Electronic Properties of Flat-Band Semiconductor Heterostructures

S. R. White and L. J. Sham
Physics Department, University of California at San Diego, La Jolla, California 92093
(Received 15 April 1981)

A new theory of the electronic properties of heterostructures is proposed. Linear combinations of Bloch waves, both propagating and evanescent, are matched across the interface. This leads to simple continuity conditions on the envelope functions, which can be used to solve any heterostructure problem. Calculated optical transitions in GaAs-AlGaAs and InAs-GaSb heterostructures show good agreement with experiment.

PACS numbers: 73.40.Lq, 73.90.+f

A superlattice of alternating layers of two semiconductors can now be fabricated.[1,2] The theory of the electronic properties of these systems may be approached in two complementary ways. First-principles band-structure calculations,[3-8] treating atoms in two dissimilar layers as constituting a supercell, can handle layer thicknesses up to a few atomic planes without exceeding present-day computer capacity. For thicker layers, an effective-mass approach becomes preferable.[1,2,9] Each layer behaves like a macroscopic crystal, modified at most by a slowly varying potential. The wave function is an amplitude modulation of a Bloch wave with the envelope governed by a Schrödinger-like equation. The major problem is joining the solution from layer to layer.

The most naive approach makes the envelope function and its derivative continuous across the layer interface. This appears to work quite well for certain type-I superlattices, e.g., GaAs-AlGaAs, in which the respective conduction and valence-band edges are close in energy.[1] For type-II superlattices, e.g., GaSb-InAs, in which the valence-band edge of one semiconductor is above the conduction-band edge of the other, this approach to envelope-function matching is completely meaningless.[2]

We report here a theory in the effective-mass genre. The amplitude modulation is extended to include both conduction and valence bands in the same energy range for the whole heterostructure by using Kane's three-band Hamiltonian.[10] There are evanescent waves which decay away from the interface so quickly that they do not contribute to the effective-mass wave function. They do play an indispensable role in matching the wave function and its normal derivative at the interface.[11] The conditions for joining the envelope function in the bulk of one layer with that in another layer are derived. They turn out to be remarkably simple and are very useful as boundary conditions for the envelope functions.

For simplicity, take the wave vector normal to the interfaces. Then the Kane Hamiltonian[10] decouples into a single band for the heavy holes and a 2×2 $\vec{k}\cdot\vec{p}$ Hamiltonian for the conduction and light-hole valence bands:

$$H_k=\begin{bmatrix} E_c+Ak^2 & Pk \\ Pk & E_l-Ak^2 \end{bmatrix}, \tag{1}$$

where k is the wave vector and E_c and E_l are the conduction and light-hole band-edge energies. P is the momentum matrix element between the conduction and light-hole valence bands. E_c-E_l and P are fitted to the known bulk band structure.

A is a positive parameter which represents schematically the effects of bands not represented in the basis for the Kane Hamiltonian. We introduce these terms so that the effective-mass equations retain the character of second-order differential equations. This makes the wave function and its normal derivative continuous across an interface. To recover the Kane model, we let $A\to 0$ after establishing the boundary conditions. A is in fact small for all materials of interest.

For small A, at a given energy E, two of the wave vectors, which correspond to evanescent waves, become very large. We denote these by $\lambda\to\pm iP/A$, and call these branches of the wave vector the "wing" bands. The other two wave vectors reduce to the usual two-band result. We denote these by

$$k\to\pm[(E-E_c)(E-E_l)]^{1/2}/P. \tag{2}$$

We call these branches the "middle" bands. They include the conduction and light-hole valence bands, where k is real, and the evanescent states in the gap, for which k is imaginary.

Consider an ideal interface between two semiconductors at the plane $z=z_0$. To match the wave function across the interface, we need to relate the two basis functions on the left to those on the right. Two assumptions are made to establish a

simple relationship. The first is that, in each material, the two basis functions are linearly independent functions of x and y at $z = z_0$. This is true for all tetrahedral crystals because these two functions of x and y do not belong to the same irreducible representation of the two-dimensional space group of the interface. The second assumption is that, for all x and y at $z = z_0$, the corresponding conduction band-edge wave functions from the two materials, and their normal derivatives, are equal, and similarly for the light-hole band-edge wave functions. Examination of the pseudopotential representation of these basis functions justifies this approximation.[12,13]

Express the wave function at energy E in terms of an incident wave from the "middle" bands of the material on the left, and reflected and transmitted waves in the "middle" and "wing" bands. The two reflection and two transmission coefficients are determined by the continuity of the wave function and its normal derivative. In terms of the basis of the two-band model, these continuity conditions yield four boundary-condition equations. In the limit that $A \to 0$ uniformly in both materials, the evanescent waves from the "wing" bands are vanishingly small everywhere except at the interface. So, away from the interface, the total wave function may be written as a linear combination of scattering functions which exclude the waves from the "wing" bands. This can be written as

$$\psi(\vec{r}) = F_c(z)u_c(\vec{r}) + F_l(z)u_l(\vec{r}). \quad (3)$$

F_c and F_l are envelope functions which modulate the Bloch basis functions u_c and u_l. Two of the four boundary-condition equations turn out to be independent of the wing-band components in this limit, and are equivalent to the continuity of $F_c(z)$ and $F_l(z)$ at z_0. (Their z derivatives are not, in general, continuous!) The other two equations, which determine the wing-band components, become irrelevant. Thus the continuity of the two envelope functions replaces the continuity of the total wave function and its derivative as the appropriate boundary condition for heterostructure problems.

Using the new two-component boundary conditions, the eigenvalue equation for the bound states of a sandwich heterostructure can be found:

$$i\frac{\beta_I(k_I)}{\beta_O(k_O)} = \begin{cases} \cot(\frac{1}{2}k_I a) \\ -\tan(\frac{1}{2}k_I a) \end{cases} \quad (4)$$

for symmetric (antisymmetric) conduction-band and antisymmetric (symmetric) light-hole-band envelope functions. k is the wave vector from Eq. (2). Subscripts I and O refer, respectively, to the inside and outside materials of a sandwich of layer width a. The quantity

$$\beta(k) = \sigma(k)\sigma(E - E_l)|(E - E_c)/(E - E_l)|^{1/2} \quad (5)$$

is the ratio of the coefficients of the eigenfunction of Eq. (1) at energy E, and $\sigma(x) \equiv x/|x|$.

Using the material parameters in Table I, we have calculated optical transition energies as a function of sandwich layer thickness for a GaAs-$Al_{0.2}Ga_{0.8}As$ sandwich. The results are shown in Fig. 1, along with the experimental values.[1] Using $\Delta E_c = E_{cO} - E_{cI}$ as an adjustable parameter, we find a good fit for $\Delta E_c = 225$ meV, which is the same value as obtained from the square-well

TABLE I. Material parameters used in calculating optical transition energies.

Material	E_g (eV)	m_c (m_0)	m_h (m_0)
GaAs	1.511[a]	0.067[a]	0.45[a]
$Al_{0.2}Ga_{0.8}As$	1.770[a]	···	0.5524[b]
GaSb	0.810[c]	0.042[c]	0.431[d]
InAs	0.420[c]	0.023[c]	0.396[d]

[a]Ref. 1.

[b]Weighted average of AlAs heavy-hole mass in H. C. Casey, Jr., and M. B. Panish, *Heterostructure Lasers Part B: Materials and Operating Characteristics* (Academic, New York, 1978), p. 12, and GaAs heavy-hole mass in Ref. 1.

[c]Casey and Panish, Ref. b.

[d]From Casey and Panish (Ref. b) with use of $m_h^{3/2} = m_v^{3/2} - m_l^{3/2} = m_v^{3/2} - m_c^{3/2}$.

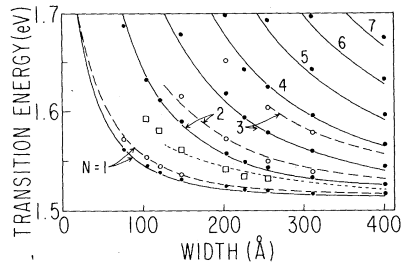

FIG. 1. Optical transition energies vs sandwich layer width for GaAs–$Al_{0.2}Ga_{0.8}As$ sandwich. Data are from Ref. 1. Transitions between the light-hole and conduction bands: open circles, experiment; dashed lines, theory. Transitions between the heavy-hole and conduction bands: solid circles, experiments; solid lines, theory. Weak transitions between the $n = 2$ light-hole state and the $n = 1$ conduction state: squares, experiment; dotted line, theory.

model.[1] The differences between Eq. (4) and the square-well model are masked by the large contribution of the band gap to the transition energy. In terms of energy values measured from the band edges, our results are systematically lower than the square-well model by 5% to 10%. More accurate measurements would be needed to see such discrepancies. Neglecting these differences, our theory provides a theoretical justification for the square-well model in certain type-I cases.

The eigenvalue equation for a superlattice with layers of width a and b is

$$R^2 = (P^2 + DPQ + Q^2)/(1 + DPQ + P^2Q^2), \qquad (6)$$

where $P = i\tan(\frac{1}{2}k_1 a)$, $Q = i\tan(\frac{1}{2}k_2 b)$, $R = i\tan[\frac{1}{2}k(a+b)]$, $D = [\beta_1(k_1)/\beta_2(k_2)] + [\beta_2(k_2)/\beta_1(k_1)]$, and k is the superlattice wave vector.

For homojunctions, if the energy is close to a given band edge in both materials, Eqs. (4) and (6) reduce to the eigenvalue equations derived from the square-well model.[1] Our theory does not reduce to the one-band model,[9] nor to the square-well model,[1] for heterojunctions, where simply matching the envelope function and its derivative is invalid.

Calculations of the optical gap as a function of superlattice layer thickness were performed with the material parameters from Table I for an InAs-GaSb superlattice, a type-II structure. The results are shown in Fig. 2, along with the optical data.[14] We obtain a good fit of the optical data with a value of $E_s = E_{c\,\mathrm{InAs}} - E_{l\,\mathrm{GaSb}} = -175$ meV, which is slightly larger than that given by the linear combination of atomic orbitals (LCAO) theory.[14]

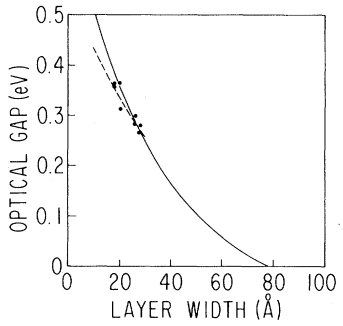

FIG. 2. Optical gap vs layer width for an InAs-GaSb superlattice. The transition is from the highest heavy-hole–like miniband maximum to the lowest conduction-like miniband minimum. Data are from Ref. 14. The solid line is our result. The dashed line is the tight-binding result from Ref. 6.

This superlattice system exhibits a semiconductor-to-semimetal transition at the interfaces for $a = b \approx 80$ Å.[15,16] We interpret this as the point at which the optical gap goes to zero. Our theory is in excellent agreement with the location of this transition, even though its value depends very sensitively on the value of E_s. In contrast, the LCAO result is 115 Å.[8]

We made several simplifications to illustrate our wave-function matching method. The method may be used with a more general bulk band structure, in which limits like $A \to 0$ are not necessary, or in systems with many electrons in the subbands, which cause the addition of a self-consistent potential. Such systems include modulation-doped superlattices,[17] isolated heterojunctions,[18] and the semimetallic interface phase of type-II superlattices.[15,16] For such systems, self-consistent calculations based upon an extension of this work are currently in progress.

This work was supported in part by National Science Foundation Grant No. DMR 80-018440.

[1]R. Dingle, in *Festkörperprobleme: Advances in Solid State Physics*, edited by H.-J. Queisser (Pergamon-Vieweg, Braunschweig, 1975), Vol. XV, p. 21.
[2]G. A. Sai-Halasz, R. Tsu, and L. Esaki, Appl. Phys. Lett. 30, 651 (1977).
[3]E. Caruthers and P. J. Lin-Chung, Phys. Rev. B 17, 2705 (1978).
[4]J. Ihm, P. K. Lam, and M. L. Cohen, Phys. Rev. B 20, 4120 (1980).
[5]W. Andreoni and R. Car, Phys. Rev. B 21, 3334 (1980).
[6]A. Madhukar and R. N. Nucho, Solid State Commun. 32, 331 (1979).
[7]J. N. Schulman and T. C. McGill, Phys. Rev. B 19, 6341 (1979).
[8]G. A. Sai-Halasz, L. Esaki, and W. A. Harrison, Phys. Rev. B 18, 2812 (1978).
[9]D. Mukherji and B. R. Nag, Phys. Rev. B 12, 4338 (1975).
[10]E. O. Kane, in *Physics of III-V Compounds*, Vol. 1 of *Semiconductors and Semimetals*, edited by R. K. Willardson and Albert C. Beer (Academic, New York, 1966), p. 75.
[11]L. J. Sham and M. Nakayama, Phys. Rev. B 20, 734 (1979).
[12]M. L. Cohen and T. K. Bergstresser, Phys. Rev. 141, 789 (1966).
[13]E. Hess, I. Topol, K.-R. Schulze, H. Neumann, and K. Unger, Phys. Status Solidi (b) 55, 187 (1973).
[14]G. A. Sai-Halasz, L. L. Chang, J.-M. Welter, C.-A. Chang, and L. Esaki, Solid State Commun. 27, 935 (1978).
[15]L. L. Chang, N. Kawai, G. A. Sai-Halasz, R. Lu-

deke, and L. Esaki, Appl. Phys. Lett. 35, 939 (1979).
[16]L. L. Chang, N. J. Kawai, E. E. Mendez, C.-A. Chang, and L. Esaki, Appl. Phys. Lett. 38, 30 (1981).
[17]R. Dingle, H. L. Störmer, A. C. Gossard, and W. Wiegmann, Surf. Sci. 98, 90 (1980).
[18]G. Abstreiter, Surf. Sci. 98, 117 (1980).

Anderson Localization in Two Dimensions

Patrick A. Lee and Daniel S. Fisher
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 27 April 1981)

The conductance for a two-dimensional tight-binding model with on-site disorder is calculated numerically with use of the Kubo formula. For weak disorder logarithmic localization is observed, in agreement with the scaling theory. The magnetoresistance is found to be negative in both the logarithmic and exponential localization regimes. Results for a model with random complex hopping matrix elements are also presented.

PACS numbers: 72.10.Bg, 71.55.Jv

In the last two years, significant advances have been made in understanding the scaling behavior of Anderson localization.[1,2] Much of the work has been based on the idea[3] that the behavior as a function of length scale L is determined by a single scaling variable, the dimensionless conductance at scale L, $g(L)=\Gamma(L)/(e^2/\hbar)$, where $\Gamma(L)$ is the conductance of a system with linear dimension L. The renormalization-group differential recursion relation which describes the changes in g as a function of length scale can be written as $d\ln g/d\ln L=\beta(g)$. The β function has been computed in two dimensions by perturbation theory in powers of g^{-1} for weak disorder. For spinless electrons it is found[4] that $\beta(g)=-(2\pi^2 g)^{-1}+O(g^{-4})$ where the absence of the zeroth-order term is unique to two dimensions (2D) and suggests that two is the lower critical dimensionality for the Anderson transition. In 2D, localization is predicted for any amount of disorder, since g always decreases as a function of L corresponding to insulating behavior. For weak disorder, however, the effects of localization will only decrease $g(L)$ logarithmically.

Numerical tests of these ideas have so far been based on rather small sample sizes and are not conclusive.[5-7] In particular, an approximate numerical study of the scaling behavior by one of us[8] failed to show the expected logarithmic localization in 2D. More recently several other approximate numerical calculations have come out in support of the one-parameter scaling theory.[9,10] The present work is aimed at helping to resolve the controversy.

We consider a tight-binding Anderson model on a 2D square lattice,

$$H=\sum_{j,k} V_x{}^{jk} a_{j+1,k}{}^{\dagger} a_{j,k} + V_y{}^{jk} a_{j,k+1}{}^{\dagger} a_{j,k} + \text{c.c.} + \sum_{j,k} E_{j,k} a_{j,k}{}^{\dagger} a_{j,k}, \tag{1}$$

where j and k label the sites in the x and y directions and E_{jk} is a random site energy distributed uniformly between $\pm W/2$. We initially take $V_x=V_y=1$. The parameter W thus provides a measure of the disorder. The frequency-dependent conductance of an $L\times L$ sample is given by the Kubo formula

$$\Gamma(\omega)=(\pi/\omega L^2)\int dE' \sum_{\alpha,\beta} |\sum_j \langle\alpha|J(j)|\beta\rangle|^2 \delta(E'+\omega-E_\beta)\delta(E'-E_\alpha), \tag{2}$$

where the current operator is $J(j)=ie\sum_k V_x{}^{jk}(a_{j,k}{}^{\dagger}a_{j-1,k}-\text{c.c.})$ and $|\alpha\rangle, |\beta\rangle$ are the eigenstates of the system with $E_\alpha<E<E_\beta$, where E is the Fermi energy. For an isolated sample the eigenvalues are discrete and $\Gamma(\omega)$ consists of a series of δ functions so that some procedure for averaging over ω must be introduced.[7,11] Furthermore the numerical computation of the current matrix elements is time consuming. We thus take a somewhat different approach by extending the disordered sample to infinity in the $\pm x$ directions by affixing an ordered tight-binding lattice on each side. We take periodic boundary conditions in the y direction for all x, and apply an electric field in the x direction *only* in the disordered region. The energy spectrum will now be continuous and the $\omega\to 0$ limit of the conduc-

