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Bound quantum states in crossed-wire systems

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Abstract. I have calculated the ground-state energy of an electron which is trapped at the intersection of a cross formed by two quantum wires. The widths of the wires forming the cross are assumed to vary independently. When the widths are equal, a bound state with energy below the energy continuum exists. The energy corresponds to the value obtained by Schult *et al*. When the ratio of the two widths is varied, the energy changes. The variation in the energy with the ratio of the widths is obtained and is shown graphically. It is observed that the energy decreases as one of the widths is allowed to increase. Numerical calculation indicates that the binding energy approaches zero asymptotically and the bound electronic state merges with the energy continuum. I have also calculated the energy of an electron trapped by a double cross. There are two bound states of the electron corresponding to symmetric and antisymmetric configurations. The energy of these states is calculated numerically. The possibility that the electron oscillates between the centres of the double cross is discussed and the frequency of oscillations is estimated.

1. Introduction

With advances in fine-line lithography, it is possible to construct and study quantum effects in semiconductors which simulate the properties of wires with extremely small widths. In these structures, the state of the electron in the direction perpendicular to the length of the wire is quantized with sufficiently large separations in energy levels and the motion of the electron parallel to the length is that of a quasi-free electron. The present-day technology is capable of producing wires with widths as small as 50 nm. Calculation of energy states of the electron in systems formed by the quantum wires has received much attention in literature [1–5] in view of their technological applications. When a cross formed by two quantum wires intersecting at right angles is constructed, the energy levels of the electron form an energy continuum with the minimum energy corresponding to the lowest energy of the quantized level in the transverse direction, but in addition to the energy continuum a bound state of the electron also exists near the intersection of the two wires. The bound-state wavefunction of the electron is large near the intersection and decreases away from it. The difference between the energy of this localized state and the energy continuum is the binding energy of the state. The binding energy of this state has been obtained recently by Schult *et al* [5], assuming that the widths of the wires forming the cross are equal. In this paper we consider that the widths are not necessarily equal and that they can be varied independently. The evaluation of energy in such situations is relevant since the differences between the two widths are likely to be more frequent in experimental situations than in situations when they are equal. We have also

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considered for the first time the possibility of a bound state trapped by a double cross in which a quantum wire is intersected at right angles by two other quantum wires. In this case the electron state can be described by wavefunctions which are symmetric and antisymmetric with respect to the two cross centres. The energies of these two states are close to each other but not equal unless the separation is approaching infinity. Combinations of the symmetric and antisymmetric wavefunctions can be formed by taking the sum of and the difference between them, giving rise to two non-stationary states which have the property that in these states the electron is localized near one centre or the other and is expected to oscillate between the two centres. We have calculated the energies of the symmetric and antisymmetric states as a function of the separation between the two crosses. The frequency of the electron oscillating between the centres is estimated.

2. Procedure

A numerical procedure useful for the evaluation of the energy of the electron in quantum wire systems has recently been proposed by Press *et al* [6]. Although other methods exist, the method given by these workers is particularly simple and as a numerical procedure very interesting. The elements of this method which were described earlier by Schult *et al* [5] are given in the following.

In the time-dependent Schrödinger equation, if we replace the time variable t by a pseudo-time τ such that $\tau = it$, then the equation takes the form

$$(\partial/\partial\tau)\Psi(X, Y, \tau) = (\partial/\partial X^2 + \partial/\partial Y^2)\Psi(X, Y, \tau) \tag{1}$$

where $X = 2mx^2/\hbar$ and $Y = 2my^2/\hbar$. If the eigenvalues and the eigenfunctions of the Laplacian are given by $-k_n^2$ and u_n, respectively, then any arbitrary wavefunction $\Psi(X, Y, \tau)$ can be expressed by

$$\Psi(X, Y, \tau) = \Sigma a_n u_n(X, Y) \exp(-k_n^2\tau) \tag{2}$$

where k_n^2 is positive and a_n is the expansion coefficient. As τ increases, the exponential terms decrease but the term containing k_0 corresponding to the ground-state energy would be the slowest to decrease provided that a_0 is not zero. Thus, for sufficiently large τ, $\Psi(X, Y, \tau)$ would approach the unnormalized ground-state wavefunction. Thus the procedure allows us to filter out the ground-state wavefunction from any arbitrary wavefunction so long as it is not orthogonal to the ground state. The ground-state energy can be obtained using the time-independent Schrödinger equation.

I apply the procedure for obtaining the ground-state wavefunction and its energy. For the cross geometry, I assume that the potential inside the quantum wires is zero and infinite outside. The electron is thus constrained to the insides of the wires. The cross wires are divided into a mesh of uniformly distributed points and an arbitrary wavefunction is defined over these points. If a bound state is expected, then it is natural to choose the arbitrary wavefunction such that it is large near the centre and is decreasing away from it. The evolution of the wavefunction in pseudo-time τ is obtained numerically by discretizing the pseudo-time over small intervals and using equation (1). The same procedure is also employed to obtain the energy of the electron attached to a double cross. The results of the numerical calculations are described in the following section.

3. Results

3.1. Bound state in a cross geometry

First we consider a cross formed by two quantum wires. The width of one wire is W and of the other W'. I assume that W' is a variable and is equal to or greater than W so that the ratio W'/W is unity or greater than unity. The energy is evaluated using the method of Press *et al* [6]. The ground-state energy E is expressed in units of $E_{\text{std}} = \hbar^2\pi^2/2mW^2$. When W'/W is unity, the bound-state energy of the electron is given by $E/E_{\text{std}} = 0.688$, a value which is in reasonable agreement with the result of Shultz *et al* [5]. When W'/W is allowed to vary, E/E_{std} decreases and is shown graphically in figure 1. Also shown in the figure is the edge of the energy continuum. The bound-state energy is defined as the difference between the energy E and the energy continuum. It is observed that the binding energy of the electron decreases from its value when W'/W is unity as the ratio of the widths W'/W is increased. For W'/W equal to about 1.75, E/E_{std} approaches the energy continuum. For values of W'/W greater than 1.75 the difference between E/E_{std} and the energy continuum is finite but is so small that it cannot be distinguished on the energy scale used in the figure. As expected, for values of W'/W greater than about 1.75 the spread of the wavefunction in the broader channel away from the centre of the cross is significant. Numerical evaluation in these situations is increasingly lengthy but, by repeated checking of the results, I conclude that the energy of the electron does merge asymptotically with the energy continuum and that the binding energy of the electron approaches zero as the ratio of the widths are increased. The spread of the wavefunction in the narrower channel away from the centre decreases as the ratio of the widths is increased.

3.2. Bound states in a double cross

I assume that the widths of all the wires forming the double cross are the same and this width is denoted by W. The distance separating the two centres of the double cross is given by W'. The ratio W'/W is therefore greater than unity. In this geometry, two energy states are possible and they are obtained by choosing the trial wavefunction which is symmetric and antisymmetric with respect to the centres of the crosses. When the pseudo-time τ is allowed to increase, the electronic energies approach the minimum energies appropriate to their symmetries. We express these energies in units of E_{std} as a function of the ratio W'/W.

I denote the symmetric state by Ψ_s and the antisymmetric state by Ψ_a and their energies by E_s and E_a, respectively. Two non-stationary states Ψ_L and Ψ_R are obtained by combining Ψ_s and Ψ_a according to

$$\Psi_L = (\tfrac{1}{2})^{1/2}(\Psi_s + \Psi_a) \tag{3}$$

and

$$\Psi_R = (\tfrac{1}{2})^{1/2}(\Psi_s - \Psi_a). \tag{4}$$

Here Ψ_L is centred around the left-hand side and Ψ_R is centred around the right-hand

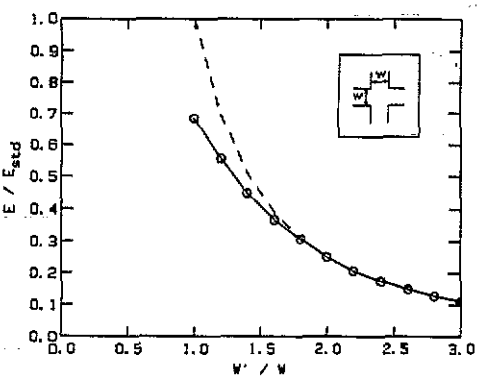

Figure 1. The continuous curve gives the variation in the energy of the electron in units of E_{std} as a function of the ratio of the widths W'/W, for the cross geometry: ---, variation in the edge of the energy continuum.

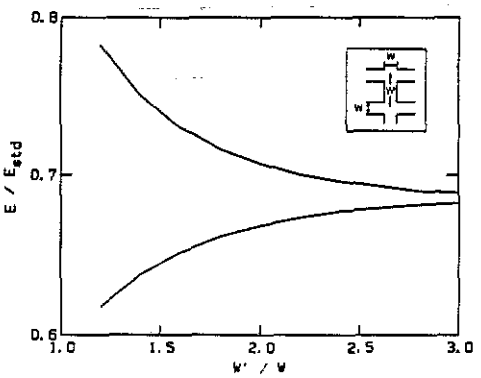

Figure 2. The upper curve shows the energy of the electron in the antisymmetric state and the lower curve gives the variation in the energy in the symmetric state in units of E_{std} as a function of the separation between the centres of the crosses in the double-cross geometry.

side of the double cross. If the electron is centred on the left-hand side of the double cross at time $t = 0$, then the time variation of the wavefunction is given by

$$\Psi(t) = (\tfrac{1}{2})^{1/2}[\Psi_s \exp(-iE_s t/\hbar) + \Psi_a \exp(-iE_a t/\hbar)] \tag{5}$$

that is

$$\Psi(t) = (\tfrac{1}{2})^{1/2} \exp(-iE_s t/\hbar)\{\Psi_s + \Psi_a \exp[-i(E_a - E_s)t/\hbar]\}. \tag{6}$$

At time $t = 0$, $\Psi(t)$ is equal to Ψ_L as required and, at time $t = \pi\hbar/(E_a - E_s)$, $\Psi(t)$ becomes Ψ_R. As the time progresses, the electron oscillates between the centres of the double cross. The frequency ν of the oscillations is given by

$$\nu = |E_a - E_s|/2\pi\hbar. \tag{7}$$

In figure 2, I have shown the variation in E_s and E_a as a function of the ratio W'/W. The absolute difference $Z = |E_a - E_s|/E_{std}$, obtained from figure 2 varies from about zero when the separation between the centres is large to about 0.164 when the separation is the smallest. If the electron mass is taken to be the same as in free space and $W = 75$ nm, the value for ν is given by

$$\nu = 1.5Z \times 10^{+10}\ s^{-1}. \tag{8}$$

The value of ν can change from the above estimate if the width W is altered or the mass of the electron is different from its free-space value.

4. Conclusions

Energies of bound electronic states are obtained numerically for a single cross formed by two quantum wires with unequal widths, and for a double cross. In the case of a single cross it is found that, as the ratio of the widths is changed, the energy of the bound state decreases. For the double cross, two states are found corresponding to symmetric and

antisymmetric configurations with respect to the centres of the double cross. The energies of these states are obtained. The possibility that the electron oscillates between the two centres is proposed, and the value of the frequency of oscillations is estimated.

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