THE INFLUENCE OF THE EFFECTIVE MASS DISCONTINUITY ON WAVEFUNCTIONS IN A QUANTUM WELL IN ELECTRIC FIELD

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Abstract.

The influence of the effective mass discontinuity on wavefunctions in a quantum well in electric field is analysed in this paper. Using asympthotic expansions of Airy functions we found that for large or low enough energies, the wavefunctions behaviour is primarily determined by the effective mass discontinuity at well boundaries, and not its potential. E.g. for low enough energies the wavefunctions penetration depth increases considerably with increasing the barrier/well effective mass ratio.

1. INTRODUCTION

The effects of high electric fields on the electronic structure of quantum well (QW) systems is a topic of considerable current interest. A number of approximate calculations[1,2)] have been performed in which the confined states are viewed as bound states and their field-induced broadering is ignored. Recently, in[3)] presented strong-field calculations for an isolated QW, however, with the effective mass discontinuity neglected.

In this paper, we shall analyse the influence of this discontinuity on asympthotic (in energy) wavefunctions behaviour.

2. ASYMPTHOTIC BEHAVIOUR OF WAVEFUNCTIONS

The energy band diagram of a quantum well (QW) in electric field perpendicular to QW plane is given in Fig. 1. Introducing E_{oe} and E_{oh} as the difference between the total electron (hole) energy $E_e(E_h)$ and their transversal components calculated in the barrier ($\hbar^2 k_t^2 /2m_{1e,h}$), the envelope electron wavefunctions take the form[4)]:

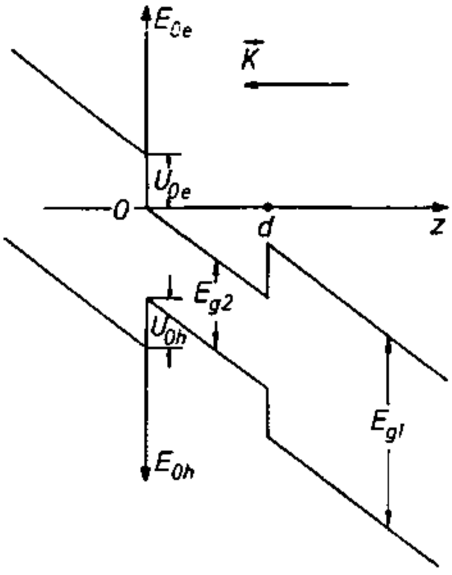

Fig. 1. Energy band diagram of a quantum well in perpendicular electric field.

The constants C_{21}, C_{22}, $C_{\alpha e}$ and $C_{\beta e}$ are determined from matching conditions of wavefunctions and their first derivatives at the interface. The multiplicative constant in (1) is determined from normalization condition, and as shown in[4] is proportional to $(C_{\alpha e}^2 + C_{\beta e}^2)^{-1/2}$

The functions Ai and Bi are the two linearly independent solutions of Airy equation (e.g.[5]). The corresponding expressions for holes have completely analogous

$$\psi_{e1}(z) = \text{const} \cdot \text{Ai}(\xi_1),\ z \leqslant 0 \tag{1}$$

$$\psi_{e2}(z) = \text{const} \cdot [C_{21}\text{Ai}(\zeta_2) + C_{22}\,\text{Bi}(\zeta_2)],\ 0 < z \leqslant d$$

$$\psi_{e3}(z) = \text{const} \cdot [C_{\alpha e}\text{Ai}(\xi_1) + C_{\beta e}\text{Bi}(\xi_1)],\ z \geqslant d.$$

The variables ξ_1 and ζ_2 are given by:

$$\xi_1 = -\left(\frac{2m_{1e}K}{\hbar^2}\right)^{1/3} \left(z + \frac{E_{oe} - U_{oe}}{eK}\right) \tag{2}$$

$$\zeta_2 = -\left(\frac{2m_{2e}K}{\hbar^2}\right)^{1/3} \left(z + \frac{E_{oe} + E_{tre}}{eK}\right),$$

where U_o is the conduction band edge discontinuity and E_{tre} is transversal energy difference in barrier and well layers.

form to those for electrons, and shall not be explicitely given. The constants C_α and C_β (index e is omitted) determine both resonance energies and widths, as well as, the asympthotic behaviour of wavefunctions for large z. For apart from resonance energies we may asympthotically expand these constants, for large positive and negative electron energies.

(i) Large negative electron energies. Taking the first leading terms of asymptho-tic expanssions for Ai, Bi, Ai' and Bi'[5] we get:

$$C_\alpha(E_0) = \frac{1}{4}(2 + \frac{1}{r} + r) \exp[-\frac{3}{2}(-E_0)^{1/2}(\frac{2}{\hbar^2})^{1/2}(m_1^{1/2} - m_2^{1/2}) d] + \tag{4}$$

$$+ \frac{1}{4}(-2 + \frac{1}{r} + r) \exp[-\frac{3}{2}(-E_0)^{1/2}(\frac{2}{\hbar^2})^{1/2}(m_1^{1/2} + m_2^{1/2}) d] +$$

+ higher order terms,

and:

$$C_\beta(E_0) = \frac{1}{8}(r - \frac{1}{r}) \exp[(\frac{2}{\hbar^2})^{1/2}(-E_0)^{1/2}(m_2^{1/2} - m_1^{1/2}) d - \tag{5}$$

$$- \frac{2}{3}(\frac{2m_1}{\hbar^2})^{1/2}(-E_0)^{1/2}(2 - \frac{3U_0}{E_0}) d] + \textit{higher order terms,}$$

where higher order terms contain power of $(-E_0)$ equal to or less than $-1/2$, therefore being negligible as compared to the terms in (4) and (5), and $r \equiv (m_1/m_2)^{1/2}$.

If $r = 1$ (position independent effective mass; $m_1 = m_2$), C_α tends to unity and C_β to zero, as $E_0 \to -\infty$. However, if $r \neq 1$ wavefunctions behaviour is qualitatively different. If barrier effective mass is greater than that in the well (as in GaAs QW in $Al_xGa_{1-x}As$ bulk), as one can see from (4) and (5), C_α tends to zero as well as C_β. It can be shown that absolute value of ratio C_α/C_β tends to infinity, as $E_0 \to -\infty$, therefore the multiplicative constant (in (1)) behaves as C_α^{-1} implying the deeper wavefunction penetration in the classically forbidden region ($z < 0$) than would be the case for position independent effective mass. In the opposite case, if the well effective mass is greater than that in the barrier, C_α tends to infinity, and C_β to zero. Making the above argumentation ($r < 1$ case) we can see that the wavefunction penetration in classically forbidden region is now highly supressed. It should be stressed, as one can see from (4) and (5) that such wavefunctions behaviour is determined primarilly by the effective mass difference and not by the existance of the well potential.

(ii) Large positive electron energies. Using the same method as in (i) we get:

$$C_\alpha(E_0) = \cos(\theta_1 - \theta_2 - \theta_3 + \theta_4) + [1 - \frac{1}{2}(r + \frac{1}{r})] \sin(\theta_3 - \theta_1) \sin(\theta_2 - \theta_4) -$$

$$- \frac{1}{2}(\frac{1}{r} - r) \cos(\theta_1 + \theta_3) \sin(\theta_2 - \theta_4) + \textit{higher order terms,} \tag{6}$$

$$C_\beta(E_o) = \sin(\theta_1 - \theta_2 - \theta_3 + \theta_4) + [1 - \frac{1}{2}(r + \frac{1}{r})] \cos(\theta_3 - \theta_1) \sin(\theta_2 - \theta_4) - \tag{7}$$

$$- \frac{1}{2}(\frac{1}{r} - r) \cos(\theta_1 + \theta_3) \sin(\theta_2 - \theta_4) + \textit{higher order terms,}$$

where

$$\theta_{1,2} = \frac{2}{3}(-\xi_{1,2})^{3/2} + \frac{\pi}{4} \text{ at } z = 0 \text{ and} \tag{8}$$

$$\theta_{3,4} = \frac{2}{3}(-\xi_{3,4})^{3/2} + \frac{\pi}{4} \text{ at } z = d \tag{9}$$

If $r = 1$ ($m_1 = m_2$) C_α would tend to unity and C_β to zero, while for $r \neq 1$ both constants complicated, but purely *oscillatory* behaviour (nondecaying with energy). The wavefunction multiplication constant (in (1)) now contains an oscillatory term plus unity, i.e.:

$$\text{const} \sim 1 + \frac{r_-}{\sqrt{2}} \sin[(\frac{2m_2E_o}{\hbar^2})^{1/2}d] \cos[(\frac{2m_1}{\hbar^2})^{1/2} \frac{E_o^{3/2}}{eK} \cdot (2 - \frac{3U_o}{E_o} + \frac{3eKd}{E_o})] \cdot \tag{10}$$

$$\cdot \sin[(\frac{2E_o}{\hbar^2})^{1/2} (m_2^{1/2} - m_1^{1/2}) d + \frac{\pi}{4}] + \textit{higher order terms,}$$

where $r_- = 0.5(r^{-1} - r)$, implying a high oscillatory depth of wavefunctions penetration with varying energy E_o, such behaviour being more pronounced for larger effective masses difference.

Although, the above expression were derived by making use asympthotic expansions of Airy functions, being most accurate for large values of their arguments, they remain valid even for realistic values of electron energy in typical GaAs – $Al_xGa_{1-x}As$ system. Upon setting the condition that using the first leading term in the asympthotic expansion should not introduce an error greater than 1% we get that $\xi_{1,2}$ should exceed 5, for large negative E_o. Taking as a typical example a 10 nm thick GaAs QW in $Al_{0.3}Ga_{0.7}As$ bulk that the above condition is fulfilled for: $E_o < -0.27$ eV($K = 10^7$ V/m), $E_o < -0.46$ eV ($K = 2 \cdot 10^7$ V/m) and $E_o < -0.65$ eV ($K = 3 \cdot 10^7$ V/m). These „limiting" energy values decrease with decreasing field and well thickness. For large positive energies, and also for holes we get similar results.

3. CONCLUSION

In this paper we analysed the wavefunctions properties in QW in electric field. Using the conventional asympthotic expansion of Airy function we derived the expressions for coefficients C_α and C_β in (1) for large negative energies (4,5) and for large positive energies (6,7). As one can see from these expressions, C_α and C_β depend strongly on the effective masses ratio, e.g. C_α for large negative energies tends to zero, unity or infinity if the barrier/well effective masses ratio is less than, equal to or greater than unity, respectivelly, with decreasing energy. These results imply qualitativelly different behaviour of wavefunctions (speciffically the penetration depths beyond the well), than would be the case without the effective mass discontinuity.

Acknowledgements

We wish to express our thanks to Lj. Radoja and G. Andjelković for high quality technical presentation.

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