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Two-electrons in a quantum dot: Tunnelling rate under a magnetic field

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ABSTRACT

This paper analyses a model of a pair of electrons collected by means of harmonic confinement $V(x, y)$ and subjected to a magnetic field $\mathbf{B} = B\hat{z}$ perpendicular to the quantum dot layer. Under these circumstances there exists a coupling between $\mathbf{B}$ and the harmonic potential which is going to alter both the effective length of the electronic functions and the tunnelling rates. The main conclusion of this paper is that, by using a finite potential barrier, a treatable expression of tunnelling rate is likely to be obtained. Likewise, another outcome is that, by increasing the magnetic fields, the harmonic confinement equalises the electronic effective widths, that is, both the x-width and the y-thickness tend to the same asymptotic value. Last but not least, one concludes that the magnetic field can be used to control the tunnelling rate.

1. Introduction

Quantum confinement develops discrete levels of electrons which are called quantum dots (QD). As a consequence, the shape of the confinement plays an important role both in the shell energy and in the electronic correlation. In fact, one of the most frequent topics in QD literature is precisely the analysis of the impact of different types of confinement on quantum dots [1–4], in an attempt to achieve electron tunnelling and eventually to build quantum processors.Within the quantum dots scope, the interest aroused by the local magnetic fields would be due to the fact that they affect the quantum levels and also involve the spin dynamics. Some effects of applying magnetic fields to QD would be spin–orbit interaction, spin flip, cyclotron and Zeeman effects. In general, quantum dots have been associated with magnetic fields under different angles: tilted [3,5] and perpendicular [6–9] magnetic fields. The aim of this paper is to analyse the magnetic field influence upon the tunnelling rate. The article begins by considering a pair of electrons in a harmonic confinement with two levels, and it continues by defining the tunnelling rate by means of a finite potential barrier. Finally, the paper analyses the influence of the magnetic field on the electronic states and on the tunnelling rate.

2. Electronic functions and tunnelling

The model developed in this paper considers a pair of electrons that are collected by means of harmonic confinement in order to form a quantum dot. Each electron can be in a fundamental state –it will be labelled by the subscript α– or in the first excited state –specified by β– and, in addition, electrons can have two different spins. The basis is composed of six states, each of them has an orbital component and a spin term. Thus the singlet state shares the spin $\chi_s = |\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2$ but not the orbital terms, which are symmetrical combinations of wave functions $\phi_n(\mathbf{r})$, where $n = \alpha, \beta$ is used to designate the electronic level. Then, the singlet state is given by

$$|\phi\rangle^1 = \frac{1}{\sqrt{2}}\phi_\alpha(\mathbf{r}_1)\phi_\alpha(\mathbf{r}_2)\chi_s\,, \tag{1}$$

$$|\phi\rangle^2 = \frac{1}{\sqrt{2}}\phi_\beta(\mathbf{r}_1)\phi_\beta(\mathbf{r}_2)\chi_s\,, \tag{2}$$

$$|\phi\rangle^3 = \frac{1}{2}[\phi_\alpha(\mathbf{r}_1)\phi_\beta(\mathbf{r}_2) + \phi_\beta(\mathbf{r}_1)\phi_\alpha(\mathbf{r}_2)]\chi_s\,, \tag{3}$$

here $\mathbf{r}_1$ and $\mathbf{r}_2$ are position vectors of electrons 1 and 2. Reciprocally, the triplet state shares the orbital term $\Phi_t = [\phi_\alpha(\mathbf{r}_1)\phi_\beta(\mathbf{r}_2) - \phi_\beta(\mathbf{r}_1)\phi_\alpha(\mathbf{r}_2)]$ but not the symmetrical spin terms

$$|\phi\rangle^4 = \frac{1}{2}\Phi_t\,[|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2]\,, \tag{4}$$

$$|\phi\rangle^5 = \frac{1}{\sqrt{2}}\Phi_t\,|\uparrow\rangle_1|\uparrow\rangle_2 \quad \text{and} \tag{5}$$

$$|\phi\rangle^6 = \frac{1}{\sqrt{2}}\Phi_t\,|\downarrow\rangle_1|\downarrow\rangle_2\,. \tag{6}$$

Both electrons will be confined by means of a harmonic potential $V(x, y)$, inside a thin conduction layer on plane XY, and negligible thickness $|Z|^2 = \delta(z)$: thin QD approximation [2,10]. Therefore, the time independent Hamiltonian determines the basis with equations (1)–(6) be formed from Hemite polynomials. From here on, the procedure consist in studying the individual electronic behaviour

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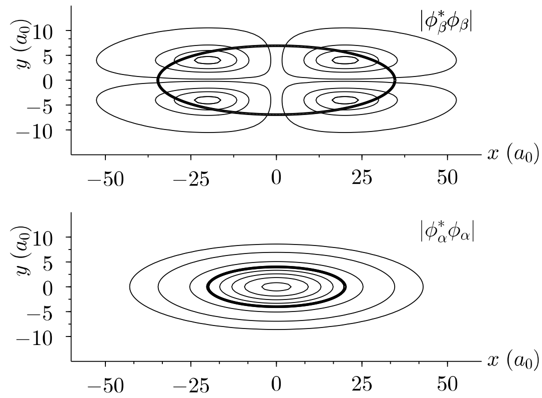

Fig. 1. Probability distribution of the electronic states ϕ_α and ϕ_β which correspond to the ground state and the excited state, respectively. The effective widths are $l_y = 4\,a_0$ and $l_x = 20\,a_0$. The innermost line corresponds to $9.5\ 10^{-4}$ for the α-state and $5.0\ 10^{-4}$ for the β-state. On the other hand, the thick line illustrates the ellipse of confinement.

considering the eigenstate properties as the combination of the single electronic magnitudes, such as energy or tunnelling rate. Fig. 1 shows the probabilities of the electronic ground state ϕ_α and of ϕ_β, the first excited state. The effective widths are $l_y = 4\,a_0$ along the y direction and $l_x = 20\,a_0$ along x, where a_0 is the effective Bohr radius,

$$a_0 = \frac{4\pi\varepsilon_0\varepsilon_b\hbar^2}{m^* e^2} = 10.35 \quad \text{nm.} \tag{7}$$

In addition, the isolines of the figure follow the sequence $9.5\ 10^{-4}$, $8.0\ 10^{-4}$, $6.5\ 10^{-4}$, $5.0\ 10^{-4}$, $3.5\ 10^{-4}$, $2.0\ 10^{-4}$, $0.5\ 10^{-4}$ and $0.1\ 10^{-4}$.

2.1. Tunnelling

The following lines concern the tunnelling, which will be modelled by means of a finite potential barrier [11–13]; obviously, this assumption involves the fact that electrons emerge somewhere. Fig. 2 describes this situation. The electronic functions ϕ_n spread along the whole space, however these wave functions will become decreasing exponential $\zeta_n(x, y) = \zeta_n(x)\zeta_n(y)$ beyond the harmonic confinement. Thus, the border line separating the harmonic functions from the exponential behaviour is an ellipse with semi-axis coincident with the effective widths $l_x = 20\,a_0$ (or $\sqrt{3}\ l_x$), and $l_y = 4\,a_0$ (or $\sqrt{3}\ l_y$), where the values in brackets are applied to the electronic excited state, see Fig. 1. It is precisely along these ellipses where both $\phi_n(\mu)$ and the exponential function must fulfil the continuity conditions:

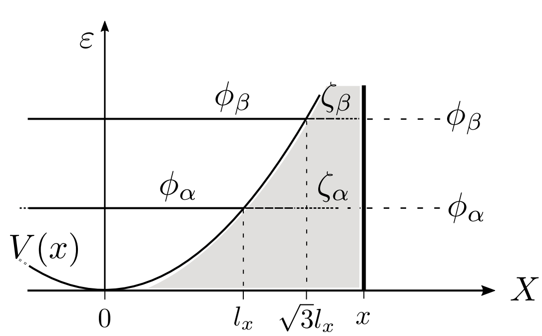

Fig. 2. Graphic description of tunnelling along x. The electronic wave functions ϕ are separated from the potential barrier (the grey area) at the coordinates l_x and $\sqrt{3}\,l_x$, forming an elliptic border on the plane XY. A generic coordinate x is used to mark the barrier end; beyond x the wave functions become again harmonic.

$$\phi_n(\mu) = A\,\exp(-b\,\mu) \qquad \text{and} \qquad \frac{d}{d\mu}\phi_n(\mu) = \frac{d}{d\mu}A\,\exp(-b\,\mu), \tag{8}$$

with $n = \alpha, \beta$ and $\mu = x, y$. For the sake of clarity, the decreasing exponential functions along x are given by

$$\zeta_\alpha(x) = \frac{1}{(\sqrt{\pi}\,lx)^{\frac{1}{2}}}\exp\left(-\frac{x}{l_x} + \frac{1}{2}\right), \tag{9}$$

$$\zeta_\beta(x) = \frac{\sqrt{6}}{(\sqrt{\pi}\,lx)^{\frac{1}{2}}}\exp\left(-\frac{2x}{\sqrt{3}\,l_x} + \frac{1}{2}\right) \tag{10}$$

where x starts at lx for ζ_α, and at $\sqrt{3}\,l_x$ for ζ_β. To obtain $\zeta_n(y)$ it is enough to replace l_x with l_y and x with y in equations (9) and (10). Fig. 2 shows a potential barrier stretching over the grey region to a generic coordinate x; the electronic distribution outside the barrier is again harmonic functions.

In this study the tunnelling rate is defined by means of the sum of two terms: the electronic probability of finding electrons inside the confinement, and the electronic probability of reaching the potential barrier end. This way, the tunnelling rates along x direction for a generic end is given by:

$$\Gamma_\alpha(x) = \int_{-l_x}^{l_x}\left|\phi_\alpha\right|^2 dx + \int_{l_x}^{x}\left|\zeta_\alpha\right|^2 dx$$
$$= =erf\,(1) + \tfrac{1}{2\sqrt{\pi}}\left[e^{-1} - \exp\left(-\tfrac{2x}{l_x} + 1\right)\right] \tag{11}$$

$$\Gamma_\beta(x) = \int_{-\sqrt{3}l_x}^{\sqrt{3}l_x}\left|\phi_\beta\right|^2 dx + \int_{\sqrt{3}l_x}^{x}\left|\zeta_\beta\right|^2 dx = erf\,(\sqrt{3}) - \sqrt{\frac{12}{\pi}}\,e^{-3}$$
$$+ \frac{3\sqrt{3}}{2\sqrt{\pi}}\left[e^{-3} - \exp\left(-\frac{4x}{\sqrt{3}\,l_x} + 1\right)\right] \tag{12}$$

where the subscripts α and β refers to ground state and excited level. Once more, it is enough to exchange x for y to obtain the y-rates. Both tunnelling equations exhibit a dependence on the effective widths, which will be the focus of the next section. Fig. 3 depicts these rates showing, among other things, that:

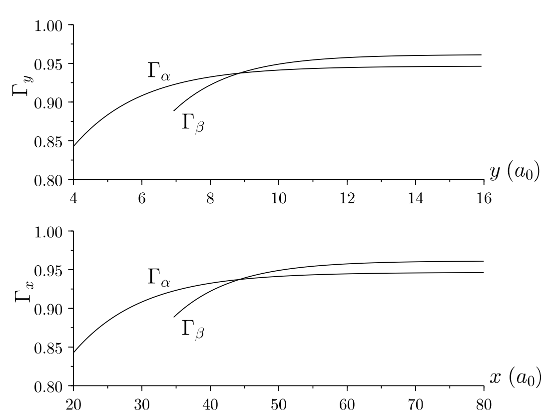

Fig. 3. Tunnelling rate as it was defined in equations (11) and (12). While Γ_α starts at l_μ, Γ_β does at $\sqrt{3}\,l_\mu$, with $\mu = x, y$. Both graphics show maximums that become constant for large widths. While Γ_y's are linked to high energies, Γ_x's are related to low energies.

1. The terms $|\phi_n|^2$ are constant so the variableness of Γ_n is essentially due to $|\zeta_n|^2$,
2. The tunnelling rates reach maximum values, which become constant for large distances, and these maximums depend neither on the effective widths nor on the direction,
3. And there exists a gap between both rates, which in a temporal analysis would be connected to the time delay between levels.