates can be identified. For the computations, we have taken $a = 5.86 \text{ \AA}$.

In order to obtain the effective-mass results from equation (11), $m_c(z)$ and $V_c(z)$, which stem from the atomic potential $V(z)$, must be calculated first. The corresponding expressions are given in [12] and can be easily computed. We have then integrated equation (11) and matched $F(z)$ and $(1/m_c)dF/dz$ at the interfaces. The single QW case is standard and no special method is required. The double QW case (and, in general, the case of a MQW structure with a significant number of elements) can be solved by the YY method. For a rectangular potential $V_c(z)$, the envelope function will have the exponential form $F(z) = a_0 \exp(ik_b z) + b_0 \exp(-ik_b z)$ for $z < 0$, with k_b the energy-dependent constant in the barrier, and $F(z) = a_2 \exp[ik_b(z - 2L_w - L_b)] + b_2 \exp[ik_b(z - 2L_w - L_b)]$ for $z > 2L_w + L_b$ [see Fig. 1(b)], and, if M is the transfer matrix relating the column vector (a_2, b_2) to (a_0, b_0) , the condition for evanescent wavefunction at both ends of the structure implies setting $M_{22} = 0$, which gives the energy. (However, equation (12.2-4) of [15] is incorrectly applied in this reference, because a finite structure such as that shown in Fig. 1(b) in solid line is not just composed of an integer number of identical elements. Therefore, we obtain a different expression for M and a different transcendental equation for E .)

The first four envelope functions for $k = 0$ are shown in Fig. 3 for the single QW case and in Fig. 4 for the double QW case. In both cases, they are seen to be evanescent at the ends of the structures, which, as said above, is achieved by taking L_{end} large enough; this should be checked *a fortiori*. The envelope function of the effective-mass approximation has been computed for the conduction band by the YY method and is also plotted in Figs. 3 and 4. In both cases we see that the approximate envelope function is very close to the exact one. Table I displays the quantization energy of the heterostructure for the two finite structures as obtained by the exact and approximate methods. The quantization energy is defined as the energy at the bottom of the conduction band of the heterostructure, taking the energy at the bottom of the conduction band of the bulk semiconductor (barrier) as the zero-energy reference. We see that, for both the single and double QW, the relative error of the energy remains small ($\leq 3\%$). The case of an actual superlattice (*i.e.* not intended to simulate a finite

structure) has also been calculated for comparison purposes. Specifically, the superlattice cell has been taken as a single square well; the structure is the same as that in dotted line in Fig. 1(a) but with $L_w = 2L_{end} = 10a$. There is no evanescent wavefunction in the barriers; the effective-mass equation (11) has been solved by the KP method using sinusoidal envelopes in both layers. As shown in Table I, the relative error of the energy (3.4 %) is small and of similar size those of the single and double QW.

4. APPLICATION TO GRADED WELL STRUCTURES

In this section, we shall be concerned with the application of the effective-mass method to a structure with graded-potential profile. Such a structure can be analyzed "exactly" by the k -space equations, whose results, again, will be taken as a reference to assess the effective-mass method. With the techniques of disordering, for example, the atoms of the elements of the barrier diffuse into the well [17,18]; a typical potential profile considered for this case is the error function profile. We shall employ here an atomic potential such that $V_c(z)$ resembles this function, although the method would be valid for any arbitrary potential shape. Specifically, we shall now have:

$$V(z) = V_0(z) + V_1(z) \cos\left(\frac{2\pi}{a}z\right), \quad (16)$$

where

$$V_0(z) = 0.7174 \left[\operatorname{erf} \left(\frac{L_w + 2(z - 35a)}{4L_d} \right) + \operatorname{erf} \left(\frac{L_w - 2(z - 35a)}{4L_d} \right) \right] \quad (17)$$

$$V_s(z) = 2.7512 + 2.1084 \left\{ 1 - 0.9617 \left[\operatorname{erf} \left(\frac{L_w + 2(z - 35a)}{4L_d} \right) + \operatorname{erf} \left(\frac{L_w - 2(z - 35a)}{4L_d} \right) \right] \right\}, \quad (18)$$

with a well length $L_w = 10a$ and a diffusion length $L_d = 30 \text{ \AA}$. We have plotted $V(z)$ and the resulting $V_c(z)$ in Fig. 5.

The calculation procedure with the "exact" equations (3) is entirely analogous to that of the square well case. Here we have needed to set $N_B = 70$, $L = L_w + 2L_{end} = 70a$ [see Fig. 5(b)]. The virtual potential may be taken to be (13) again; its particular form is irrelevant as long as it does not differ very much from any local potential of the structure (in which case the concept of "slowly-varying" envelopes would be meaningless). Fig. 6 shows the first four envelopes at $k = 0$. The envelope of the conduction band as computed from equation (11) is also plotted for comparison. Equation (11), as mentioned before, was solved using the finite-element method (FEM) [16]. As with the square well structures analyzed in Section 2, the approximate envelope closely follows the shape of the exact one. The energy error of the effective-mass method is 0.78 % (see Table I).

5. CONCLUSIONS

We have employed the exact k -space method to analyze square well heterostructures. Although this method is intended for periodic structures, we have seen that the evanescent form of the envelope functions at the ends of a finite structure can be truly reproduced. We have also computed the conduction band envelope function of these structures in the effective-mass approximation. The approximate envelopes are very close to the exact ones —it is worth noting that the former were computed by the YY

method, which explicitly imposes evanescent wavefunction at the ends of the structure; this, in turn, confirms the ability of the k -space method to describe finite structures. The quantization energy obtained by the effective-mass model is reasonably close to the exact value. This good agreement is to be expected in view of the applicability of the envelope-function method for abrupt heterostructures, as discussed and justified in [11]. The case of a true periodic superlattice was also included in the calculations and the quantization energy error given by the effective-mass method is much of the same size as that of the finite heterostructures.

By using a suitable atomic potential, we have extended the k -space analysis to a QW structure with graded-potential profile. Again, a very good agreement is found between the exact and effective-mass results. The relative error of the quantization energy is smaller than that of the abrupt heterostructures. In fact, as said above, the envelope-function approach has been justified to work quite well even for abrupt heterostructures, so its behavior with graded structures should be satisfactory.

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	Single QW	Double QW	Superlattice	Graded QW
"Exact" quantization energy	5.7963 eV	5.7957 eV	5.7952 eV	5.7794 eV
KP absolute error	---	---	1.5 meV	---
Relative error	---	---	2.4 %	---
YY absolute error	1.9 meV	1.8 meV	---	---
Relative error	3 %	2.9 %	---	---
FEM absolute error	---	---	---	0.33 meV
Relative error	---	---	---	0.78 %

TABLE I. The "exact" quantization energies of the four heterostructures considered are shown in the upper row. The energy errors introduced by the effective-mass model are displayed in the lower rows. Explicit mention to the method used to implement this model is made in each case.

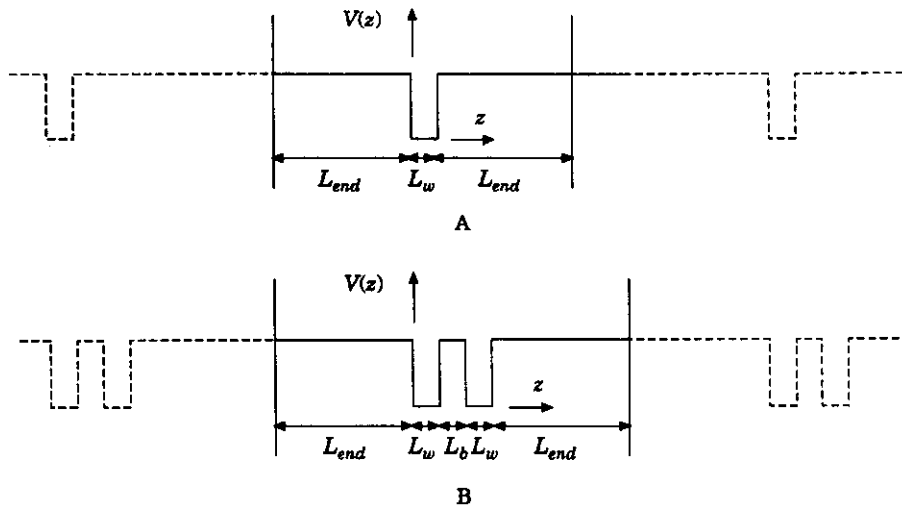


Fig. 1. A, Potential of a single square quantum well (—) and periodic structure actually described when the k -space equations are used (---). B, Same as (A) for a double square quantum well.

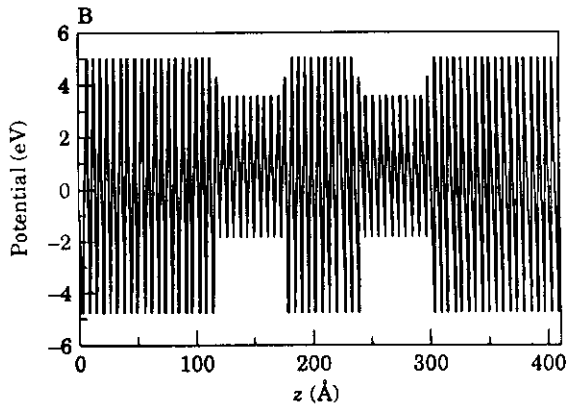
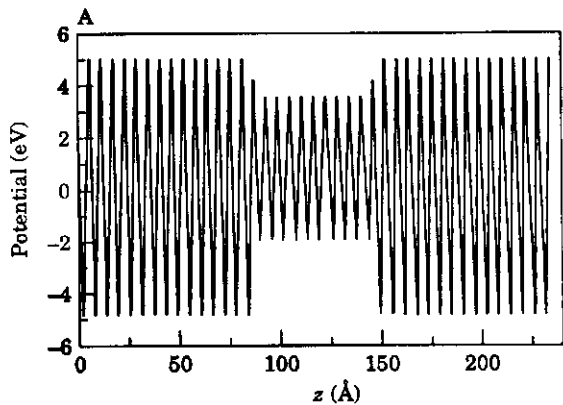


Fig. 2. A, Atomic potential of the single quantum well of Fig. 1A. B, Atomic potential of the double quantum well of Fig. 1B.

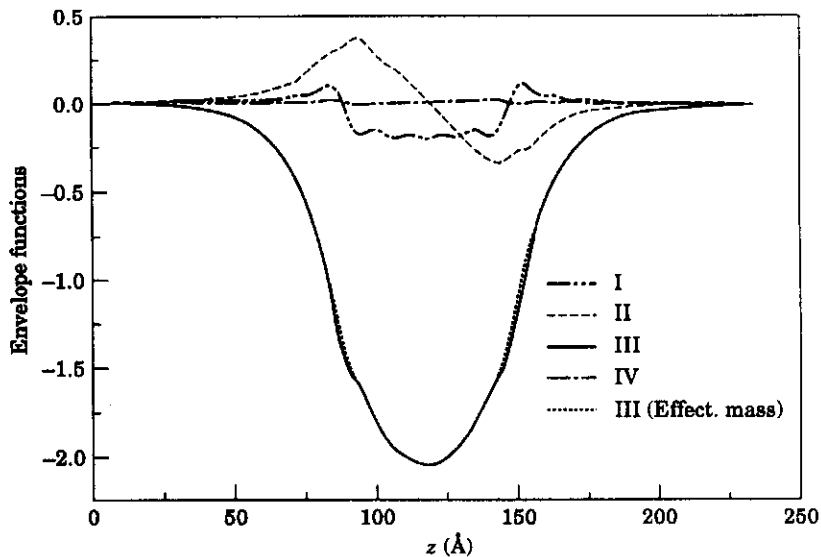


Fig. 3. The first four envelope functions of the single quantum well of Fig. 1A for $k=0$, and the approximate envelope function obtained from the effective-mass model for the conduction band.

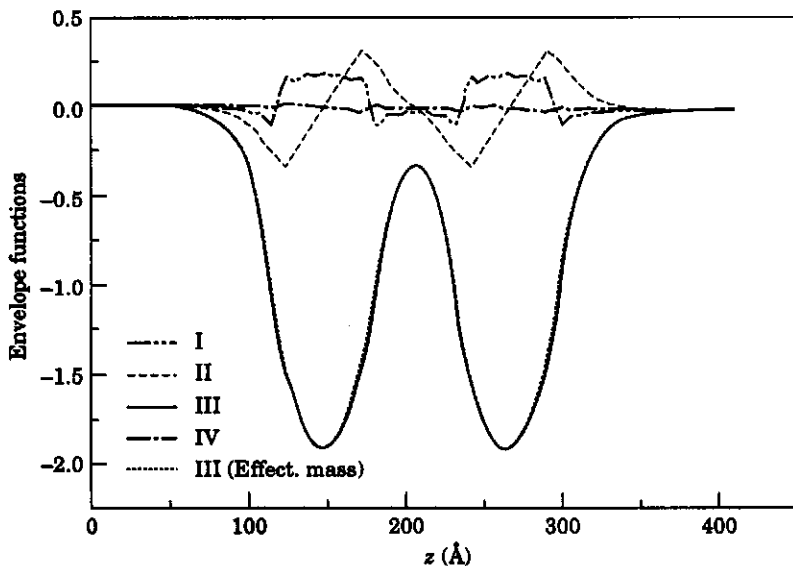


Fig. 4. The first four envelope functions of the double quantum well of Fig. 1B for $k=0$, and the approximate envelope function obtained from the effective-mass model for the conduction band.

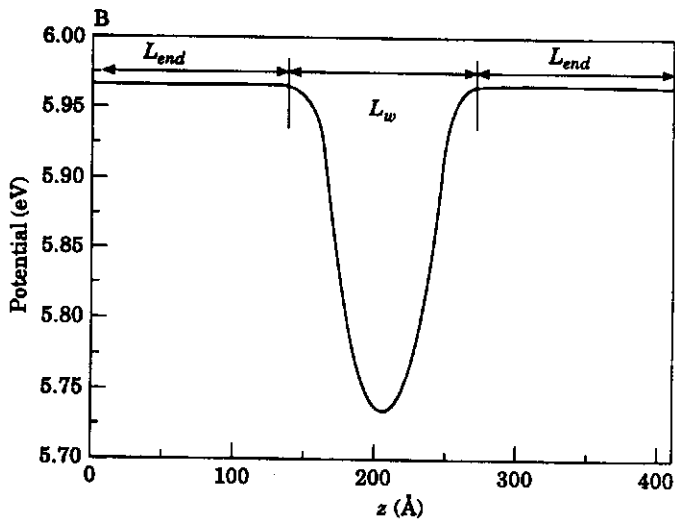
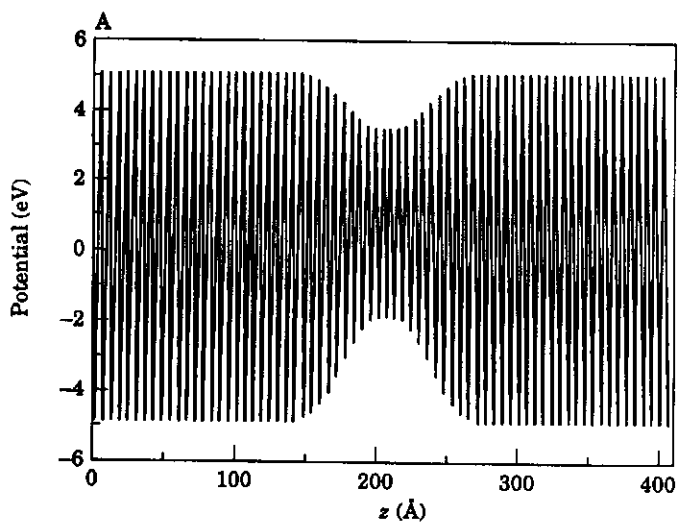


Fig. 5. A, Atomic potential of the single quantum well with graded-potential profile. B, Effective potential.

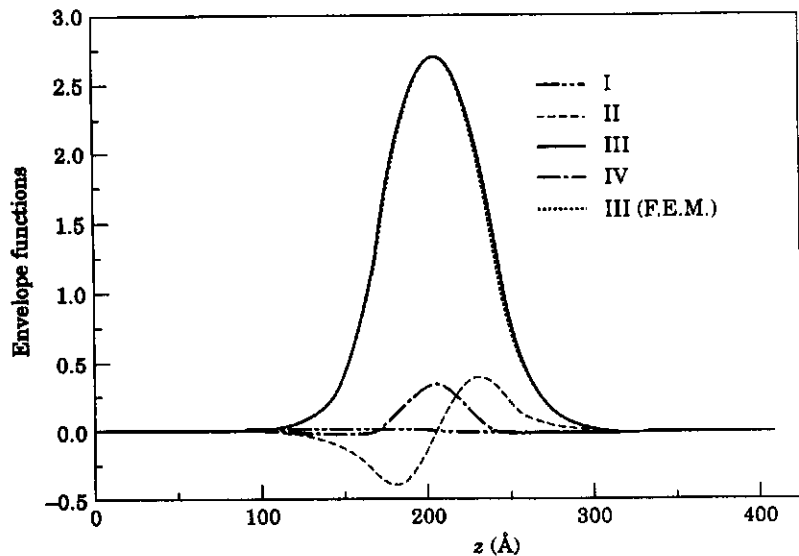


Fig. 6. The first four envelope functions of the single graded quantum well of Fig. 5 for $k=0$, and the approximate envelope function obtained from the effective-mass model for the conduction band.