Analytical closed form expressions for the effective band edges in shallow quantum wells

Jasprit Singh
Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, Michigan 48109-2122

(Received 2 December 1993; accepted for publication 22 February 1994)

Shallow quantum wells are widely used in electronic and optoelectronic heterostructure devices. However, to determine the effective band edges, one needs numerical techniques unless the barrier height is infinite. In this letter the nearly free electron approach used in periodic structures is exploited to provide accurate energy level expressions for the electronic ground state in a number of important quantum wells with different shapes. These include the square quantum well without and with an applied transverse electric field.

High quality heteroepitaxy of semiconductors has allowed one to fabricate arbitrary shaped quantum wells from semiconductors. If the quantum well has a "square well" form and the potential barrier is infinite, the ground state energy of the electron is known in a closed form:

$$E_1=\frac{\pi^2\hbar^2}{2m^*W^2}, \tag{1}$$

where m^* is the effective mass and W the well size. However, if the barrier height V_0 is finite, one has to solve a transcendental equation iteratively.[1]

If the quantum well is under the presence of an electric field or if the shape of the quantum well is not a square but triangular, for example, the problem must be solved numerically. A number of important devices require the study of quantum wells under an applied field.[2-5] A simple observation allows us to provide an analytical result for rather complicated potential wells. The observation is the following: *the electronic levels of a single quantum well are almost the same as that of a periodic array of multiquantum wells as long as the barrier is large enough.* Thus, if instead of solving a single quantum well problem one solves a periodic multiquantum well problem, the results should not be too different.

By converting a single quantum well problem to a periodic potential problem we can exploit the much simpler and elegant mathematics of Fourier transforms to solve the problem.[6] In Fig. 1 we show two simple cases of a square quantum well of well width W and barrier height V_0. An equivalent periodic structure of periodicity "a" is also shown. In Fig. 1(a) the quantum well is shown without an external electric field, while in Fig. 1(b) a field is applied. Other potentials can be similarly represented. The ground state of this system will be obtained by simply calculating the lowest Fourier coefficients of this periodic potential.

The periodic potential can be written quite generally as[6]

$$U(x)=\sum_G U_G e^{iGx}, \tag{2}$$

where G represents the reciprocal lattices of the periodic potential and U_G are the Fourier transform coefficients

$$G=\frac{2n\pi}{a}, \tag{3}$$

$$U_G=\frac{1}{a}\int_0^a U(x)e^{-iGx}dx. \tag{4}$$

The electronic states obey the k-space Schrödinger equation (see, for example, Chap. 7 in Ref. 6)

$$\left(\frac{\hbar^2}{2m^*}\left|k-G\right|^2-E\right)C_{k-G}+\sum_{G'} U_{G'-G}C_{k-G'}=0, \tag{5}$$

where the general solution has the form

$$\Psi_k(x)=\sum_G C_{k-G}e^{i(k-G)x}. \tag{6}$$

As noted earlier, if the barrier width is large, the resulting solution represents the uncoupled well problem quite accurately. We are interested in the lowest energy state that oc-

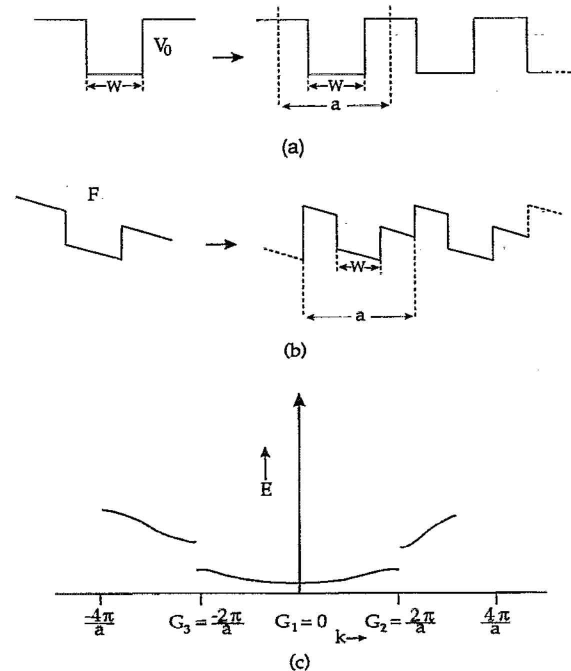

FIG. 1. (a) A square well potential represented as a periodic multiquantum well structure; (b) A square quantum well under an applied field represented by a periodic structure; (c) the nearly free electron description of a general periodic structure. If the barrier widths are large the miniband widths are essentially zero.

 © 1994 American Institute of Physics

curs at $k-G_1=0$. To a good approximation we need to only include the coefficients C_{k-G_1}, C_{k-G_2} and C_{k-G_3} in the Schrödinger equation where as shown in Fig. 1(c),

$$G_2-G_1=\frac{2\pi}{a},$$
$$G_3-G_1=\frac{-2\pi}{a}. \tag{7}$$

The other coefficients are negligible at the zone center point. We get three coupled equations from Eq. (5):

$$(E-E^0_{k-G_1})C_{k-G_1}=U_{G_2-G_1}C_{k-G_2}+U_{G_3-G_1}C_{k-G_3},$$
$$(E-E^0_{k-G_2})C_{k-G_2}=U_{G_1-G_2}C_{k-G_1}+U_{G_3-G_2}C_{k-G_3}, \tag{8}$$
$$(E-E^0_{k-G_3})C_{k-G_3}=U_{G_1-G_3}C_{k-G_1}+U_{G_2-G_3}C_{k-G_2},$$

Here,

$$E^0_k=\frac{\hbar^2k^2}{2m^*}. \tag{9}$$

To solve for the energy levels, we solve the determinant (at $k=G_1$), denoting $U_{2\pi/a}$ by U_1 and $E^0_{2\pi/a}$ by E^0_1, and ignoring $U_{4\pi/a}$.

$$\begin{vmatrix} E & -U_1 & -U_1^* \\ -U_1 & E-E^0_1 & 0 \\ -U_1^* & 0 & E-E^0_1 \end{vmatrix}=0. \tag{10}$$

The ground state is found to be,

$$E=\frac{E^0_1-\sqrt{E^{02}_1+8U_1^2}}{2}. \tag{11}$$

Noting that the electron energy is measured from the dc Fourier coefficient U_0, we get for the ground state or the effective band edge:

$$E_1=U_0-\frac{1}{2}E^0_1\left(\sqrt{1+\frac{8U_1^2}{E^{02}_1}}-1\right). \tag{12}$$

This expression is accurate if the higher order coefficients U_n are small which is true for the potentials shown in Fig. 1 and most smooth potentials. The component U_1 is given by Eq. (15) below with the field F zero.

Focusing on the potential of Fig. 1(b), if F is the applied electric field, the potential may be written as (using say $a=2W$ for simplicity where W is the well size),

$$V(x)=\Delta E+(eFa/2)-eFx \quad 0\leqslant x\leqslant a/4,$$
$$V(x)=(eFa/2)-eFx \quad a/4<x<3a/4,$$
$$V(x)=\Delta E+(eFa/2)-eFx \quad 3a/4<x<a, \tag{13}$$

where ΔE is the potential barrier height. We need to find the dc and the first Fourier coefficient of this potential. These are simply found to be

$$U_0=\Delta E/2, \tag{14}$$

$$U_{2\pi/a}=U_1=\frac{\Delta E}{\pi}-\frac{ieFa}{2\pi}. \tag{15}$$

Thus we have

$$|U_1|^2=(\Delta E/\pi)^2+(eFa/2\pi)^2. \tag{16}$$

The band edge positions are now given by: zero field square well potential:

$$E_1=\frac{\Delta E}{2}-\frac{\pi^2\hbar^2}{4m^*W^2}\left[\left(1+\frac{32\Delta E^2W^4m^{*2}}{\pi^6\hbar^4}\right)^{1/2}-1\right]; \tag{17}$$

square well under an applied transverse electric field F:

$$E_1=\frac{\Delta E}{2}-\frac{\pi^2\hbar^2}{4m^*W^2}\left(\left\{1+32\left[\left(\frac{\Delta E}{\pi}\right)^2+\left(\frac{eFW}{\pi}\right)^2\right]\frac{W^4m^{*2}}{\hbar^4\pi^4}\right\}^{1/2}-1\right). \tag{18}$$

Note that these rules are derived using the case $a=2W$, which is a good choice since for the square well $U_{4\pi/a}=0$ and our approximation which ignores higher harmonies is good.

Let us now consider how accurate the expressions derived above are. We apply the results to two important cases: (i) the well size dependence of the effective band edge in a $GaAs/Al_{0.3}Ga_{0.7}As$ quantum well; (ii) quantum confined Stark effect in a 100 Å $GaAs/Al_{0.3}Ga_{0.7}As$ quantum well. We use a 65:35 rule for the conduction band to valence band discontinuity ratio, so that $\Delta E_c=244$ meV and $\Delta E_v=131$ meV. The conduction and valence band mass values used are $0.067m_0$ and $0.45m_0$.

In Fig. 2, we show the comparison of the approximate analytical result of Eq. (12) with the exact results for the GaAs/AlGaAs quantum well. Also shown is the result for an infinite barrier case. The agreement between the exact results and the results from Eq. (12) are quite good over the range of well sizes from 30 to 150 Å. Below 30 Å, our assumption $a=2W$ leads to minibands so that one simply needs to relax this to say $a=5W$ which requires one to evaluate the Fourier coefficients U_0 and U_1 for the new potential. Beyond 150 Å well size, there is a small discrepancy which arises from ignoring the higher Fourier coefficients $U_{4\pi/a}$ in the central coupled equation solution. However, since 30–150 Å wells represent a range normally used for most device applications, Eq. (12) provides an accurate and useful result.

In Fig. 3, we show that shift in the effective band edges of a 100 Å $GaAs/Al_{0.3}Ga_{0.7}As$ quantum well as a function of applied field. This shift is primarily responsible for quantum confined Stark effect. We show a comparison between our analytical results. The exact results are obtained by solving the Schrödinger equation in the quantum well profile by finite difference method. Once again very good agreement is seen between the simple results presented in this letter and the exact results. Also shown in Fig. 3 is a result from a perturbative calculation using an infinite barrier.[7] The infinite barrier calculation is seen to show a smaller shift since the electron and hole states are not able to penetrate the barrier regions.

As a final case, we consider a very shallow conduction band well corresponding to a $GaAs/Al_{0.1}Ga_{0.9}As$ structure. The conduction band discontinuity is taken to be 75 meV for the structure. This structure allows us to further test the va-

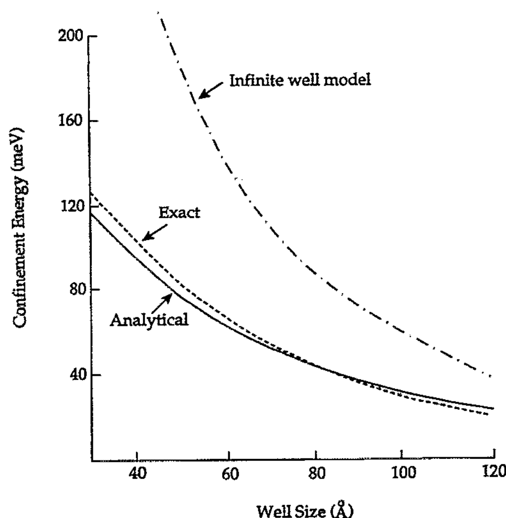

FIG. 2. A comparison of the well size dependence of the effective band edge in $GaAs/Al_{0.3}Ga_{0.7}As$. Results are shown for an exact calculation, analytical results based on this letter and an infinite well calculation.

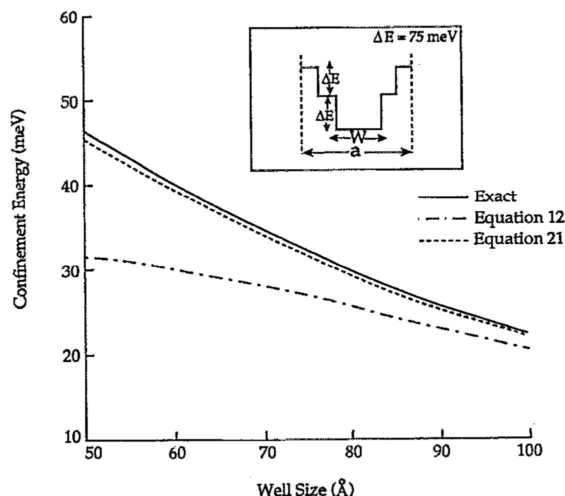

FIG. 4. The confinement energy of a $GaAs/Al_{0.1}Ga_{0.9}As$ well as a function of well size. The exact calculation is shown along with results of Eqs. (12) and (21). The inset shows the potential profile used to obtain Eq. (21). The artificial barrier suppresses miniband formation and gives very good agreements for narrow shallow wells. The periodicity distance $a=2W$.

lidity of our results and to make a simple improvement. In Fig. 4 we show the exact results for the conduction band confinement energy as a function of well size. Also shown are results based on Eq. (12). Once again we see good agreement at larger well sizes and a smaller value than the exact results at smaller well size. To avoid the miniband formation we artificially change the barrier potential as shown in the inset of Fig. 4. With this choice we have

$$U_0=\frac{3}{4}\,\Delta E, \tag{19}$$

$$U_1^2=\frac{5\Delta E^2}{2\pi^2}\,. \tag{20}$$

The value of E_1^0 remains the same. By artificially doubling the barrier away from the well region, we suppress the miniband formation. With a choice of the surrounding potential given by the insert of Fig. 4, the results can be extended to shallow and narrow wells. The new choice of the potential gives

$$E_1=\frac{3\Delta E}{4}-\frac{\pi^2\hbar^2}{4m^*W^2}\left[\left(1+\frac{80\Delta E^2W^4m^{*2}}{\hbar^4\pi^6}\right)^{1/2}-1\right]. \tag{21}$$

In Fig. 4 we show the exact results for a 75 meV barrier for GaAs quantum wells and the results obtained from Eq. (21). The results are found to be in very good agreement. Thus, Eq. (21) is an improvement over Eq. (12) for the effective band edge and has a greater applicability.

In summary, we have provided analytical closed form results for the effective band gap of shallow quantum wells. The analytical closed form results are quite accurate for shallow wells where the infinite barrier solution is invalid. The results are not so accurate for wide wells where the infinite well solution is quite reasonable. However, the accuracy of this method can be improved by including higher order Fourier terms.

This work was supported by an Air Force Grant (Contract No. AFOSR-91-0434).

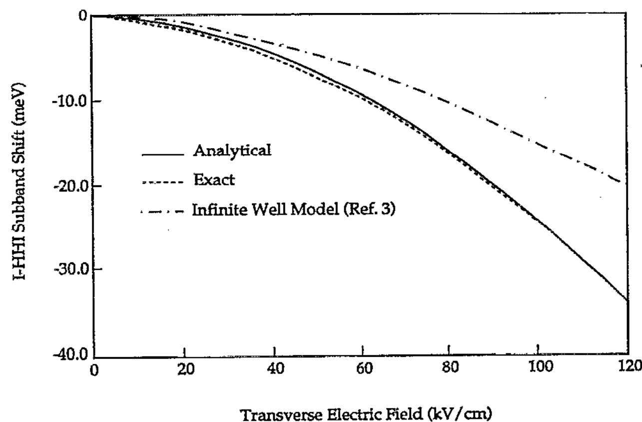

FIG. 3. The shift in the effective band gap of a 100 Å $GaAs/Al_{0.3}Ga_{0.7}As$ well as a function of electric field.

[1] See, for example, *Quantum Mechanics*, edited by L. I. Shiff (McGraw–Hill, New York, 1968).
[2] R. Dingle, W. Wiegman, and C. H. Henry, Phys. Rev. Lett. **33**, 827 (1974).
[3] D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegman, T. H. Wood, and C. A. Burrus, Phys. Rev. Lett. B **32**, 1043 (1985).
[4] K. W. Goosen, L. M. F. Chirovsky, R. A. Morgan, J. E. Cunningham, and W. Y. Jan, IEEE Photon. Technol. Lett. **3**, 448 (1991).
[5] S. W. Lee, T. M. Kim, K. V. Chu, S. Park, M. S. Jeong, and O. D. Kwon, Appl. Phys. Lett. **62**, 1176 (1993).
[6] See, for example, *Introduction to Solid State Physics*, edited by C. Kittel (Wiley, New York, 1986).
[7] E. E. Mendez, G. Bastard, L. L. Chang, and L. Esaki, Phys. Rev. Lett. B **26**, 7101 (1982).