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Renormalization formalism in the theory of the electronic structure of superlattices: Application to silicon superlattices

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A renormalization formalism for the calculation of electronic states in nontrivial superlattices is discussed for the first time. Starting from a microscopic tight-binding description of the crystal electron Hamiltonian using localized orbitals, we show how the renormalization techniques are implemented and easily applied to the study of superlattices of arbitrary width. As an example of the renormalization procedure, we consider silicon crystals in the presence of an additional superlattice potential in the [001] direction. We study the dependence of the energy gap upon superlattice width, and describe how relevant parameters drive the change from an indirect- to direct-band-gap material. Moreover, a peculiar effect due to zone folding of inequivalent valleys in the conduction band is found. The advantages of the present procedure relative to other computational tools available from the literature are discussed.

I. INTRODUCTION

Methods for the calculation of electronic states in crystals having three-dimensional translational symmetry have a long and well established tradition. The basic framework of these methods[1] was established early but significant improvements have been made. With the increasing availability of powerful computer facilities, a high degree of sophistication can be achieved in calculating physical quantities of interest without the limitations of restrictive assumptions. In principle all of the traditional methods can be applied to superlattices; in practice, however, they rapidly become impractical as the superlattice width increases. Only for ultrathin superlattices where the layer width is a few atomic planes do we find theoretical calculations based upon traditional methods. Among these are calculations using the empirical pseudopotential method[2] and the empirical tight-binding method.[3]

Significant advances have been made in the past few years toward finding alternative and workable procedures for calculating the electronic structure of superlattices of arbitrary width. Not surprisingly, parallel progress has occurred in the closely related problem of finding efficient computational procedures for the electronic structure of surfaces and interfaces. In these systems there is only two-dimensional translational symmetry because of symmetry breaking due to the presence of a surface or heterostructure. In the case of superlattices the translational symmetry remains in the growth direction but the number of atoms in the supercell is generally high. This makes the applicable computational techniques closer to those of surfaces and heterostructures than to standard three-dimensional crystals.

Presently two of the more common methods dealing with superlattices of arbitrarily large width are the envelope function method[4] and the tight-binding method combined with a complex-**k** procedure[5,6] (also referred to as the energy-dependent tight-binding method). More recently the pseudopotential method, limited in earlier work to ultrathin superlattices, has been applied to the study of medium-size superlattices. This was made possible by considering the presence of one constituent as a "perturbation" on an otherwise perfect material.[7]

The principle purpose of this paper is the presentation of a new approach to the problem of superlattices based upon powerful renormalization techniques. We present the first discussion and application of a renormalization formalism to the study of the electronic structure of realistic superlattices. As an example of the method, we study a prototype silicon superlattice. This simplest of the elemental group-IV superlattices has both an intrinsic interest, and serves as a reasonable test of our new procedure prior to its adaptation to more complicated systems.

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II. THE RENORMALIZATION APPROACH FOR SILICON SUPERLATTICES

Before presenting the new method and applying it to silicon, we briefly summarize some relevant aspects of the envelope-function approach and the complex-**k** procedure for superlattices. This discussion is relevant since these are the only methods leading to secular equations whose order is independent of the superlattice width.

The envelope function method[4] is based upon an averaged description of the two constituent crystals of the superlattice system. The underlying strategy is to avoid a detailed microscopic description of the component crystals. In a small region of the Brillouin zone the band structure is approximated using a $\mathbf{k}\cdot\mathbf{p}$ matrix, of reasonably small order, whose parameters are determined semiempirically from the bulk effective masses, momentum matrix elements, and band edges of the component materials. An effective generalized Schrödinger equation, with appropriate boundary conditions, is then constructed for the envelope function. Of course, such a procedure has a limited range of validity, being confined to energies in close proximity to the band edges and to materials with similar electronic structure. There is the additional difficulty of nonrigorous boundary conditions and the inability to treat compounds with a multivalley band structure. Despite these drawbacks, the envelope function procedure is useful in a number of cases for a qualitative determination of the electronic states, and in selected other cases, a quantitative description can be obtained.

A second method capable of treating superlattices with arbitrary width is the semiempirical tight-binding method in conjunction with the complex-**k**-vector procedure.[5] In applications of the standard tight-binding method to three-dimensional crystals, one selects a real **k** vector and determines the corresponding eigenvalues $E_n(\mathbf{k})$. In the complex-**k**-vector method the energy E is fixed and the corresponding complex **k** vectors are found that satisfy the determinantal tight-binding equation. The decaying and growing waves of the component crystals in the direction of the superlattice are thereby determined. These energy-dependent wave functions are used to expand the superlattice states, and the eigenvalues are found by imposing boundary conditions at the interface and at the border of the superlattice unit cell. The procedure is not routine, involving the evaluation of energy-dependent basis functions, complicated expressions of the matrix elements, and a trial-and-error search for eigenvalues. The method is closely related to the transfer matrix method.[8]

The renormalization formalism was originally proposed in condensed-matter physics in connection with the problem of phase transitions and critical phenomena.[9] Among applications fostering further extensions, we mention its surprising success in the numerical evaluation of the critical properties of the two-dimensional Ising model.[10] Subsequently, renormalization techniques were applied to a wide range of electronic problems[11] including disordered systems, surfaces, and interfaces. A step toward systematic application of the renormalization techniques (and the closely related recursion[12] and moment methods[13]) is contained in review articles.[14,15] The only superlattice application of the renormalization method to appear in the literature was confined to a very simple one-dimensional lattice.[16]

To illustrate the renormalization procedure we consider the case of an ideal silicon crystal with a superimposed superlattice potential in the [001] direction. We study this case because of its importance as a prototype of the class of group-IV superlattices. Recently, experimental results[17] have been accumulating on Si-$\mathrm{Si}_{1-x}\mathrm{Ge}_x$ superlattices, and the potential of graded elemental group-IV superlattices could become of experimental interest as in the case of III-V compound concentration-graded superlattices.[7] Furthermore, silicon superlattice selection simplifies the testing procedure since other calculations are available in the literature.[6]

The starting point is a tight-binding Hamiltonian for the bulk silicon crystal. We adopt a well-known parametrization[18] using five orbitals per site (s,p_x,p_y,p_z,s^*); the introduction of an excited s^* state into the minimum basis set with nearest-neighbor interactions provides a reasonably good description of all valence bands, and also of the lowest conduction band with its six equivalent minima. We consider a superlattice with a superperiodic external potential in the z direction. For simplicity this potential is approximated by a finite-depth rectangular well of height V_s. For each localized orbital we construct a corresponding two-dimensional Bloch sum with a fixed vector parallel $(\mathbf{k}_\parallel)$ to the planes comprising the superlattice. The one-electron Hamiltonian is then expressed in the basis of the two-dimensional Bloch sums. For any $\mathbf{k}_\parallel$ vector we have a multisite linear "ring" Hamiltonian with only nearest-neighbor interactions. The Hamiltonian can be written in the form

$$H=\sum_{\substack{n=1\\ \alpha,\beta}}^{N_p}(A_{n,n})_{\alpha\beta}\,|\phi_{n\alpha}\rangle\langle\phi_{n\beta}|+\sum_{\substack{n=1\\ \alpha,\beta}}^{N_p-1}(B_{n,n+1})_{\alpha\beta}\,|\phi_{n\alpha}\rangle\langle\phi_{n+1,\beta}|+\sum_{\substack{n=1\\ \alpha,\beta}}^{N_p-1}(B_{n+1,n})_{\alpha\beta}\,|\phi_{n+1,\alpha}\rangle\langle\phi_{n\beta}|$$
$$+\sum_{\alpha,\beta}(B_{1,N})_{\alpha\beta}\,|\phi_{1\alpha}\rangle\langle\phi_{N\beta}|+\sum_{\alpha,\beta}(B_{N,1})_{\alpha\beta}\,|\phi_{N\alpha}\rangle\langle\phi_{1\beta}|\ . \qquad (1)$$

In the above expressions we have used latin letters ($n=1,\ldots,N_p$ or N_p-1) for the site indices and greek letters (α or β, ranging from 1 to 5) for the on-site orbital indices. The A's and B's are matrices of order 5×5. The A's are diagonal and the B's can be easily expressed in terms of $\mathbf{k}_\parallel$ and the few independent parameters reported in Ref. 18. The additional superlattice potential is accounted for by introducing a shift V_s in all of the di-

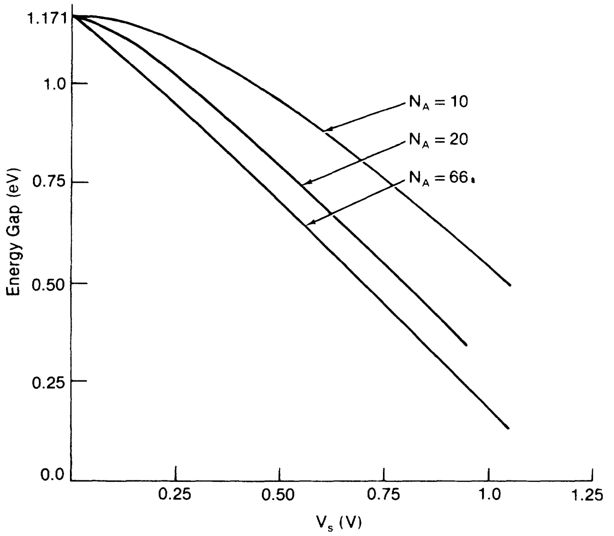

FIG. 1. The dependence of the energy gap upon the superlattice potential V_s for superlattices of three different widths.

agonal matrix elements for half of the sites of the supercell. For sake of simplicity the total number of sites N_p in the supercell is taken to be a multiple of 4 so that the stacking in the [001] direction is an even number of layers, each layer having two planes. The wave vector k_z of the superlattice Brillouin zone has the bounds $-\pi/\tau < k_z < \pi/\tau$ where $\tau = 0.25 a_0 N_p$, a_0 being the lattice parameter of silicon.

A particular feature of a Hamiltonian such as (1) is the presence of corner matrices B_{1N} and B_{N1} containing interactions between adjacent planes and a multiplicative phase factor $\exp(-ik_z\tau)$. Without these matrices, the problem of finding the Green's function of the Hamiltonian (1) would lead to a matrix continued fraction.[15] The corner blocks mathematically account for the essential differences between a finite slab of material and a superlattice.

To this point, only group theory has been used to reduce the three-dimensional superlattice problem to a one-dimensional ring Hamiltonian in block form. We now show how to systematically renormalize the Hamiltonian and obtain the Green's function. Suppose for simplicity that a single site is eliminated; site 2 for example. A renormalized Hamiltonian is obtained with renormalized matrix elements

$$
\begin{aligned}
\tilde{A}_{1,1} &= A_{1,1} + B_{1,2}\frac{1}{E - A_{2,2}}B_{2,1} , \\
\tilde{A}_{3,3} &= A_{3,3} + B_{3,2}\frac{1}{E - A_{2,2}}B_{2,3} , \\
\tilde{A}_{1,3} &= B_{1,2}\frac{1}{E - A_{2,2}}B_{2,3} , \\
\tilde{A}_{3,1} &= B_{3,2}\frac{1}{E - A_{2,2}}B_{2,1} .
\end{aligned}
\qquad (2)
$$

An efficient FORTRAN program has been implemented that simultaneously eliminates all equivalent sites. Suppose N_A planes of silicon are in part A with superimposed potential V_s, and N_B planes are in part B. As an added simplification, we assume that N_a and N_b are even and equal. In part A we eliminate all even-numbered equivalent sites except the one numbered N_a. Most of the remaining sites are equivalent and the few inequivalent sites at the border are stored away. We again eliminate the even numbered sites and save inequivalent sites. This renormalization procedure is repeated until no equivalent sites remain. Not more than $1+\mathrm{int}[\log_2(N_A)]$ inequivalent sites will remain. The same procedure is repeated for part B again generating no more than $1+\mathrm{int}[\log_2(N_B)]$ inequivalent sites. The small number of remaining sites are then individually eliminated until only a 2×2 site Hamiltonian remains which yields the Green's-function matrix elements upon inversion. For a superlattice with $N_p = N_a + N_b$ planes, the number of renormalizations to be performed to obtain the Green's function at a given energy E is on the order of $2\log_2(N_p)$. Note that each renormalization requires a simple inversion of a 5×5 matrix and a few related products of matrices of the same order. Thus for a superlattice of 1000 atomic planes, approximately 20 renormalizations can reduce the initial Hamiltonian to a single-site renormalized matrix.

We now present some results obtained with this procedure. Figure 1 shows the dependence of the energy gap upon the applied bias V_s for various superlattice widths. The case of $N_A = N_B$ tending toward infinity (not shown) is a straight line with a slope of negative one connecting the points (0.0, 1.171) and (1.171, 0.0); however, level quantization effects introduce an upward bending that is larger for small superlattice widths. This effect was first pointed out by Krishnamurthy *et al.*,[6] who used a minimal basis set with first- and second-nearest-neighbor interaction, and a complex-**k**-vector procedure. It would be of interest to examine more carefully the region near $V_s = E_G$ and to explore the possibility of a semiconductor-metal transition of the silicon superlattice.

Another interesting feature is the transition from an indirect gap to a direct gap material as the width and the value of V_s is changed. Figure 2 shows a portion of the folded dispersion curves of an ideal perfect crystal with $N_p = 40$. Notice the presence of the degeneracies in the conduction band. The valence band associated with the p_x and p_y orbitals is doubly degenerate. At Γ and at the edge of the Brillouin zone (in the [001] direction) where the band was folded, there is a fourth-order degeneracy. Figures 3(a) and 3(b) show dispersion curves with $V_s = 0.50$ and $N_p = 40$. We see that the superlattice has nearly become a direct-band-gap material. The doublet of levels arising from the conduction band is a peculiar effect due to zone folding of inequivalent valleys in the [001] and $[00\bar{1}]$ directions. The ground state is also an almost-degenerate doublet, a fact verified by considering the gradual deformation of the folded conduction bands with increasing superlattice potential [see Figs. 4(a) and 4(b)]. This effect, though small, bears a resemblance to intervalley effects arising in impurity problems.[19]

Figure 4(c) shows the quantum-well doublets of the heavy-hole valence band (p_x,p_y) resulting from the reduced degeneracy. These results show the convenience of the renormalization procedure to deal not only with materials with minima (or maxima) at Γ, but also to treat complicated multivalley semiconductors.

III. CONCLUSIONS

In conclusion, the renormalization procedure has been shown to successfully describe the electronic states in superlattices of arbitrary size. The required number of renormalizations increases logarithmically with superlat-

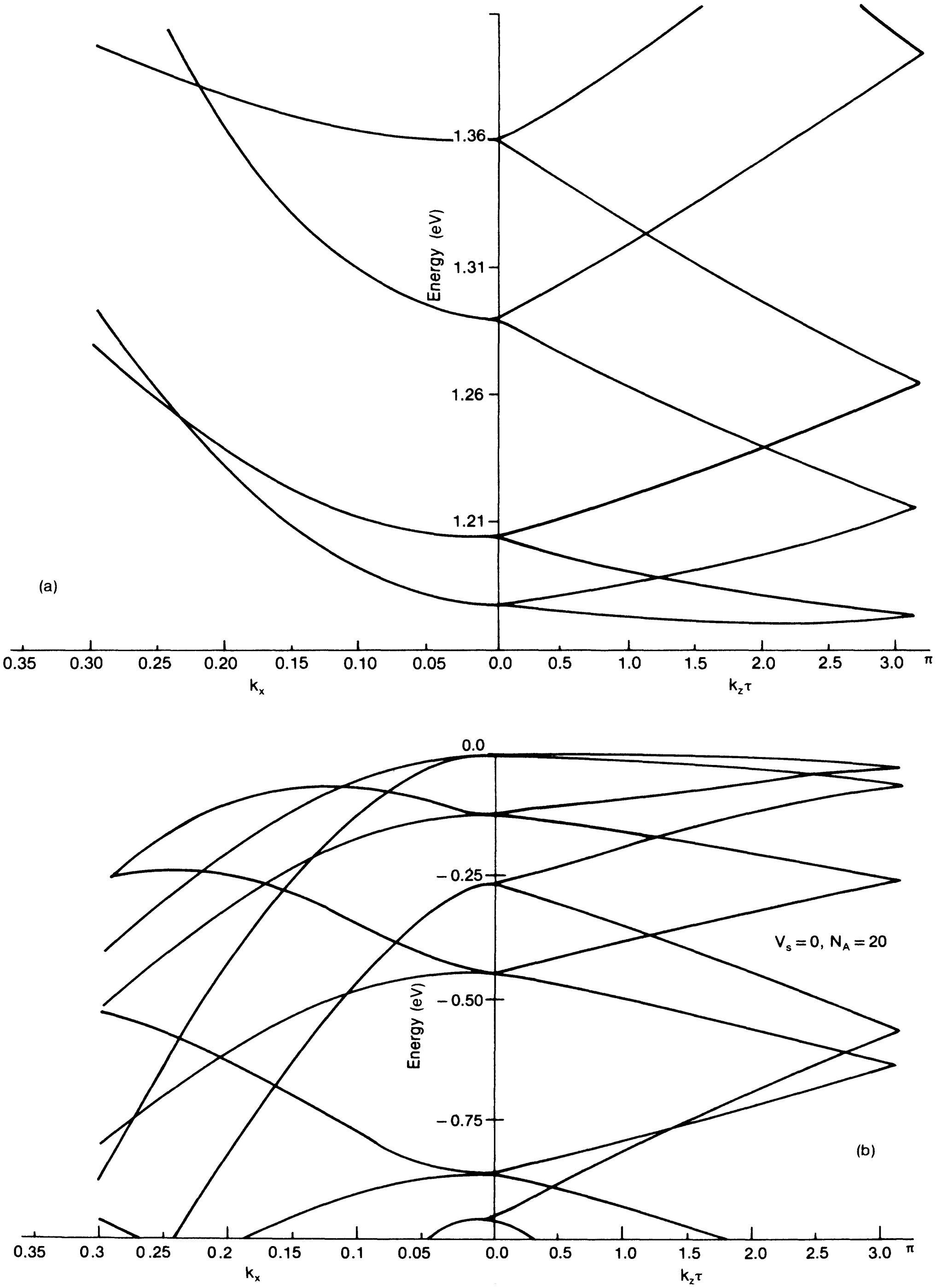

FIG. 2. Dispersion curves for conduction (a) and valence (b) states along k_z and k_x directions for the perfect crystal. $N_p = 40$ such that the unit cell has a length $10a_0$ in the z direction. (a_0 is the lattice parameter of silicon, and is scaled to be 4.)

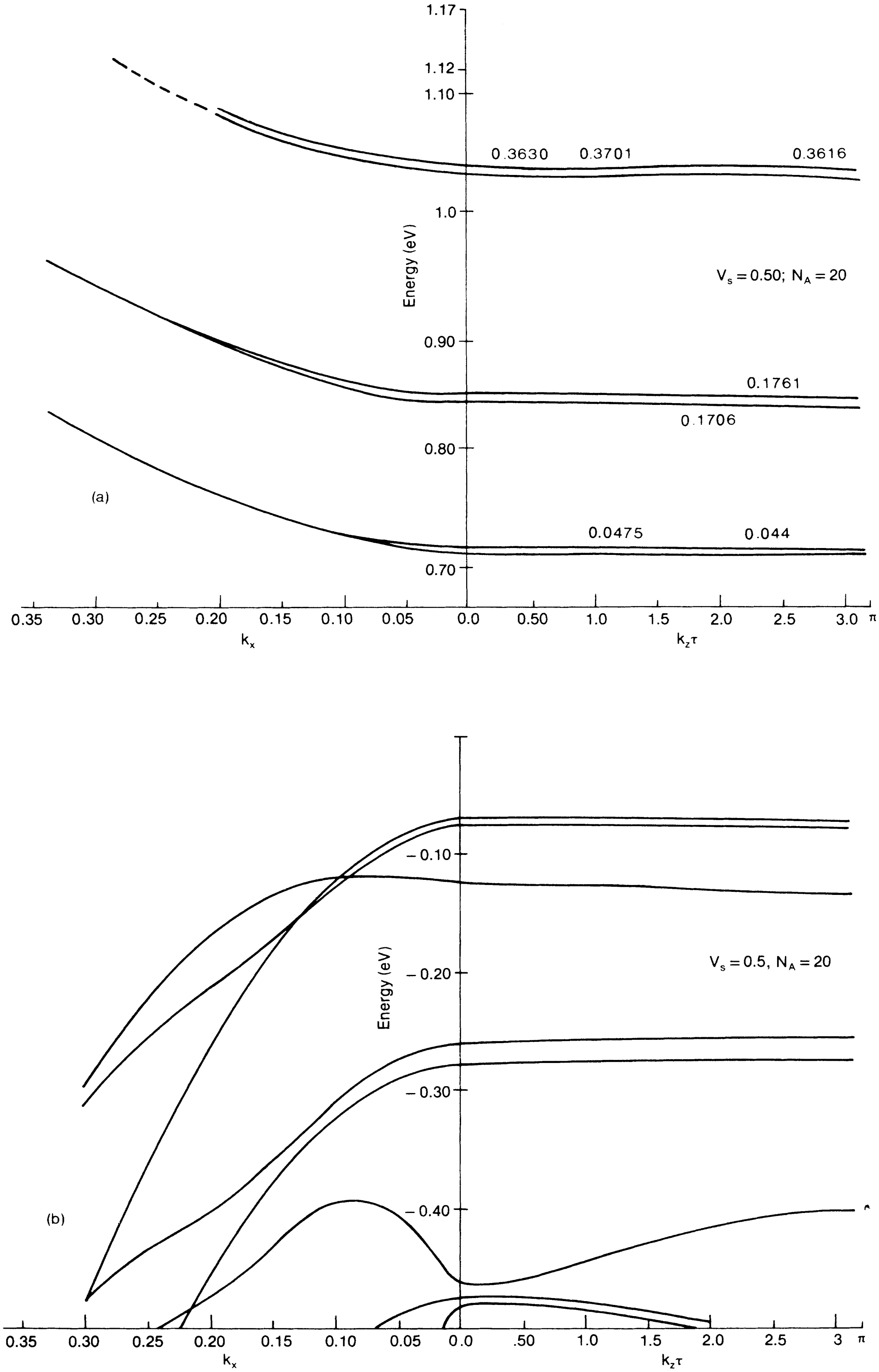

FIG. 3. Dispersion curves for conduction (a) and valence (b) states with $N_p = 40$ and superlattice potential $V_x = 0.50$. In (a) the spacing of the doublet levels starting with the lowest one is approximately 0.0035, 0.0055, and 0.008 eV. A portion of the dispersion curves along the k_x direction is also shown. From (b) we estimate the effective mass of the heavy hole to be about 1.8 times that of the light hole. In (a) the energies along the conduction bands are referenced to the bottom of the wells (at 0.67 eV from the top of the valence band).

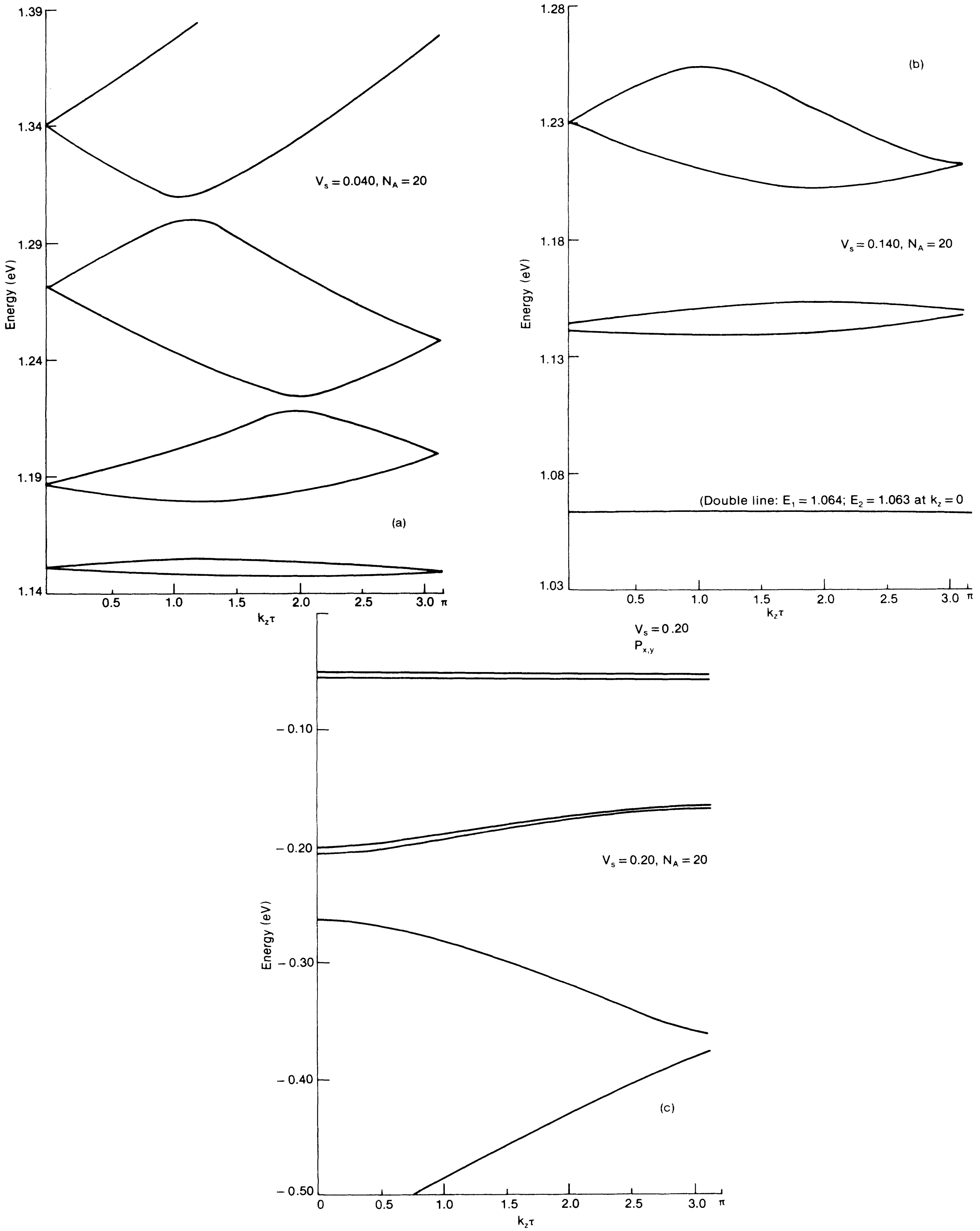

FIG. 4. This set of figures shows doublet formation in the quantum wells by the gradual deformation of the folded bands as the superlattice potential increases. The conduction bands with $V_s = 0.04$ and $V_s = 0.14$ are shown in (a) and (b) while the heavy-hole valence band with $V_s = 0.20$ is shown in (c).

tice size. The parametrization of the silicon energy bands was taken from the literature and included nearest-neighbor interactions only. However, the method can be adapted to include spin-orbit interaction and/or more distant neighbor interactions. A more accurate parametrization could be useful to look for semiconductor-metal transitions in silicon superlattices. We are presently applying this technique to other elemental group-IV superlattices including silicon-germanium alloys and superlattices.

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