Kinetic Energy Operators and Electron Transmission in Nonabrupt Heterojunctions

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Transmission properties of electrons through abrupt and nonabrupt $GaAs/Al_xGa_{1-x}As$ heterojunctions are studied using several forms of the kinetic energy operator with a position dependent effective mass. The nonabrupt interface potential and electron effective mass are obtained by assuming a linear variation of the aluminum molar fraction through the interface. For a given interface width, the electron transmission is shown to depend considerably on the form of the kinetic energy operator. Different kinetic energy operators are shown to be equivalent when the interface width of the $GaAs/Al_xGa_{1-x}As$ heterojunction is of the order of sixteen GaAs lattice parameters.

I. Introduction

The most used scheme for calculation of the properties of abrupt and nonabrupt semiconductor heterostructures is the effective-mass theory (EMT). Since EMT is justified only when smooth variations of the alloy composition are considered, one may question its use in the case of abrupt semiconductor interfaces. If nonabrupt interfaces are taken into account, the exact form of the kinetic energy operator (KEO) with a position dependent effective mass and the continuity condition of the wave function and its derivative at the interfaces still are open problems[1-6].

Despite the uncertainties related with the form of the KEO, few works have studied its influence on the properties of semiconductor heterostructures. Csavinszky and Elabsy[7] considered the influence of the form of the KEO on the binding energy of a hydrogenic donor placed at the centre of a $Al_xGa_{1-x}/GaAs/Al_xGa_{1-x}As$ quantum well. They found that the binding energy of the donor is a sensitive function of the form of the KEO. Galbraith and Duggan[8] calculated optical transition energies of GaAs/(Al, Ga)As quantum wells, and showed their dependence on the forms of the KEO that they have used. On the other hand, both Morrow and Browstein[9], as well as Einevoll and Hemmer[10] argued that the difference among KEOs is not important when the interface is very smooth. However, they do not have proved their hypothesis, nor obtained indications on how slowly graded have to be the interfaces to the validity of their assumption.

The influence of different KEOs in the transmission properties of electrons through abrupt and nonabrupt $GaAs/Al_xGa_{1-x}As$ heterojunctions is studied in this work. The purpose is to find an indication of the interface width at which different KEOs become equivalent. The $GaAs/Al_xGa_{1-x}As$ interface region is described accordingly the model previously proposed by Freire, Auto, and Farias[11,12]. KEOs with $\gamma = \alpha$ are used, like those of BenDaniel and Duke[13], and Zhu and Kroemer[14].

A general form for the KEOs is presented in Section II, as well as a description of the potential and electron effective mass through the $GaAs/Al_xGa_{1-x}As$ interface that characterizes the nonabrupt interface model used in this work. In Section III, numerical results show the influence of the interface width and KEO on the electron transmission through $GaAs/Al_xGa_{1-x}As$ heterojunctions. It is obtained the interface width at which different KEOs become equivalent. Finally, this work finishs in Section IV with comments on its limitations and consequences.

II. Kinetic energy operators and interface model

After the proposition of the effective-mass theory by Wannier[15], Slater[16], and Luttinger and Kohn[17], several works tryed to extend the EMT beyond the constant effective-mass picture to study crystals with graded composition. Several forms were proposed for the KEO with position dependent effective mass, $m = m(z)$, including those of: BenDaniel and Duke[13], $K_{BDD} = p[m(z)]^{-1}p/2$; Zhu and Kroemer[14], $K_{ZK} = [m(z)]^{1/2}p^2[m(z)]^{1/2}/2$; Gora and Williams[18] and/or Bastard[19] $K_{GW(B)} = p^2[m(z)]^{-1} + [m(z)]^{-1}p^2/4$; Liu and Khun[20], $K_{LK} = p[m(z)]^{-1}p[m(z)]^{-1} + [m(z)]^{-1}p[m(z)]^{-1}p/4$.

The most general KEO was proposed by von Roos[21], and is given by:

$$K_{vR} = \frac{1}{4}[m(z)^{\alpha}pm(z)^{\beta}pm(z)^{\gamma} + m(z)^{\gamma}pm(z)^{\beta}pm(z)^{\alpha}], \quad (1)$$

with $\alpha + \beta + \gamma = -1$. The continuity conditions are imposed on $m^{\alpha}\psi(z)$ and $m^{\alpha+\beta}\psi'(z)$, where $\psi(z)$ is the envelop function. Morrow an Browstein[9] showed that only single-term forms with $\alpha = \gamma$ are viable candidates to be a KEO in the case of abrupt semiconductor heterojunctions. No restriction seems to exist for γ when graded semiconductor interfaces are considered.

Today it seems that the KEO with $\beta = -1$, $\gamma = 0$ (the BenDaniel and Duke[13] KEO) is the most used, although not definitively accepted. Recently, Hagston *et al.*[3] have argued that the KEO of BenDaniel and Duke[13] leads to a violation of the Heisenberg Uncertainty Principle. They suggested that the KEO of Zhu and Kroemer[14] does not suffer this deficience.

Accordingly Eq. (1), the influence of the KEO on the properties of semiconductor heterostructures is determined by the spatial dependence of the effective mass of carriers. Ribeiro Filho *et al.*[22] have developed a GaAs/Al_xGa_{1-x}As interface model where both the potential and the electron effective mass through the interfacial region is obtained as a function of the growth pattern of the interfacial aluminum molar fraction. In the case of a linear variation of the aluminum molar fraction through the GaAs/Al_xGa_{1-x}As interface localized at the limits $z = \pm a$, the interface potential and electron effective mass are given, respectively, by[11,12,22]

$$V_x(z) = V_x^{(0)} + V_x^{(1)}\left(\frac{z}{2a}\right) + V_x^{(2)}\left(\frac{z}{a}\right)^2 \quad (2)$$

$$\frac{m_x(z)}{m^*} = m_x^{(0)} + m_x^{(1)}\left(\frac{z}{2a}\right) \quad (3)$$

where

$$V_x^{(0)} = \frac{x}{2}\left(\epsilon_1 + \epsilon_2\frac{x}{2}\right)Q_e\ , \quad (4)$$

$$V_x^{(1)} = V_x = x\left(\epsilon_1 + \epsilon_2 x\right)Q_e\ , \quad (5)$$

$$V_x^{(2)} = \epsilon_2\left(\frac{x}{2}\right)^2 Q_e\ , \quad (6)$$

$$m_x^{(0)} = \mu_1 + \mu_2\frac{x}{2}\ , \quad (7)$$

$$m_x^{(1)} = \mu_2 x\ , \quad (8)$$

In the above equations, Q_e is the band offset for electrons, $\epsilon_i(\mu_i)$ are experimental constants associated with the compositional dependence of the $Al_xGa_{1-x}As$ gap energy in the Γ-direction (electron effective mass) at 300 K[23], and m^* is the electron mass in the free-space.

III. Effects of KEOs in the electron transmission

To have an indication of how smooth has to be the interfaces to the equivalence of different KEOs with $\alpha = \gamma$, transmission properties of electrons through abrupt and nonabrupt GaAs/$Al_{0.3}Ga_{0.7}$As heterojunctions of several interface widths are calculated. The interface potential and electron effective mass are described by Eqs. (2, 3). Wave equations with KEOs are obtained by taking $-2 \leq \alpha \leq +2$, and solved numerically with the multistep potential approximation of Ando and Itoh[24]. It is considered a band offset $Q_e = 0.6$.

Figs. 1 and 2 show that the dependence of the electron transmission coefficiente T_e on the form of the KEO is bigger when the interface width is small. This could be seen by comparing the electron transmission through abrupt and nonabrupt interfaces. For a given interface width (curves with the same type of line in the figures), T_e is highly dependent on the form of the KEO.

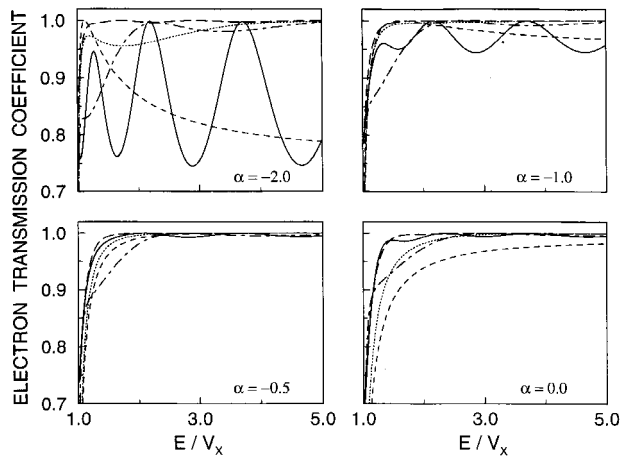

Figure 1. Electron transmission through abrupt and nonabrupt GaAs/$Al_{0.3}Ga_{0.7}$As heterojunctions calculated considering the spatial dependence of the interface potential and electron effective mass and a band offset $Q_e = 0.6$. Kinetic energy operators with $\alpha = 0.0, -0.5, -1.0, -2.0$ were used, as well as interface widths of: 0LP (dashed); 4LP (dotted); 8LP (dotted dashed); 16LP (long dashed). The continuous line shows the electron transmission calculated considering the constant interfacial effective-mass approximation, and an interface width of 16 LP.

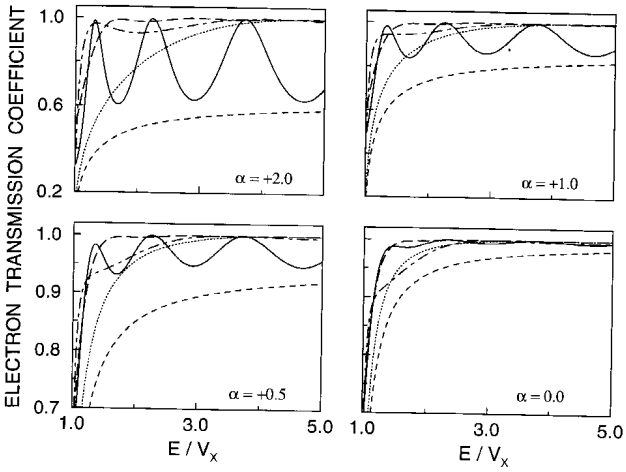

Figure 2. Electron transmission through abrupt and nonabrupt GaAs/$Al_{0.3}Ga_{0.7}$As heterojunctions calculated considering the spatial dependence of the interface potential and electron effective mass and a band offset $Q_e = 0.6$. Kinetic energy operators with $\alpha = 0.0, +0.5, +1.0, +2.0$ were used, as well as interface widths of: 0LP (dashed); 4LP (dotted); 8LP (dotted dashed); 16LP (long dashed). The continuous line shows the electron transmission calculated considering the constant interfacial effective-mass approximation, and an interface width of 16 LP.

T_e changes considerably with α when the interface width ℓ is as small as four GaAs lattice parameters (LP). However, when ℓ is greater or of the order of sixteen GaAs lattice parameters (see long dashed lines in the figures), T_e does not change its behavior, being almost independent of α. Consequently, different KEOs are shown to be equivalent in the case of electrons when the interface width of the GaAs/$Al_{0.3}Ga_{0.7}$As heterojunction is $\gtrsim$ 16 LP.

To highlight the importance of the way the spatial dependence of the effective mass is considered, T_e is also calculated assuming that $m(z) = m_x^{(0)}$, i.e., $m(z)$ is constant through the interface region of width ℓ = 16LP (see continuous line in the figures). The constant mass approximation is responsible for the existence of resonances in the transmission. These resonances increase strongly with the value of $|\alpha|$. On the other hand, if the complete spatial dependence of the electron effective mass is considered, the transmission resonances never occur when the interface width is smaller than 4LP and $-1 \leq \alpha \leq +1$.

The KEO of Zhu and Kroemer ($\alpha = -1/2$)[14] produces the smallest dependence of T_e on the interface width, as well as the smallest resonances generated with the constant effective mass approximation. The dependence of T_e calculated with the KEO of BenDaniel and Duke ($\alpha = 0$)[13] on the interface width is a little stronger than that shown by Te when calculated with the KEO of Zhu and Kroemer[14].

It is worth to be observed that if $\alpha \geq 0$, the electron transmission decreases with α for a given interface width. The rate of decreasing is big when the interface width is small.

IV. Concluding remarks

In this work, it was obtained that kinetic energy operators with $-2.0 \leq \alpha \leq +2.0$ are all equivalent when the width of the graded semiconductor interface is of the order of 100Å. Since the best interface widths of semiconductor samples are nowadays at least of two lattice parameters[25,26], one can conclude that more fundamental results are needed to indicate the validity and range of applicability of the effective-mass theory, as well as the correct form of the kinetic energy operator in the domain of the semiconductor physics of reduced dimensionality.

The limit of 100 Å obtained here for the equivalence of several KEOs is a consequence of the semiconductor data used in the calculations, the growth pattern of the interface, and the approximations that were done (for example, the assumption $\gamma = \alpha$). However, the

result agrees with that of Wolfe *et al.*[27] on the limitations of the effective-mass approximation. Based in simple arguments related with the Heisenberg uncertainty principle, Wolfe *et al.*[27] have argued that, in the case of GaAs, the effective-mass approximation is a very reliable tool only when semiconductor dimensions bigger than 300 Å are involved. Consequently, more fundamental results are necessary to explain the considerable success of the effective-mass approximation in the estimation of the properties of semiconductor heterostructures.

Considerable progress has been achieved by Burt toward obtaining an effective-mass equation from first principles, i.e., microscopic Scroedinger equations that are valid even for abrupt semiconductor interfaces[28,29]. However, his final version of the effective-mass equation was obtained by neglecting terms that would contribute to the KEO. Consequently, a comparison between Burt's kinetic energy operator[28] and those previously proposed arguing hermiticity[16] does not indicate conclusively the form of the KEO with a position dependent effective-mass.

References

1. M. G. Burt, Appl. Phys. Lett. **65**, 717 (1994).
2. A. Brezini and M. Sebbani, Phys. Stat. Sol. (b) **178**, 141 (1993).
3. W. E. Hagston, P. Harrison, T. Piorek, and S. Stirner, Superlatt. Microstruct. **15**, 199 (1994).
4. M. R. Geller and W. Kohn, Phys. Rev. Lett. **70**, 3103 (1993).
5. C. Schnittler and M. Kirilov, Phys. Stat. Sol. (b) **176**, 143 (1993).
6. J. Thomsen G. T. Einevoll and P. C. Hemmer, Phys. Rev. **B47**, 12760 (1993).
7. P. Csavinszky and A. M. Elabsy, Semicond. Sci. Technol. **3,** 1010 (1988).
8. I. Galbraith and G. Duggan, Phys. Rev. **B38**, 10057 (1988).
9. R. A. Morrow and K. R. Browstein, Phys. Rev. **B30**, 678 (1984).
10. G. T. Einevoll and P. C. Hemmer, J. Phys. **C21**, L1193 (1993).
11. V. N. Freire, M. M. Auto and G. A. Farias, in *Proceedings of the 5th Brazilian School on Semiconductor Physics*, edited by J. R. Leite A. Fazzio and A. S. Chaves, p. 356 (World Scientific, Singapore, 1992).
12. V. N. Freire, M. M. Auto and G. A. Farias, Superlatt. Microstruct. **1**, 17 (1992).
13. D. J. BenDaniel and C. B. Duke, Phys. Rev. **152**, 683 (1966).
14. Q.-G Zhu and H. Kroemer, Phys. Rev. **B27**, 3519 (1983).
15. G. H. Wannier, Phys. Rev. **52**, 191 (1937).
16. J. C. Slater, Phys. Rev. **76**, 1592 (1949).
17. J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).
18. T. Gora and F. Williams, Phys. Rev. **177**, 1179 (1969).
19. G. Bastard, Phys. Rev. **B24**, 5693 (1981).
20. T. L. Li and K. J. Kuhn, Phys. Rev. **B47**, 12760 (1993).
21. O. von Roos, Phys. Rev. **B27**, 7547 (1983).
22. J. Ribeiro Filho, G. A. Farias and V. N. Freire, unpublished.
23. S. Adachi, J. Appl. Phys. **S8**, R1 (1985).
24. Y. Ando and T. Itoh, J. Appl. Phys. **61**, 1497 (1987).
25. A. Ourmazd, D. W. Taylor, J. Cunningham and C. W. Tu, Phys. Rev. Lett. **62**, 933 (1989).
26. O. Albrektsen, D. J. Arent, H. P. Meier and H. W. M. Salemink, Appl. Phys. Lett. **57**, 31 (1990).
27. C. M. Wolfe, N. Holonyak, Jr. and G. E. Stillman, in *Physical Properties of Semiconductors*, (Prentice-Hall, 1989) p. 68.
28. M. G. Burt, J. Phys: Condens. Mat. **4**, 6651 (1992).
29. M. G. Burt, Appl. Phys. Lett. **65**, 717 (1994).