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Lifetime of resonant state in a spherical quantum dot*

Li Chun-Lei(李春雷)† and Xiao Jing-Lin(肖景林)

College of Physics and Electromechanics, Inner Mongolia National University, Tongliao 028043, *China*

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This paper calculates the lifetime of resonant state and transmission probability of a single electron tunnelling in a spherical quantum dot (SQD) structure by using the transfer matrix technique. In the SQD, the electron is confined both transversally and longitudinally, the motion in the transverse and longitudinal directions is separated by using the adiabatic approximation theory. Meanwhile, the energy levels of the former are considered as the effective confining potential. The numerical calculations are carried out for the SQD consisting of GaAs/InAs material. The obtained results show that the bigger radius of the quantum dot not only leads significantly to the shifts of resonant peaks toward the low-energy region, but also causes the lengthening of the lifetime of resonant state. The lifetime of resonant state can be calculated from the uncertainty principle between the energy half width and lifetime.

Keywords: spherical quantum dot, lifetime of resonant state, transmission probability
PACC: 3270F, 7200

1. Introduction

Resonant tunnelling of a particle is a pure quantum phenomenon due to the description of particle motion derived from wave theoretical interpretation. In quantum mechanics, the particle (e.g. electron) can be regarded as a wave packet marked distribution of probability. After confronting a potential barrier, it splits into a reflected wave packet and a trapped wave packet, and the latter is transmitted into a resonant transmission system. After a very short span of time, a part of the latter is thrown into the right of the resonant transmission system. Since the 1930s, a number of investigations have been carried out. In 1932, MacColl[1] concluded that the lifetime of a wave packet tunnelling through a potential barrier is not longer obviously than vacuum; Wigner[2] calculated the lifetime of an electron tunnelling through a potential barrier by using a method of peak value of wave packet; Hartman[3] proved MacColl's conclusion and Wigner's calculation. Over the past three decades, resonant tunnelling has been more widely studied following the pioneering work by Tsu and Esaki.[4,5] Most research papers on the resonant tunnelling problem have been written by using the time-independent Schrödinger equation[6−10] or time-dependent Schrödinger equation.[11−14] Naoki and Shigeru[15] derived the lifetime of the time evolution of an electron wave packet in a double barriers resonant tunnelling system. With the rapid progress in crystal growth and microfabrication techniques, it is now possible to explore the transmission problem in nanometre-scale semiconductor structures, and leads to the idea of transmission through zero-dimensional 'quantum dot' structures. Recently, Li Shu-Shen *et al*[16−19] researched into the transport properties in quantum dot by using a recursion method. Li *et al*[20,21] studied electronic transport properties of molecular junctions. Dai *et al*[22] studied radiative lifetimes of Rydberg 6pnd $J = 2$ state of Pb I by multichannel quantum defect theory. Gao *et al*[23] researched the effect of magnetic field on the transmission properties of electrons in a four-terminal quantum waveguide.

The purpose of this paper is to calculate the lifetime of resonant state and the transmission probability in a SQD. Our results should be useful to design optimum high-speed resonant- transmission devices.

2. Model and calculation

Throughout the paper the units of energy will be given in terms of the effective Rydberg constant $R_{\rm y} = \hbar^2/(2m_{\rm e}^* a_{\rm B}^2)$ and lengths are given in terms of the Bohr radius $a_{\rm B} = \hbar^2\varepsilon/(m_{\rm e}^* e^2)$, where $m_{\rm e}^*$ is the electron's effective mass.

The Schrödinger equation describing the motion

*Project supported by the National Nature Science Foundation of China (Grant No 10347004).
†E-mail: lichunleimm@sohu.com

of a single electron can be written in cylindrical coordinates as follows:

$$\Big[-\frac{1}{r^2}\Big(r\frac{\partial}{\partial r}r\frac{\partial}{\partial r}+\frac{\partial^2}{\partial\theta^2}\Big)-\frac{\partial^2}{\partial z^2}+V_{\rm e}(r)\Big] \times \Psi(r,\theta,z)=E\Psi(r,\theta,z), \quad (1)$$

where E is the incident energy of the electron, the confining potential $V_{\rm e}(r)$ is zero inside the SQD, and is V_0 outside the SQD. Using the adiabatic approximation theory, we can write the wavefunction as a product:[24]

$$\Psi(r,\theta,z)=\frac{1}{\sqrt{2\pi}}{\rm e}^{{\rm i}m\theta}g_r^n(z)f_m^n(r), \quad (2)$$

where $g_r^n(z)$ is a slightly varying function of r. n,m are the radial and angular momentum quantum number respectively. In the following calculations, we set $m=0$ due to radial symmetry in our structure. The functions $g_r^n(z)$ and $f_m^n(r)$ satisfy the system of equations

$$\Big[-\frac{\partial^2}{\partial z^2}+E_n^m(z)\Big]g_r^n(z)=Eg_r^n(z), \quad (3)$$

$$\Big[-\frac{1}{r^2}\Big(r\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-m^2\Big)+V_{\rm e}(r)]f_m^n(r) = E_n^m(z)f_m^n(r). \quad (4)$$

It is first needed to calculate the energy levels $E_n^m(z)$. Build the radial wavefunctions on Bessel functions, where we have divided the SQD into slices along axis z and R is the radius of each part. The wavefunctions must equal zero when $r\to\infty$ and be finite when $r=0$, so it can be written as

$$f_m^n(r)=A_mJ_m(k_1r), \quad 0<r<R,$$

$$k_1=\sqrt{E_n^m(z)}, \quad (5)$$

$$f_m^n(r)=B_mK_m(k_2r), \quad r>R,$$

$$k_2=\sqrt{V_0-E_n^m(z)}, \quad (6)$$

where z, R and the radius of the SQD R_0 satisfy the relation: $R=\sqrt{z(2R_0-z)}$.

Using the boundary condition for $r=R$, we can obtain a series of quantized energy levels $E_n^m(z)$, and then we treat them as the effective confining potentials in the following calculations. Now we calculate the transmission probability of the electron tunnelling through the SQD. In the SQD, Eq.(3) can be written as

$$\frac{\partial^2}{\partial z^2}g_r^1(z)+[E-E_1^0(z)]g_r^1(z)=0. \quad (7)$$

The wavefunction in the jth region of the SQD is written as

$$g_r^1(z_j)=A_{1,j}\exp({\rm i}k_jz_j)+A_{2,j}\exp(-{\rm i}k_jz_j), \quad (8)$$

$$g_r^1(z_{\rm in})=A_{1,{\rm in}}\exp({\rm i}k_{\rm in}z)+A_{2,{\rm in}}\exp(-{\rm i}k_{\rm in}z), \quad \text{(emitter region)} \quad (9)$$

$$g_r^1(z_{\rm out})=A_{1,{\rm out}}\exp({\rm i}k_{\rm out}z)+A_{2,{\rm out}}\exp(-{\rm i}k_{\rm out}z), \quad \text{(collector region)} \quad (10)$$

where

$$k_j=\sqrt{E-E_1^0(z)}, \quad \text{and} \quad k_{\rm in}=k_{\rm out}=\sqrt{E}.$$

Current flux density conservation requires the continuity for both $g_r^1(z)$ and its derivative at each interface. This leads to relationships between the coefficients $A_{1,{\rm in}}$, $A_{2,{\rm in}}$, $A_{1,{\rm out}}$ and $A_{2,{\rm out}}$:

$$\begin{pmatrix}A_{1,{\rm in}}\\A_{2,{\rm in}}\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1 & -{\rm i}k_{\rm in}^{-1}\\1 & {\rm i}k_{\rm in}^{-1}\end{pmatrix} \times M\begin{pmatrix}1 & 1\\{\rm i}k_{\rm out} & -{\rm i}k_{\rm out}\end{pmatrix}\begin{pmatrix}A_{1,{\rm out}}\\A_{2,{\rm out}}\end{pmatrix}, \quad (11)$$

where $M=\prod_j M_j$ is the product of a series of transfer matrix M_j with 2×2 dimensions.

If $E>E_1^0(z)$, then $k_j=\sqrt{E-E_1^0(z)}$ and the transfer matrices are

$$M_j=\begin{pmatrix}\cos(k_jz_j) & -\dfrac{1}{k_j}\sin(k_jz_j)\\ k_j\sin(k_jz_j) & \cos(k_jz_j)\end{pmatrix}, \quad (12)$$

and if $E<E_1^0(z)$, then $k_j=\sqrt{E_1^0(z)-E}$ and the transfer matrices are

$$M_j=\begin{pmatrix}\cosh(k_jz_j) & -\dfrac{1}{k_j}\sinh(k_jz_j)\\ -k_j\sinh(k_jz_j) & \cosh(k_jz_j)\end{pmatrix}, \quad (13)$$

where z_j is the width of the jth region. Finally, the transmission probability T is $T=|A_{1,{\rm out}}|^2/|A_{1,{\rm in}}|^2$.

The time-dependent wavefunction of the electron wave packet can be written as

$$g(z,t)=\frac{1}{\sqrt{\Delta k}}\int g_r^1(z) \times\exp[-(k-k_0)^2/2\Delta k^2-{\rm i}Et]{\rm d}k, \quad (14)$$

where $k=\sqrt{E}$. Distribution of the electron wave packet in k-space is Gaussian, which is centred at k_0 and has a finite width Δk.

3. Results and discussion

In the following calculations we set the SQD's confining potential to be 0.6 eV and $m_e^* = 0.053m_0$, where m_0 is the free-electron mass. We treat $E_1^0(z)$ as the effective confining potential. The radius of the SQD's R_0 is 5 nm. In calculations, we set the centre of the SQD at $z = 5$ nm, when $t = 0$ fs, the centre of the electron wave packet lies at $z = 0$ nm. The numerical calculations are carried out for Eq.(14) as shown in Fig.1 (note that wavefunction is not normalized).

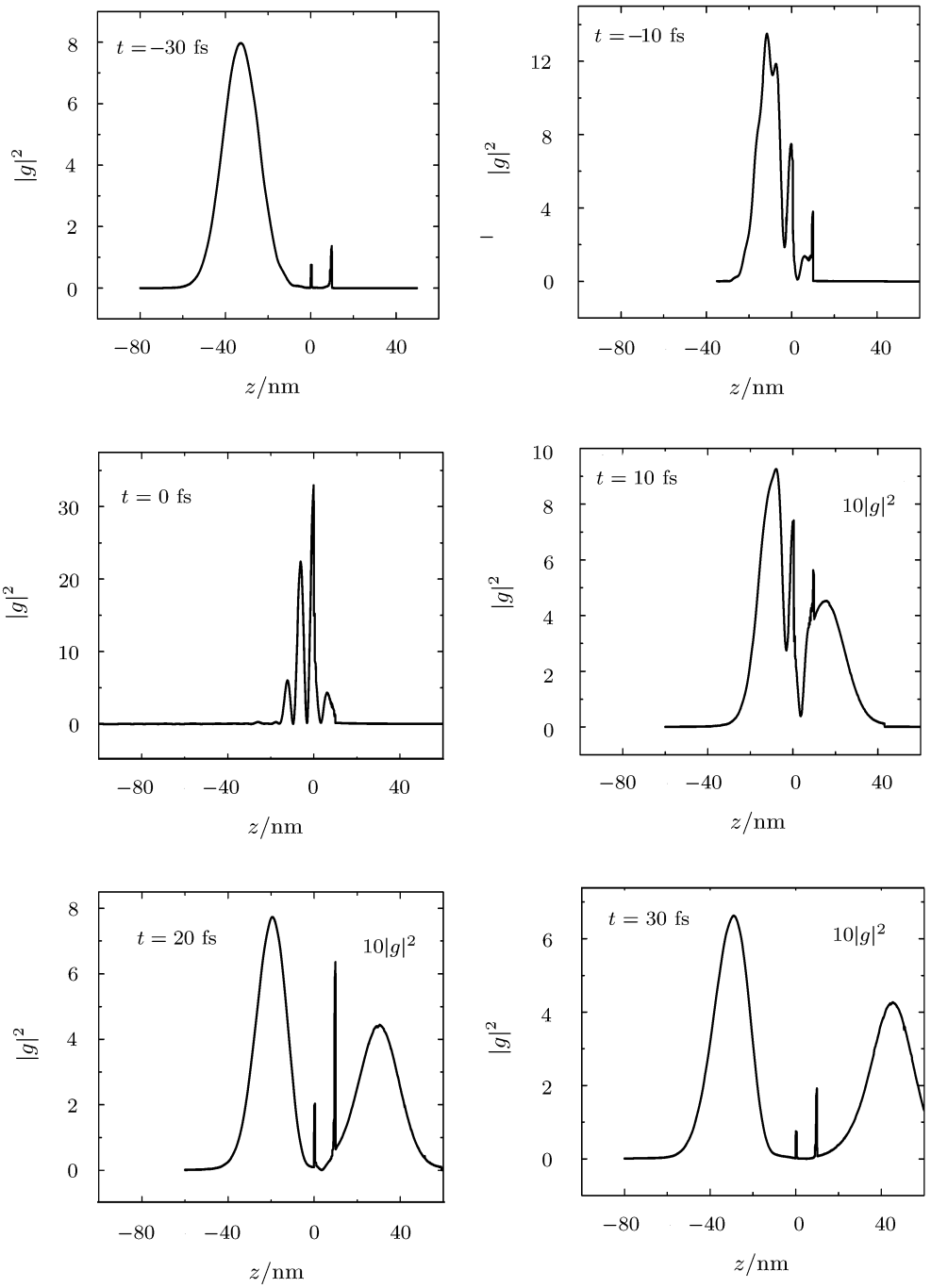


Fig.1. The time evolution of the electron wave packet in the SQD, where $R_0 = 5.0$ nm, $k_0 = 5.0 \times 10^8$ m^{-1} and $\Delta k = 1.5 \times 10^8$ m^{-1}.

When $t = -10$ fs, the wave packets hits the SQD. When $t = 0$ fs, the wavefunction shows a spatial oscillation due to interaction between the reflect wave packet and the incident one. After that, when $t = 20$ fs, a part of the wave packet is transmitted to the right of the SQD. It can be clearly seen that the lifetime of resonant state in the SQD, i.e. from $t = 0$ fs to $t = 20$ fs, is about 20 fs. This conclusion can be seen from Fig.2.

Figure 2 shows the time dependence of amplitude of the wave packet at the centre of the SQD. In Fig.2, from $t = 0$ fs to $t \approx 8$ fs, the amplitude of the wave packet at the centre of the SQD becomes greater and greater. The reason is that the wave packet throws into the SQD in the span of time. From $t \approx 8$ fs to $t \approx 20$ fs, $|g|^2$ decreases exponentially. This is because the wave packet transmits to the right of the SQD in the span of time.

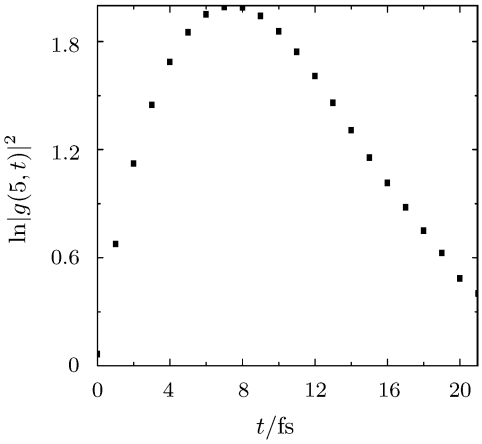


Fig.2. The time dependence of the amplitude of the wave packet at the centre of the SQD.

In the textbook about quantum mechanics,[25] the uncertainty principle between the energy half width and the lifetime is $\tau \cdot \Gamma \approx \hbar$. According to the above relation, we can obtain the lifetime of resonant state in the SQD. Figure 3 shows transmission probability T as a function of electron energy E for the different SQD radii. The solid, dashed, and dotted lines correspond to $R_0 = 20, 10$, and 5 nm, respectively. Meanwhile, we can calculate the energy half width Γ and the lifetime τ in Fig.3 for $R_0 = 5$ nm as, $\Gamma = 0.1968 - 0.1649 = 0.0319$ eV, and $\tau \approx \hbar/\Gamma = 20.636$ fs. The value of lifetime coincides very well with that obtained from simulation of the wave packet, it indicates that the lifetime in the SQD can be calculated from the energy half width Γ. Because the width Γ can be obtained by an analysis of the stationary state, this facilitates the procedure of calculating the lifetime of resonant state in the SQD. From Fig.3, with the radius of the SQD variation from 5nm to 20nm, the transmission peaks move toward the lower-energy region, accompanied by the increase of number of the peaks. The reason is that the resonance energy levels will decrease for a larger SQD radius. We next calculated the lifetime of resonant state in the SQD.

Figure 4 shows the lifetime of resonant state as a function of the radius of the SQD. From this figure, we find that the lifetime is strongly dependent on the radius of the SQD. This is because the energy half width Γ will decrease sharply as increasing the radius of the SQD.

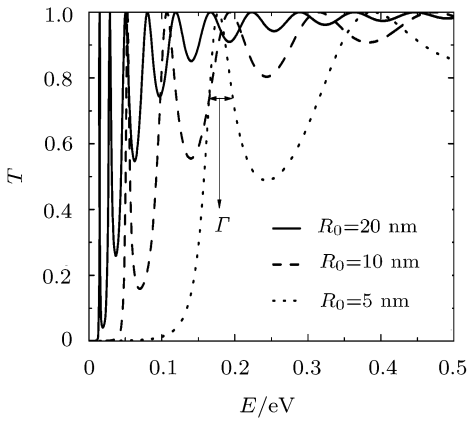


Fig.3. The transmission probability T as a function of the electron energy E for different radius of the SQD.

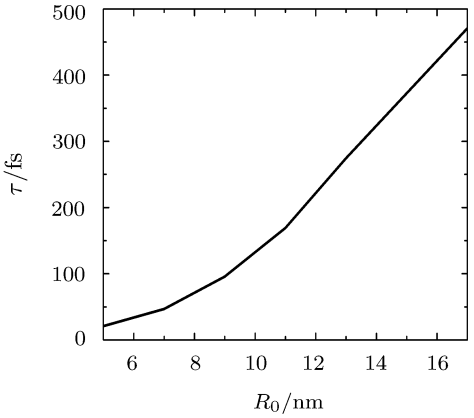


Fig.4. The lifetime τ of the resonant state as a function of the radius of the SQD.

4. Conclusions

In this paper, we have studied the lifetime of resonant state and transmission probability through a

SQD by using the transfer matrix technique. The results show that the big size of the SQD not only leads significantly to the shifts of resonant peaks toward the lower-energy region but also causes the lengthening of the lifetime of resonant state. To get the lifetime of resonant state in the SQD, time evolution of an electron wave packet is calculated. Meanwhile, the lifetime of resonant state in the SQD was calculated by using the uncertainty principle between the energy half width and the lifetime. Because the lifetime of the resonant state eventually limits the operation speed of transmission devices, our results should be useful to design optimum high-speed resonant-transmission devices.

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