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Electronic States Associated with Extended Defects in Quantum Well Structures*

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A simple model for the calculation of bound states associated with extended defects in quantum well structures is developed. We consider a particle confined between two plane parallel potential walls and determine the conditions for existence of bound states for two types of defects: infinite "trench-like" and cylindrical. We show that in a Ga(Al, As) - GaAs - Ga(Al,As) quantum well structure defects capable of producing appreciably bound states must have lateral dimensions of the order of 0,1 μm.

Desenvolvemos um modelo simples para o cálculo dos estados ligados associados a defeitos extensos em uma estrutura de poço de potencial quântico. Estudamos o caso de uma partícula confinada entre duas paredes paralelas de potencial infinito, sendo que uma delas contém um defeito, seja sob a forma de uma trincheira, seja sob a forma de um cilindro. Mostramos que para produzir um estado fortemente ligado, os defei-

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tos no sistema Ga(Al,As) - GaAs - Ga(Al,As) devem ter dimensões laterais da ordem de 0,1 ym.

1. INTRODUCTION

Low dimensional physical systems have attracted considerable attention from both experimentalists and theorists in the past few years. One of the most interesting such systems are electrons confined to thin layers. Modern growth techniques, in particular molecular beam epitaxy, allow for the "engineering" of semiconductor heterostructures formed by layers, the thicknesses of which may be as small as a few atomic planes. The GaAs-(Ga,Al)As heterostructure is a well studied example of these materials, in which regular bandgap variations (forming the so-called superlattices) lead to the confinement of electron and holes to well defined regions in space[1-3]. Another well studied example of a superlattice is In As-GaSb.[4]

Recent photoluminescence experiments performed on InAs-GaSb[5] and GaAs-(Ga,Al)As[6] have shown that defects in the interface of the heterostructures may be detected. Such defects are produced when, after the growth of any particular layer is concluded the surface is not perfectly smooth but presents protuberances and reentrances which affect the thickness of the next layer when it is grown.

The aim of the present work is to investigate in a simple model the electronic structure associated with defects of the type described above. For simplicity sake we limit ourselves to a single quantum well with infinitely high walls. As discussed later on, such a model is good for eiectrons confined to GaAs wells of not too small width ($L > 80$Å), such as are actually produced[3,6].

In Section 2, we describe our model and write down the basic equations. In Section 3, we present and discuss some numerical results with emphasis on their relevance to the interpretation of photoluminescence data. Finally, in Section 4 we presrnt some brief conclusions.

2. THE MODEL

We adopt the semiclassical approach in which the different energy gaps in the different heterostructure components produce potential barriers for the electron and hole's. This extremely simplified picture, which neglects the details of the crystalline potentials, has been applied with remarkable successes in the interpretation of the single and multiple quantum well structures of GaAs-(Ga,Al)As[2,3]. We also neglect charge transfer effects which may alter the energy gap variation profile and all many body effects such as exchange, correlation and exciton formation. Within these approximations, the single perfect quantum well problem reduces to that of a particle confined between two plane potential barriers. We limit ourselves to the infinite potential barrier limit. This is done in order to simplify the computations and because we are mainly interested in states which lie reasonably far from the top of the actual potential well. We are hence limited to treat electrons confined to not too narrow GaAs layers ($L > 80$Å) in GaAs-(Ga,Al)As heterostructures.

The solution to the infinite potential barrier, perfect single quantum well problem is well-known. The energy levels for a particle with quantum numbers n and $k_{||}$, where n denotes the eigenstates of a one-dimensional infinitely deep well and $k_{||}$, the wavevector parallel to the well walls, are:

$$E_n(\vec{k}_{||}) = \frac{\hbar^2\pi^2}{2m}\frac{n^2}{L^2} + \frac{\hbar^2 k_{||}^2}{2m_{||}} . \qquad (2.1)$$

In eqn. (2.1), m and $m_{||}$ denote, respectively, the effective masses of the particle in the directions perpendicular and parallel to the well walls. The length L measures the width of the well.

We consider two types of defects, which are shown schematically in Fig. 1. The first, Fig. 1 (a), is semi-infinite, trench-like, defect of width a and depth $L' \geqslant L$. The second, Fig. 1(b), is a circular cylinder of radius a and depth $L' \geqslant L$.

The method of solution is similar in both cases and we discuss it first for the trench-like defect. The well is divided into three re-

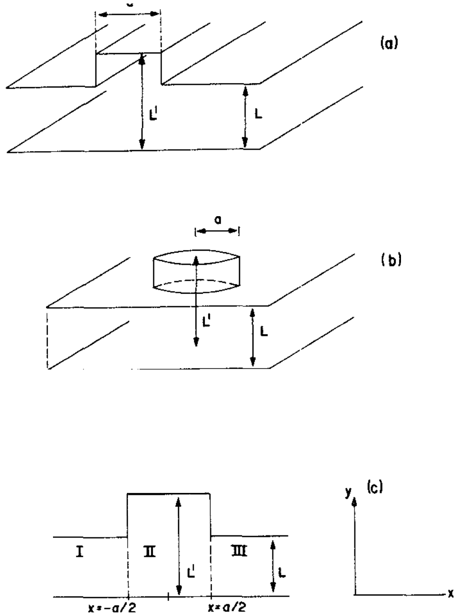

Fig.1 - (a) Perspective view of the confining potential barriers for a trench like defect. The potential is zero between the plates and infinite outside them. (b) Same for a finite size cylindrical defect. (c) Cross -section of potential barrier shown in (a).

gions, as indicated in Fig. 1(c). In each region, a solution of energy E to Schrödinger's equation is written:

$$\begin{aligned} \psi_{I}(x,y) &= \sum_n \left(A_n e^{ik_n x} + B_n e^{-ik_n x}\right) \sin \frac{n\pi y}{L} \\ \psi_{II}(x,y) &= \sum_s \left(C_s e^{iq_s x} + D_s e^{-iq_s x}\right) \sin \frac{s\pi y}{L'} \qquad (2.2) \\ \psi_{III}(x,y) &= \sum_n \left(E_n e^{ik_n x} + F_n e^{-ik_n x}\right) \sin \frac{n\pi y}{L} \end{aligned}$$

In eqns. (2.2):

$$\begin{aligned} k_n &= \sqrt{\frac{2mE}{\hbar^2} - \left(\frac{n\pi}{L}\right)^2} \\ q_s &= \sqrt{\frac{2mE}{\hbar^2} - \left(\frac{s\pi}{L'}\right)^2} \end{aligned} \qquad (2.3)$$

These solutions automatically satisfy the condition of vanishing on all horizontal plane surfaces of the well walls, as shown in Fig. 1 (a). The boundary condition that $\psi_{II}(x,y)$ should vanish on the lateral walls of the trench is not satisfied. This condition is fulfilled by appropriately matching the solutions in the various regions.

To relate the various coefficients appearing in (2.2) we apply the continuity conditions of ψ and its derivative across the planes $x = -\frac{a}{2}$ and $x = \frac{a}{2}$. These are written:

$$\psi_{II}(-\tfrac{a}{2},y) = \begin{cases} \psi_I(-\tfrac{a}{2},y) & 0 < y < L \\ 0 & \text{otherwise} \end{cases} \tag{2.4}$$

and similarly for the derivative and at $x = a/2$.

From (2.4) we obtain:

$$C_s\, e^{-iq_s a/2} + D_s\, e^{iq_s a/2} = \sum_n \alpha(s,n)\, (A_n\, e^{-ik_n a/2} + B_n\, e^{ik_n a/2}) \; . \tag{2.5}$$

In (2.5), we have:

$$\alpha(s,n) = \frac{2}{L'} \int_0^L dy\, \sin\frac{s\pi y}{L'} \sin\frac{n\pi y}{L} = \frac{2(-1)^n nLL'}{\pi}\; \frac{\sin s\pi L/L'}{s^2L^2-n^2L'^2} \; . \tag{2.6}$$

Similar equations can be easily obtained from the other matching conditions. We remark, in passing, that the difficulty in solving such an elementary quantum mechanics problem stems from the fact that the eigenfunctions are not separable in the presence of defects such as those shown in Fig. 1.

The question we want to answer is whether the defect under consideration can produce a bound state and, if so, under what conditions. The lowest energy level for the perfect well of width L is:

$$E_0 = \frac{\hbar^2\pi^2}{2mL^2} . \qquad (2.7)$$

This we take as our energy unit. On the other hand, the lowest energy level for the perfect well of width L' ($\underline{a} \to \infty$) is:

$$E_0' = \left(\frac{L}{L'}\right)^2 E_0 . \qquad (2.8)$$

Hence, any bound state localized at a defect of finite size and depth L' must have an energy $E_b = \xi E_0$ such that:

$$\left(\frac{L}{L'}\right)^2 \leqslant \xi \leqslant 1 . \qquad (2.9)$$

If such a bound state exists, eqns. (2.2) have a solution with $A_n = F_n = 0$, since for k_n purely imaginary we must have decaying solutions away from the defect for $|x| \to \infty$. Notice that k_n is a pure imaginary, for any n, if we are looking at states with energy $E_b \leqslant E_0$. Since the lowest bound state corresponds to a as smooth as possible wavefunction (no nodes), we set: $C_s = D_s$, $B_n = E_n$. With these conditions, the matching equations reduce to:

$$\begin{aligned} 2C_s\, e^{-iq_s a/2} &= \sum_n \alpha(s,n) \left(1 - \frac{iK_n}{q_s}\right) e^{-K_n a/2} B_n \\ 2C_s\, e^{iq_s a/2} &= \sum_n \alpha(s,n) \left(1 + \frac{iK_n}{q_s}\right) e^{-K_n a/2} B_n , \end{aligned} \qquad (2.10)$$

where $k_n = iK_n$ is real. These may be rewritten:

$$\sum_n \alpha(s,n) \left[\tan q_s a/2 - \frac{K_n}{q_s}\right] e^{-K_n a/2} B_n = 0 . \qquad (2.11)$$

For these equations to have a nontrivial solution the determinant of the coefficients must vanish. The energies $E_b = \xi E_0$ at which this occurs are the energies of the searched for bound states. Numerical results are discussed in the next Section.

For the finite defect shown in Fig. 1(b), we exploit cylindrical symmetry in order to write down solutions to Schrödinger's equations appropriate for the region of the defect and for the rest of the system. As before, we limit our search to highly symmetric states. In the present case these are cylindrically symmetric, i.e., are independent of the angular coordinate. Then, inside the cylinder, a solution with energy E is written:

$$\psi_I(\rho,y) = \sum_s A_s\, J_0(q_s\rho)\, \sin\frac{s\pi y}{L'}$$

and outside:

$$\psi_{II}(\rho,y) = \sum_n \left[B_n\, J_0(k_n\rho) + C_n\, N_0(k_n\rho)\right]\sin\frac{n\pi y}{L} \quad . \qquad (2.12)$$

In Eqns. (2.12), ρ is the radial coordinate, q_s and k_n are defined as in eqns. (2.3), J_0 and N_0 are respectively, Bessel and Neumann functions[7]. The functions above vanish everywhere on the walls of the well, except on the lateral walls of the cylindrical defect.

Applying matching condition and recalling that we are looking only for bound states, we arrive straightforwardly at the equivalent of eqn. (2.11):

$$\sum_n \alpha(s,n) \left[\frac{H_0^{(1)}(k_n a)}{J_0(q_s a)} - \frac{k_n H_0^{(1)\prime}(k_n a)}{q_s J_0'(q_s a)}\right] B_n = 0. \qquad (2.13)$$

where $H_0^{(1)}$ are Hankel functions and the prime denotes derivative with respect to the argument. Bound states correspond to zero of the determinant of the coefficients of the set of homogeneous linear equations (2.13). We now discuss the numerical solutions to (2.11) and (2.13).

3. RESULTS

We present initially results for the trench-like defect. When solving for the zero the determinant of (2.11), we must take only a finite number of terms corresponding to cutting off the expansion in (2.2) at some $n = N$. From (2.4) we can see that the problem is basically that of Fourier (sine) expanding a function which is zero in a finite interval - $\psi_{II}(\pm a/2, y) = 0$ for $L \leq y \leq L'$ -. The deeper the defect becomes, the larger N has to be in order to satisfy this boundary condition to a good approximation. Hence, the poorer becomes our approximation of an infinite barrier potential, because higher n's corresponds to higher excited states of the one-dimensional well. The defects which are expected to occur in good quality molecular beam epitaxy samples being reasonably shallow, we do not think that this is a serious limitation.

In Figure 2 we present a study of the convergence property of the zero of the determinant of (2.11) for a reasonably deep defect, which has $L' = 1.314L$ and $a = L$. As we see, the error made in the value of ξ by taking $N = 1$, compared with $N = 15$, is 3%. By taking $N = 4$, the error reduces to 2%. Although the convergence, mathematically speaking, is quite slow, from the physical point of view, the error made in cutting off at a small value of N is not severe. Most of the results discussed below were obtained by taking $N = 4$, i.e., solving for the determinant of a 4×4 matrix of coefficients.

In Fig. 3 we present results for ξ as a function of the trench width for two different values of L'/L. For $L' = 1.105L$, up to $a = 3L$ we find a single bound state (of s symmetry). For $a = 2.5L$ we are within 2% of the asymptotic value of $\xi = 0.819$. A bound state exists for any

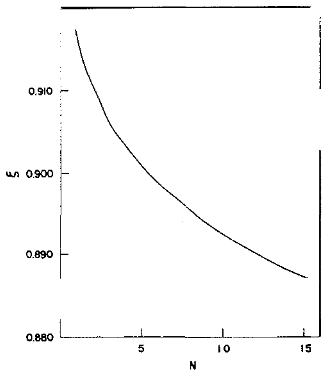

Fig.2 - Convergence of bound state energy ξ as a function of the dimension N of the determinant of the matrix of coefficients of eqn. (2.11), for $L' = 1.314L$ and $a = L$. The calculation is done for a trench-like defect

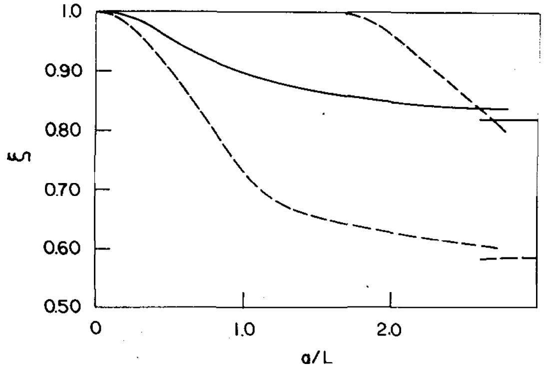

Fig.3 - Bound states energies for the trench-like defect for L' = 1.105L (dashed line) and L' = 1.314L (solid line) as a function of a/L. The continuum of states is situated above the line ξ = 1.0. The asymptotic values for ξ as $a\to\infty$ are indicated by the horizontal traces at the right hand side of the Figure.

value of a, which is a characteristic feature of a two-dimensional problem - the infinite trench reduces the problem to an effective two dimensional one. For L' = 1.314L, a second bound state splits off at about a = 1.75L. We notice that, by a = 2L, the first bound state has already practically reached the asymptotic value.

In Fig. 4 we present a similar result, but for the cylindrical defect, for L' = 1.1L and L' = 1.2L. The only important qualitative difference from the previous results is that a bound state now splits off only for a minimum radius of the defect. We are then in a "three-dimen-

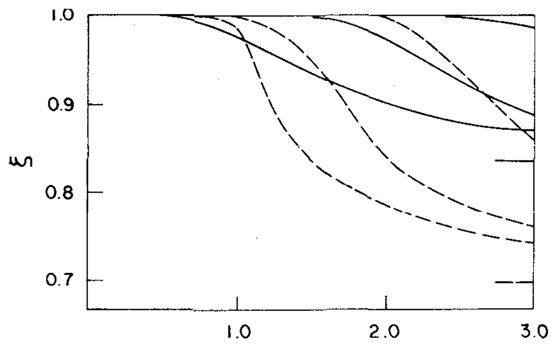

Fig.4 - Same as Fig. 3 for the cylindrical defect. with L' = 1.1L (solid line) and L' = 1.2L (dashed line).

sional" regime. There are now more bound states shown because we consider larger radii. However, as expected, the approach to the asymptotic value is slower than for the semi-infinite trench-like defect. For $a \simeq 10L$, the lowest bound state is within 4% of the limiting value.

In Fig. 5, we present results foi the bound state energy as a function of the well depth at two fixed radii. Again, the fact that a minimum size defect' is needed before a state splits off can be clearly seen.

In Fig. 6 we present a plot showing for which regions of the parameters L'/L and a/L, which characterize the dimensions of the defect we have s-symmetry bound states. In this Figure, we indicate the total number of such bound states. For $L' = 1.1L$, no bound states appear for $a < 0.8\pi L$; only one bound state exists for $0.8\pi L < a < 1.7\pi L$; etc.

Its is interesting now to consider these numbers for a typical GaAs quantum well of width $L = 100$Å. Sincs the electron potential well depth is 200 MeV and the electronic mass $m = 0.0665 m_0$, the ground state of the well $E_1 \cong 56$ MeV is low enough for the infinite well depth approximation to be reasonable. For a defect 10Å deep, the first bound state appears for $a \sim 500$Å diameter, which is a rather large defect. For its binding energy to become appreciable $a \sim 1000$Å, and we are already in the tenths of a micron size region. We emphasize that taking a more realis-

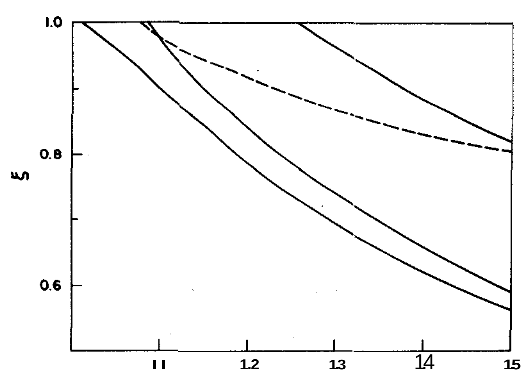

Fig.5 - Bound state energies for the cylindrical defect for $a = \pi L$ (dashed line) and $a = 2\pi L$ (solid line) as a function of L'/L. The continuum of states is situated above the line $\xi = 1.0$

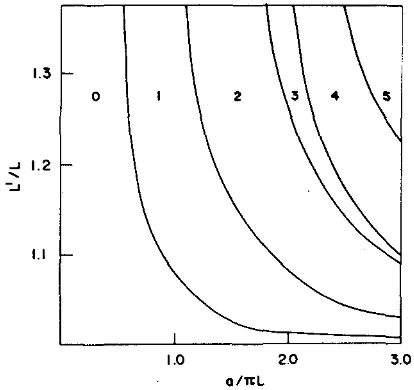

Fig.6 - Number of bound states as a function of the length parameters L'/L and $a/\pi L$ which characterize, respectively, depth and radius of a cylindrical defect. The integers indicate the number of s-symmetry bound states which exist within each parameter region.

tic potential well barrier will only lead to less localized states, and to bigger minimum size defects which can produce such states.

On the other hand, inclusion of the neglected electron-electron interaction, which leads to formation of exciton states contributes to localization of the electronic states. Such effects require a more sophisticate treatment of the problem than the one we presented here, but should not alter significantly the size estimated above.

4. CONCLUSION

In conclusion, we have presented a simple model for the electronic structure of single quanturn well with defects. In particular, we have determined the conditions for the appearance of localized states associated with two different types of defects: semi-infinite, trench-like, defects and finite size cylindrical defects. This choice of geornetry was dictated by the computational difficulty of solving a non-separable Schrödinger equation. In addition, we consider only the limiting caseof an infinite potential barrier, which yields the less stringentconditions for the existence of bound states.

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