Binding energies of hydrogenic impurities in parabolic quantum wells

Richard P. Leavitt

Martin Marietta Laboratories, 1450 South Rolling Road, Baltimore, Maryland 21227

(Received 15 June 1987)

We have calculated binding energies of simple, hydrogenic-type impurities in parabolic quantum wells as functions of the displacement of the impurity from the well center and the strength of the well potential. The calculation method is based on an expansion of the impurity wave function in a series of hydrogenic-type functions. Our results for the impurity at the well center are in excellent agreement with those obtained by a different method elsewhere.

Parabolic quantum wells can now be grown by molecular-beam epitaxy in two different types of structures: doping (or n-i-p-i) superlattices,[1] in which the potential variation arises from depletion of doped layers, and compositionally modulated GaAs/(Al,Ga)As quantum-well structures, in which the potential variation arises from systematic changes in the alloy composition. The latter type of well can be approximated by growing alternating thin layers of GaAs and $Al_xGa_{1-x}As$ (of fixed composition) with varying layer thicknesses.[2] Structures of both types are of interest both because of the potential for practical application in electro-optic and nonlinear optical devices and because of the amount of fundamental information that can be obtained from their study. Particularly in the case of doping superlattices, in which the donors and acceptors themselves determine the spatial dependence of the band structure,[3] the theoretical and experimental study of the electronic properties of shallow impurities in parabolic wells is essential for understanding the behavior of these systems.

In this Brief Report we present results of calculations of the binding energies of hydrogenic-type impurities in parabolic quantum wells. In contrast to previous calculations of this type,[4] we consider in this work the dependence of the binding energy on the position of the impurity relative to the center of the well. This refinement is made possible by our using a multiterm expansion of the impurity wave function in a series of hydrogenic-type functions of appropriate behavior about the symmetry axis. In particular, we consider the ground state of the impurity associated with the lowest electron or hole subband in the system.

Consider the following form for the Hamiltonian that describes hydrogenic impurities in the parabolic-well system:

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\epsilon|\mathbf{r}-\mathbf{r}_0|} + \tfrac{1}{2}m^*\omega^2 z^2 , \quad (1)$$

where m^* is the effective mass of the electron or hole, ϵ is the dielectric constant of the material, $\mathbf{r}_0$ is the position of the impurity, and ω is the angular frequency associated with the harmonic potential. The presence of the parabolic potential term in Eq. (1) reduces the sym-

metry of the impurity Hamiltonian from spherical to cylindrical, with the z axis as the axis of symmetry. We consider a variational solution to the Schrödinger equation, $H\Psi = E\Psi$ [with H given by Eq. (1)], of the form

$$\Psi_{mp} = \sum_{n=l+1}^{\infty}\sum_{l=m}^{n-1} c_{nl}^{mp}\psi_{nlm}[(\mathbf{r}-\mathbf{r}_0)/a] , \quad (2)$$

where ψ_{nlm} are the usual hydrogenic wave functions, n is the principal quantum number, l is the angular momentum quantum number, m is the azimuthal (magnetic) quantum number, p is an integer that distinguishes eigenstates of Eq. (1) having the same m, and a is an effective Bohr radius (treated as a variational parameter). Note that, as a consequence of the cylindrical symmetry of Eq. (1), m is a good quantum number in the presence of the parabolic well, whereas n and l are not.

Calculations of the energy of the lowest state having a given m based on Eq. (2) are performed in the following manner. The complete set of states $[nl]$ in the summation in Eq. (2) (for a given m) is truncated to the finite set having $n \le n_{max}$. Then the coefficients c_{nl}^{mp} are found, for a given a, that diagonalize the Hamiltonian, Eq. (1). Finally, the parameter a in Eq. (2) is varied until the lowest eigenvalue of Eq. (1) reaches a minimum. To en-
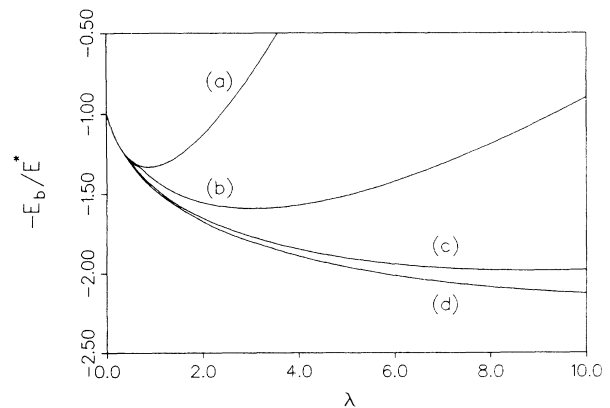

FIG. 1. Impurity binding energy as a function of the strength parameter λ for various values of n_{max}: (a) $n_{max}=1$, (b) $n_{max}=4$, (c) $n_{max}=7$, and (d) $n_{max}=10$. The impurity is at the center of the parabolic well ($u_0=0$).
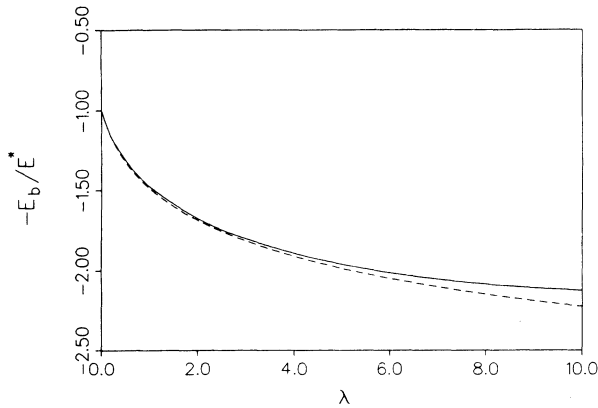
7650

FIG. 2. Comparison of hydrogenic-function approach and variational approach to calculating the impurity binding energies for a parabolic well. Solid curve: hydrogenic functions, Eq. (2); dashed curve: two-parameter variational function, Eq. (3). The impurity is at the center of the well ($u_0 = 0$).
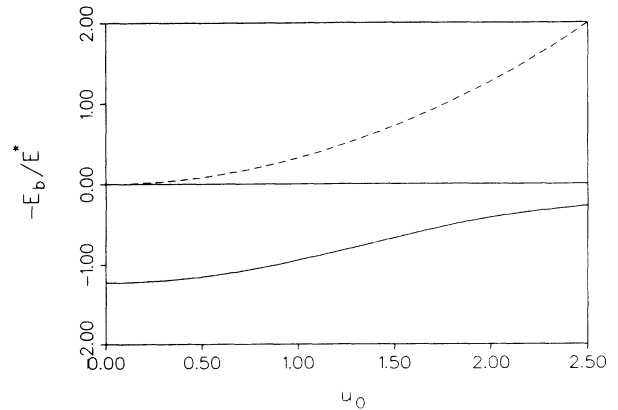

FIG. 3. Calculated binding energy for an impurity in a parabolic well as a function of the positional parameter u_0. Also shown is the harmonic potential (dashed curve). The strength parameter λ is equal to 0.32.

sure accuracy in calculating the eigenvalues, the size of the basis [given by $n_{max}(n_{max}+1)/2$] is increased until there is little change in the lowest eigenvalue of Eq. (1).

We introduce the zero-point vibrational amplitude of the parabolic well, $\alpha = (\hbar/m^*\omega)^{1/2}$; the zero-point energy of the well, $E_0 = \hbar\omega/2$; and the impurity binding energy in the absence of the well, $E^* = m^*e^4/2\epsilon^2\hbar^2$. In terms of these quantities, there are two appropriate dimensionless parameters: $\lambda = E_0/E^*$, which is a measure of the relative strengths of the well and impurity potentials, and $u_0 = \hat{z}\cdot r_0/\alpha$, which measures the displacement of the impurity from the well center in units of the zero-point vibrational amplitude. Our results are presented in terms of these parameters. Also, the impurity binding energy is defined as the difference between the zero-point energy and the lowest eigenvalue of Eq. (1), i.e., $E_b = E_0 - E$ (which is always a positive quantity).

In Fig. 1 we show the dependence of the impurity binding energy on the strength parameter λ for the case where the impurity is at the well center. In the figure we have plotted results for values of $n_{max} = 1$, 4, 7, and 10. As expected, for increasing λ, more terms must be added to the sum in Eq. (2) to achieve convergence. For all values of n_{max} greater than one, there is a discontinuity in the slope of the E_b-vs-λ curve. (In Fig. 1 the discontinuity is most apparent for $n_{max} = 4$.) The magnitude of this discontinuity decreases, and its location progresses toward lower values of λ, as n_{max} increases. The reason for the discontinuity is that there exist two minima in the $E(a)$ curve; one occurs close to the effective Bohr radius in the absence of the well, $a^* = \epsilon\hbar^2/me^2$, and the other occurs at a much smaller value of a. For sufficiently small λ or a sufficiently small number of terms in the series in Eq. (2), the first minimum is the global minimum. As λ or n_{max} increases, the second minimum becomes the global

minimum. The discontinuity in slope occurs where the two minima correspond to the same energy.

In Fig. 2 we compare our results (computed with $n_{max} = 10$) for the on-center impurity with results obtained previously[4] using a two-parameter variational function of the form

$$\Psi_{var} = C \exp(-\beta z^2 - |r - r_0|/a) , \qquad (3)$$

where β and a are treated as variational parameters. It can be seen from the figure that the superposition of hydrogenic functions gives a reasonably accurate representation of the binding energy for a wide range in λ.

In Fig. 3 we show results for the binding energy as a function of the positional parameter u_0 for $\lambda = 0.32$, where we have chosen $n_{max} = 4$ (which should be reasonably accurate for this value of λ). For comparison we also show the well potential on the same plot. For $u_0 < 1$, the binding energy follows the potential curve quite well. As u_0 increases much beyond 1, the binding energy approaches zero proportionately to u_0^{-1}.

We have illustrated a technique by which the binding energies for impurities in parabolic wells can be calculated for an arbitrary position of the impurity relative to the center of the well. Results for the impurity at the well center agree well with those obtained elsewhere by a two-parameter variational approximation.[4] Obvious extensions of the technique are to include the anisotropy of the kinetic energy term[5] for holes and coupling of heavy- and light-hole bands.[6]

[1] G. H. Dohler, H. Kunzel, D. Olego, K. Ploog, P. Ruden, H. J. Stolz, and G. Abstreiter, Phys. Rev. Lett. **47**, 864 (1981).

[2] R. C. Miller, A. C. Gossard, D. A. Kleinman, and O. Munteau, Phys. Rev. B **29**, 3740 (1984).

[3] P. Ruden and G. H. Dohler, Phys. Rev. B **27**, 3538 (1983).

[4] G. A. Luna-Acosta, Solid State Commun. **55**, 5 (1985).

[5] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).

[6] G. D. Sanders and Y.-C. Chang, Phys. Rev. B **32**, 5517 (1985).