

TUNNELLING BETWEEN TWO QUANTUM DOTS: A 1D MODEL WITH TWO DELTA-WELLS

VIKTOR BEZÁK

Department of Experimental Physics, Comenius University
84248 Bratislava, Slovakia
bezak@fmph.uniba.sk

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The 1D Schrödinger equation for an electron with the potential energy defined as a pair of equal delta-wells is analyzed. If the distance between the wells exceeds a critical value, there exist two negative eigenenergies. We focused attention on the non-stationary motion when the electron alternates periodically its position in the left and right well. The delta-wells are considered as models of quantum dots (QDs) in a quantum wire embedded in a semiconductor structure. To apprehend the motion of an electron between the QDs at low temperatures (which is evidently a tunnelling phenomenon), we employ a density-matrix formalism. We derive the solution of the Liouville (von Neumann) equation in the approximation of a relaxation time. The solution suggests that the oscillatory motion of the electron between the QDs undergoes a damping. The main cause of this damping is the electron–phonon interaction. At very low temperatures, the damping, corroborating a decoherence process, can also be effected artificially when a voltage source with a noise component is employed.

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1. Introduction

Quantum dots (QDs) are prospective building blocks of nanophysical structures promising interesting applications [1]. In this paper, we will consider a structure with two QDs. Labelling these QD1 and QD2, we will discuss the transition of an electron from QD1 to QD2 and backwards. In general, this is a complex process. At low temperatures, if the distance between the QDs is not too short, this process can be described as the tunnelling of the electron between the QDs. We assume that the QDs correspond to two exactly equal quantum wells owing to which the electron may have a negative energy, provided that the potential energy of the electron outside the QDs is put equal to zero.

Tunnelling is, of course, a familiar topic in the quantum mechanics. To present its theory in the simplest way, one used to consider the one-particle Schrödinger equation in one dimension with the potential energy in the form of a barrier defined with a given width and height (*e.g.* [2]). (Consult also the monograph [3] presenting many exactly solvable tunnelling problems.)

The standard scheme of calculating the tunnelling probability harmonizes with the scattering theory. The connection with the scattering theory becomes particularly apparent when 2D or 3D tunnelling problems are considered. For instance, if a particle tunnels across a *laterally inhomogeneous* barrier, the usual 1D calculations are insufficient. A laterally inhomogeneous barrier can occur in a quantum point contact, where a barrier has a window through which the tunnelling is easier than through the rest of the barrier (*cf. e.g.* [4, 5]). Then the tunnelling is combined with diffraction. The lateral inhomogeneity of a delta-barrier $g\delta(x)$ may be defined in a stochastic manner: the amplitude g is defined as a random function $g(y)$ or $g(y, z)$ in the 2D or 3D case. The theory of the tunnelling through randomly inhomogeneous delta-barriers was published in [6–8].

When dealing with the tunnelling between two QDs, we cannot rely on the scattering-theory approach. The objective of the present paper is to show how we can cope with the problem when the tunnelling cannot be described as a process with a given incident de Broglie wave accompanied by a reflected and transited wave. To clarify the tunnelling between two QDs, we propose a 1D model with two equal delta-wells. We speak (in the 1D case) of a delta-well centered in the point x_i , if the potential energy $V(x)$ in the vicinity of x_i is approximated as $-\Omega_i\delta(x - x_i)$ with $\Omega_i > 0$.

2. The Schrödinger equation connected with the problem

We will deal with the Schrödinger equation

$$i\hbar \frac{\partial\psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2\psi(x, t)}{\partial x^2} + V(x)\psi(x, t) \quad (1)$$

with the potential energy

$$V(x) = -\Omega [\delta(x + a/2) + \delta(x - a/2)], \quad \Omega > 0. \quad (2)$$

$a > 0$ is the distance between two equal delta-wells. The stationary Schrödinger equation associated with Eq. (1) reads

$$-\left[\frac{\hbar^2}{2m}\right] \partial^2\phi_E(x)/\partial x^2 - \Omega [\delta(x + a/2) + \delta(x - a/2)] \phi_E(x) = E\phi_E(x). \quad (3)$$

All positive values of E are eigenenergies of Eq. (3). We may index them, together with the corresponding eigenfunctions, by the real wave vector k_x

$$E \equiv E_{k_x} = \frac{\hbar^2 k_x^2}{2m}, \quad \phi_E \equiv \phi_{k_x}(x). \tag{4}$$

The set of the positive eigenenergies E is not complete and one negative energy E_0 or two negative energies E_1, E_2 must be included in the spectrum of the eigenenergies. There exists a critical distance

$$a_{\text{crit}} = \frac{\hbar^2}{m\Omega} \tag{5}$$

(cf. e.g. [9]) having the following meaning: If $0 < a < a_{\text{crit}}$, we have to consider one negative eigenenergy and if $a_{\text{crit}} < a$, we have to consider two negative eigenenergies. (*Tertium non datur*: the potential energy (2) does neither allow the spectrum in which any negative eigenenergy is absent, nor the spectrum with more than two negative eigenenergies.) The situation is plotted in Fig. 1. In this plot, α is a dimensionless parameter proportional to the distance a with the proportionality factor

$$\gamma = 2m\Omega/\hbar^2, \tag{6}$$

so that $a_{\text{crit}} = 2/\gamma$. The quantity E_{00} means the negative eigenenergy of Eq. (1) in the limiting case when $a \rightarrow +0$,

$$E_{00} = -2m\Omega^2/\hbar^2. \tag{7}$$

In the present paper, we intend to deal only with the case when $a > a_{\text{crit}}$.

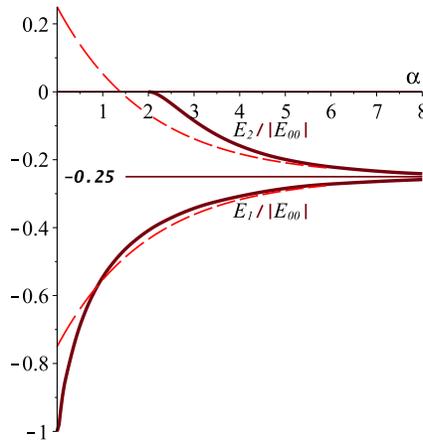


Fig. 1. The dependence of the eigenenergies E_1 and E_2 on the variable $\alpha = \gamma a$. The dashed curves are the exponentials $-1/4 \mp (1/2) \exp(-\alpha/2)$.

Figure 1 plainly suggests that asymptotically both the eigenenergies E_1 , E_2 tend to the value $-0.25|E_{00}|$ as exponential functions of the distance a .

Since Eq. (1) with potential energy (2) was treated by many authors (*cf. e.g.* the textbook [10] and the solutions manual [11]), we refrain from explaining a detailed derivation of its solutions. In Appendix A, however, we present the explicit forms of the solutions in order to make clear some symbols that are used in the main text. When writing the eigenenergies as

$$E_1(a) = -\frac{\hbar^2 \kappa_1^2}{2m}, \quad E_2(a) = -\frac{\hbar^2 \kappa_2^2}{2m}, \quad (8)$$

we can state that the two solid curves plotted in Fig. 1 correspond to the roots of the transcendental equations

$$\begin{aligned} \kappa_1/\gamma &= 0.5 [1 + \exp(-\kappa_1 a)], \\ \kappa_2/\gamma &= 0.5 [1 - \exp(-\kappa_2 a)]. \end{aligned} \quad (9)$$

Analyzing these equations, we can easily prove that

$$\begin{aligned} E_1(a) &\approx -|E_{00}| [1/4 + (1/2) \exp(-a/a_{\text{crit}})], \\ E_2(a) &\approx -|E_{00}| [1/4 - (1/2) \exp(-a/a_{\text{crit}})] \end{aligned} \quad (10)$$

for $\gamma a > 5$. Equations (1) and (3) imply that the tunnelling between the delta-wells exemplifies the quantum-mechanical coherence which expresses itself as oscillations in the tunnelling behavior. We will also deal with the question of how these oscillations can gradually become damped out when the delta-wells are incorporated in a statistical system with many degrees of freedom. This is a decoherence problem.

3. Oscillational motion of the electron between the wells

3.1. Functions $\phi_+(x)$, $\phi_-(x)$

Keeping the condition $\gamma a > 2$ in mind, we use the denotation $\phi_\mu(x)$ for the eigenfunction corresponding to E_μ , $\mu = 1, 2$. We define the functions

$$\begin{aligned} \phi_+(x) &= [\phi_1(x) + \phi_2(x)]/\sqrt{2}, \\ \phi_-(x) &= [\phi_1(x) - \phi_2(x)]/\sqrt{2}. \end{aligned} \quad (11)$$

They are mutually orthogonal, and normalized to unity

$$\begin{aligned} \int_{-\infty}^{\infty} dx \phi_+(x) \phi_-(x) &= 0, \\ \int_{-\infty}^{\infty} dx [\phi_+(x)]^2 &= \int_{-\infty}^{\infty} dx [\phi_-(x)]^2 = 1. \end{aligned} \quad (12)$$

We say that when the wave function is equal to $\phi_-(x)$, the electron is localized in the quantum well centered in the point $x_1 = -a/2$, *i.e.* in the quantum dot QD1. Similarly, the wave function $\phi_+(x)$ means the localization of the electron in the quantum dot QD2 centered in $x_2 = a/2$, see Fig. 2.

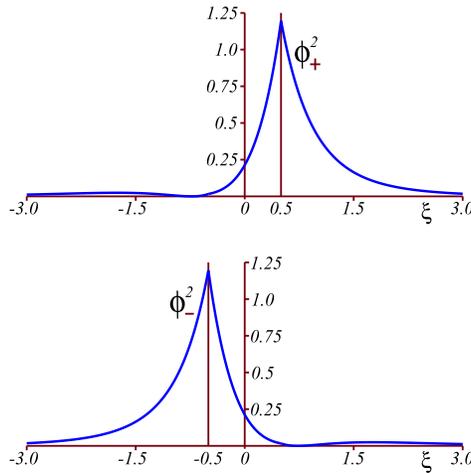


Fig. 2. The probability densities $\phi_+^2(\xi)$, $\phi_-^2(\xi)$. The variable ξ means the dimensionless position, $\xi = x/a$.

3.2. The transfer of the electron between the wells

Bearing in mind Eq. (1) and $a > a_{crit}$, we define the propagator $K(x, t; x_0)$

$$i\hbar \partial K(x, t; x_0) / \partial t = - [\hbar^2 / (2m)] \partial^2 K(x, t; x_0) / \partial x^2 - \Omega [\delta(x + a/2) + \delta(x - a/2)] K(x, t; x_0), \quad (13)$$

$$K(x, 0; x_0) = \delta(x - x_0). \quad (14)$$

Then, if $\psi_0(x)$ represents a defined initial wave function (at $t_0 = 0$), the wave function at any other time instant t is given by the integral

$$\psi(x, t) = \int_{-\infty}^{\infty} dx_0 K(x, t; x_0) \psi_0(x_0). \quad (15)$$

In our analysis, we focus attention on positive times, $t > 0$. The complete set of the eigenfunctions involves both the functions $\phi_1(x)$, $\phi_2(x)$ corresponding to the negative eigenenergies E_1 , E_2 , and an infinite number of functions

$\phi_{k_x}(x)$ corresponding to positive energies $E(k_x)$. Formally, the propagator can be written as a sum

$$K(x, t; x_0) = \sum_{\nu=1,2} \exp(-iE_\nu t/\hbar) \phi_\nu(x_0) \phi_\nu(x) + \sum_{k_x} \exp(-iE(k_x)t/\hbar) \phi_{k_x}^*(x_0) \phi_{k_x}(x). \tag{16}$$

Let the initial state $\psi_0(x)$ be $\phi_-(x) = (1/\sqrt{2})[\phi_1(x) - \phi_2(x)]$ or $\phi_+(x) = (1/\sqrt{2})[\phi_1(x) + \phi_2(x)]$. Since each function $\phi_{k_x}(x)$ is orthogonal to the functions $\phi_1(x)$, $\phi_2(x)$, and since the latter are also mutually orthogonal, we obtain the simple result

$$\psi_\pm(x, t) = \frac{1}{\sqrt{2}} [\exp(-iE_1 t/\hbar) \phi_1(x) \pm \exp(-iE_2 t/\hbar) \phi_2(x)]. \tag{17}$$

The immediate calculation of the density function

$$|\psi_\pm(x, t)|^2 = (1/2) [\phi_1^2(x) + \phi_2^2(x)] \pm 2 \cos [(E_2 - E_1)t/\hbar] \phi_1(x) \phi_2(x) \tag{18}$$

exemplifies the oscillational motion of the electron between the delta-wells with the period

$$t_{\text{per}} = \frac{2\pi\hbar}{E_2 - E_1}. \tag{19}$$

3.3. Current density in the central point between the delta-wells

For an electron with a negative energy E_{neg} , the interval between the delta-wells represents a rectangular potential-energy barrier of width a and height $|E_{\text{neg}}|$. Assuming that $a > a_{\text{crit}}$, we direct attention on the current density corresponding to $\psi_-(x, t)$ or $\psi_+(x, t)$

$$v_\pm(x, t) = \frac{i\hbar}{2m} \left[\psi_\pm(x, t) \frac{\partial \psi_\pm^*(x, t)}{\partial x} - \psi_\pm^*(x, t) \frac{\partial \psi_\pm(x, t)}{\partial x} \right] = \frac{\hbar}{m} \text{Im} \left[\psi_\pm^*(x, t) \frac{\partial \psi_\pm(x, t)}{\partial x} \right], \quad t > 0. \tag{20}$$

The functions $\psi_-(x, t)$, $\psi_+(x, t)$ are complex

$$\psi_\pm(x, t) = \left(1/\sqrt{2}\right) [\exp(-iE_1(a)t/\hbar) \phi_1(x) \pm \exp(-iE_2(a)t/\hbar) \phi_2(x)].$$

Thus we arrive at the current densities

$$v_-(x, t) = \frac{\hbar}{m} \left[\phi_1(x) \frac{\partial \phi_2(x)}{\partial x} - \phi_2(x) \frac{\partial \phi_1(x)}{\partial x} \right] \sin \left(\frac{[E_2(a) - E_1(a)]t}{\hbar} \right),$$

$$v_+(x, t) = -v_-(x, t). \tag{21}$$

Choosing $x = 0$ (the central point of the barrier between the QDs), we obtain the functions

$$\psi_-(0, t) = \frac{N_1}{\sqrt{2}} \frac{\exp(-iE_1(a)t/\hbar)}{\cosh(\kappa_1 a/2)},$$

$$\left. \frac{\partial \psi_-(x, t)}{\partial x} \right|_{x=0} = -\frac{N_2 \kappa_2}{\sqrt{2}} \frac{\exp(-iE_2(a)t/\hbar)}{\sinh(\kappa_2 a/2)},$$

where N_1, N_2 are normalizing constants. Hence,

$$v_-(0, t) = A(a) \sin\left(\frac{[E_2(a) - E_1(a)]t}{\hbar}\right), \quad (22)$$

where

$$A(a) = \frac{\hbar}{m} \frac{N_1 N_2 \kappa_2}{\cosh(\kappa_1 a/2) \sinh(\kappa_2 a/2)}. \quad (23)$$

If the time is very short in comparison with t_{per} , $|v_-(0, t)|/t$ or $|v_-(0, t)|/t$ is the tunnelling probability (per second) in the usual sense

$$P_{\text{tunnel}}(a) \approx A(a) [E_2(a) - E_1(a)]/\hbar, \quad t \ll \hbar/[E_2(a) - E_1(a)]. \quad (24)$$

In expression (23), the parameters N_μ and κ_μ are complicated functions of the distance a between the delta-wells (*cf.* Appendix A). However, if a is sufficiently large, then $\kappa_\mu \rightarrow \kappa_0$ (the value for a single delta-well) and the dependence of $N_1 N_2 \kappa_2$ on a is weak. In such a case, the dependence of the amplitude A (and the tunnelling probability P_{tunnel}) on the distance a is mainly determined by the denominator of expression (23), and so it becomes exponential, $A(a) \sim \exp(-\kappa_0 a)$, as it could be expected.

4. Interaction of the pulsating electron with environment: a formal theory of decoherence

The solution presented in the previous section has shown which consequences would follow if the electron might be considered as an isolated particle. This assumption is unrealistic if the delta-wells are to correspond to QDs. The QDs are embedded in a vibrating crystalline lattice which contains randomly distributed defects. Thus, the electron moves in a fluctuating environment. This environment is a system with a huge number of degrees of freedom, and we may legitimately define its temperature. Since this is a statistical concept, we ought to turn away from the one-electron Schrödinger equation used in the previous section. Instead, to describe plausibly the dynamics of the electron, a density-matrix theory should be applied.

We define the environment as a space $\mathcal{S}_{\mathcal{D}}$ spanned by position vectors Q . A typical crystal includes roughly 10^{20} atoms in the cubic millimeter, so the dimensionality of $\mathcal{S}_{\mathcal{D}}$ is of this order of magnitude. Then we define also the space $\mathcal{S}_{\mathcal{D}+1}$ as the set of the position vectors (x, Q) . Let $\Psi(x, Q, t)$ be the wave function defined (in the coordinate representation) in the space $\mathcal{S}_{\mathcal{D}+1}$ and let a fictitious Observer be capable to watch repeatedly over this wave function. We may enumerate the observations denoting the wave function corresponding to the j^{th} observation as $\Psi^{(j)}(x, Q)$. Because the environment fluctuates, the functions $\Psi^{(j)}(x, Q)$ differ from one another, even if they all are defined with the same initial condition $\Psi^{(j)}(x, Q, 0) = \Psi_0(x, Q)$. To construct the density matrix ρ of the electron, we have to define effective one-electron wave functions. So we write

$$\psi^{(j)}(x, t) = \int d^{\mathcal{D}}Q \Psi^{(j)}(x, Q, t), \quad \int dx |\psi^{(j)}(x, t)|^2 = 1. \quad (25)$$

Denoting the number of observations as N_{O} , we may define the density matrix of the electron as

$$\rho(x, x_0, t) = \frac{1}{N_{\text{O}}} \sum_{j=1}^{N_{\text{O}}} \psi^{(j)}(x, t) \psi^{(j)*}(x_0, t), \quad N_{\text{O}} \rightarrow \infty. \quad (26)$$

We presume that the electron wave functions are linear combinations of the basis functions $\phi_1(x)$, $\phi_2(x)$. For $a > a_{\text{crit}}$, we deem it useful to introduce the functions

$$\begin{aligned} \Phi_{11}(x_0, x) &= \phi_1(x_0)\phi_1(x), \\ \Phi_{12}(x_0, x) &= \phi_1(x_0)\phi_2(x), \\ \Phi_{21}(x_0, x) &= \phi_2(x_0)\phi_1(x), \\ \Phi_{22}(x_0, x) &= \phi_2(x_0)\phi_2(x). \end{aligned} \quad (27)$$

These four functions can be comprehended as mutually orthogonal unit vectors

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dx_0 \Phi_{\mu_1\nu_1}(x_0, x) \Phi_{\mu_2\nu_2}(x_0, x) = \delta_{\mu_1\mu_2} \delta_{\nu_1\nu_2}. \quad (28)$$

With this notation,

$$\begin{aligned} \rho(x, x_0, t) &= (1/N_{\text{O}}) \sum_{j=1}^{N_{\text{O}}} \left[C_{11}^{(j)}(t) \Phi_{11}(x_0, x) + C_{12}^{(j)}(t) \Phi_{12}(x_0, x) \right. \\ &\quad \left. + C_{21}^{(j)}(t) \Phi_{21}(x_0, x) + C_{22}^{(j)}(t) \Phi_{22}(x_0, x) \right]. \end{aligned}$$

Thus, using the average values $C_{\mu\nu}(t) = \sum_j C_{\mu\nu}^{(j)}(t)/N_O$, we may use the formula

$$\begin{aligned} \rho(x, x_0, t) = & C_{11}(t)\Phi_{11}(x_0, x) + C_{12}(t)\Phi_{12}(x_0, x) \\ & + C_{21}(t)\Phi_{21}(x_0, x) + C_{22}(t)\Phi_{22}(x_0, x). \end{aligned} \tag{29}$$

Actually, the problem of determining the density matrix is reduced to the calculation of the complex-valued matrix

$$\mathbf{C}(t) = \begin{pmatrix} C_{11}(t), & C_{12}(t) \\ C_{21}(t), & C_{22}(t) \end{pmatrix}. \tag{30}$$

Employing the matrix formalism, we observe that

$$\rho(x, x_0, t) = (\phi_1(x_0), \phi_2(x_0)) \mathbf{C}(t) \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix}. \tag{31}$$

For physical reasons, we take the density matrix as a sum of the equilibrium part and time-dependent part

$$\rho(x, x_0, t) = \rho_{\text{eq}}(x, x_0) + \rho_1(x, x_0, t). \tag{32}$$

The time-independent part $\rho_{\text{eq}}(x, x_0)$, which is the density matrix at the thermodynamic equilibrium, is known *a priori*

$$\begin{aligned} \rho_{\text{eq}}(x, x_0) = & \exp(\beta E_F) [\exp(-\beta E_1(a))\Phi_{11}(x_0, x) \\ & + \exp(-\beta E_2(a))\Phi_{22}(x_0, x)], \quad \beta = 1/(k_B T). \end{aligned} \tag{33}$$

Here, E_F is the Fermi energy and $E_1(a)$, $E_2(a)$ are the negative energies shown in Fig. 1, $E_1(a) < E_2(a)$ for $a > a_{\text{crit}}$. We assume that

$$E_F < E_1, \quad k_B T \ll |E_1 - E_F|, \tag{34}$$

so that the Fermi–Dirac function $f_0(E)$ may be replaced by $\exp[\beta(E_F - E)]$. Condition (34) justifies the omission of terms related to positive electron energies in the equilibrium density matrix $\rho_{\text{eq}}(x, x_0)$.

4.1. The Liouville equation

4.1.1. The relaxation problem

In this subsection, we consider the situation when no *external* field is present. In this case, we denote the density matrix as $\rho_0(x, x_0, t)$. This two-point function is the solution of a kinetic equation, the Liouville equation. (It used also to be called the von Neumann equation.) We assume that the

interaction of the electron with its environment has a braking effect which we may formally grasp by inserting a term with a relaxation time in the Liouville equation (*cf. e.g.* [12]). We write the Liouville equation in the form of

$$\begin{aligned} \partial\rho_0(x, x_0, t)/\partial t + \rho_1(x, x_0, t)/\tau &= \Lambda(x, x_0)\rho_0(x, x_0, t), \\ \rho_1(x, x_0, t) &= \rho_0(x, x_0, t) - \rho_{\text{eq}}(x, x_0). \end{aligned} \quad (35)$$

We reckon the relaxation time $\tau > 0$ to be a formal positive parameter. The r.h.s. of Eq. (35) involves the operator

$$\begin{aligned} \Lambda(x, x_0) &= -(i/\hbar) [H(x) - H(x_0)] \\ &= [i\hbar/(2m)] (\partial^2/\partial x^2 - \partial^2/\partial x_0^2) - (i/\hbar)[V(x) - V(x_0)]. \end{aligned} \quad (36)$$

Mathematically speaking, Eq. (35) is non-homogeneous

$$\partial\rho_0(x, x_0, t)/\partial t + \rho_0(x, x_0, t)/\tau - \Lambda(x, x_0)\rho_0(x, x_0, t) = \rho_{\text{eq}}(x, x_0)/\tau. \quad (37)$$

After defining the initial wave function of the electron as the linear combination

$$\psi_0(x) = c_1(0)\phi_1(x) + c_2(0)\phi_2(x) \quad (38)$$

with two real coefficients $c_1(0)$, $c_2(0)$, we can consider the initial density matrix

$$\begin{aligned} \rho_0(x, x_0, 0) &= C_{11}(0)\Phi_{11}(x, x_0) + C_{12}(0)\Phi_{12}(x, x_0) \\ &\quad + C_{21}(0)\Phi_{21}(x, x_0) + C_{22}(0)\Phi_{22}(x, x_0). \end{aligned} \quad (39)$$

Obviously,

$$C_{11}(0) = [c_1(0)]^2, \quad C_{22}(0) = [c_2(0)]^2, \quad C_{12}(0) = C_{21}(0) = c_1(0)c_2(0). \quad (40)$$

We can directly derive the function

$$\begin{aligned} \Lambda(x, x_0)\rho(x, x_0, t) &= -(i/\hbar)[E_2(a) - E_1(a)] \\ &\quad \times [C_{12}(t)\Phi_{12}(x_0, x) - C_{21}(t)\Phi_{21}(x_0, x)]. \end{aligned} \quad (41)$$

Let us write down the left-hand side of Eq. (37)

$$\begin{aligned} M^L &= [\partial/\partial t + 1/\tau - \Lambda(x, x_0)] \rho(x, x_0, t) = \{d/dt + 1/\tau\}C_{11}(t)\Phi_{11}(x_0, x) \\ &\quad + \{d/dt + 1/\tau + (i/\hbar)[E_2(a) - E_1(a)]\}C_{12}(t)\Phi_{12}(x_0, x) \\ &\quad + \{d/dt + 1/\tau - (i/\hbar)[E_2(a) - E_1(a)]\}C_{21}(t)\Phi_{21}(x_0, x) \\ &\quad + \{d/dt + 1/\tau\}C_{22}(t)\Phi_{22}(x_0, x). \end{aligned}$$

The right-hand side of Eq. (37) is $M^R = \rho_{\text{eq}}(x, x_0)/\tau$, with the equilibrium function given by Eq. (32). The equality $M^L = M^R$ is tantamount to two homogeneous and two non-homogeneous differential equations

$$\begin{aligned} \{d/dt + 1/\tau + (i/\hbar)[E_2(a) - E_1(a)]\}C_{12}(t) &= 0, \\ \{d/dt + 1/\tau - (i/\hbar)[E_2(a) - E_1(a)]\}C_{21}(t) &= 0. \\ (d/dt + 1/\tau)C_{11}(t) &= \exp[\beta(E_F - E_1(a))]/\tau, \\ (d/dt + 1/\tau)C_{22}(t) &= \exp[\beta(E_F - E_2(a))]/\tau. \end{aligned}$$

These equations can be solved readily

$$C_{12}(t) = c_1(0)c_2(0) \exp\{- (1/\tau - (i/\hbar)[E_2(a) - E_1(a)])t\}, \quad C_{21}(t) = C_{12}^*(t).$$

$$C_{\mu\mu}(t) = \exp\{\beta[E_F - E_\mu(a)]\} + [|c_\mu(0)|^2 - \exp\{\beta[E_F - E_\mu(a)]\}] \exp(-t/\tau),$$

$\mu = 1, 2.$

After inserting these functions in formula (29), we arrive at the complete solution of the Liouville equation

$$\begin{aligned} \rho_0(x, x_0, t) &= \rho_{\text{eq}}(x, x_0) + \{[c_1(0)]^2 - \exp\{\beta[E_F - E_1(a)]\}\}\phi_1(x_0)\phi_1(x) \\ &\quad + \{[c_2(0)]^2 - \exp\{\beta[E_F - E_2(a)]\}\}\phi_2(x_0)\phi_2(x)e^{-t/\tau} \\ &\quad + c_1(0)c_2(0)[\exp\{i[E_2(a) - E_1(a)]t/\hbar\}\phi_1(x_0)\phi_2(x) \\ &\quad + \exp\{-i[E_2(a) - E_1(a)]t/\hbar\}\phi_2(x_0)\phi_1(x)]e^{-t/\tau}. \end{aligned} \quad (42)$$

Clearly, $\rho_0(x, x_0, t)$ tends to the equilibrium density matrix $\rho_{\text{eq}}(x, x_0)$ if $t \rightarrow \infty$. The exponential function $e^{-t/\tau}$ suggests that $1/\tau$ is the rate with which the electron becomes thermalized in its environment. Synonymously, $1/\tau$ may be interpreted as the rate with which the motion of the electron undergoes the decoherence process.

4.1.2. Damped pulsations

The local density in the point x and at the time instant $t > 0$, corresponding to the alternating presence of the electron in the states with energies $E_1(a)$ and $E_2(a)$, is given by the diagonal element of the density matrix

$$\begin{aligned} \rho_0(x, x, t) &= \rho_{\text{eq}}(x, x) + \left(\{[c_1(0)]^2 - \exp\{\beta[E_F - E_1(a)]\}\}[\phi_1(x)]^2 \right. \\ &\quad \left. + \{[c_2(0)]^2 - \exp\{\beta[E_F - E_2(a)]\}\}[\phi_2(x)]^2 \right) e^{-t/\tau} \\ &\quad + 2c_1(0)c_2(0) \cos\{[E_2(a) - E_1(a)]t/\hbar\}\phi_1(x)\phi_2(x)e^{-t/\tau}. \end{aligned} \quad (43)$$

It is instructive to compare expression (43) with expression (18). We take $c_1(0) = 1/\sqrt{2}$, $c_2(0) = -1/\sqrt{2}$. If $\tau \rightarrow \infty$ and if $\beta \rightarrow +0$, we observe that $\rho_{\text{eq}}(x, x_0) \rightarrow [\phi_1(x)]^2 + [\phi_2(x)]^2$ and $\rho_0(x, x, t) \rightarrow |\psi(x, t)|^2$. Thus, expression (43) goes over exactly into expression (18).

The current density can be expressed as

$$v_-(x, t) = \frac{\hbar}{m} \text{Im} \frac{\partial \rho_0(x, x_0, t)}{\partial x} \Big|_{x_0=x}. \quad (44)$$

For $x = 0$, we obtain the expression

$$v_-(0, t) = A(a) \sin \{ [E_2(a) - E_1(a)]t/\hbar \} e^{-t/\tau} \quad (45)$$

with the amplitude $A(a)$ given by Eq. (23).

5. Influence of noise upon the pulsational behavior: theory with a fluctuating potential-energy

5.1. Abstract formulation based on the Schrödinger equation

Let us take

$$H_0(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (46)$$

in the role of the “unperturbed” Hamiltonian, with the potential energy $V(x)$ defined by Eq. (2). Correspondingly, $\psi_0(x, t)$ is the solution of the equation

$$i\hbar \frac{\partial \psi_0(x, t)}{\partial t} = H_0(x) \psi_0(x, t). \quad (47)$$

Now, our objective is to discuss what happens when a noise term is added to Hamiltonian (46). For the sake of simplicity, we define the noise term as an x -independent fluctuation of the potential energy. This means that we add a term $\mathcal{E}(t)$ to $H_0(x)$, positing that it represents a stationary stochastic process. So, we accept the Schrödinger equation

$$i\hbar \frac{\partial \tilde{\psi}(x, t)}{\partial t} = H(x, t) \tilde{\psi}(x, t) \quad (48)$$

with the Hamiltonian

$$H(x, t) = H_0(x) + \mathcal{E}(t), \quad (49)$$

supposing that $\mathcal{E}(t)$ derives from an external source. (Later on, in Sec. 7, we will reinterpret somehow the meaning of $\mathcal{E}(t)$.)

Clearly,

$$\tilde{\psi}(x, t) = \exp\left(-\frac{i}{\hbar} \int_0^t dt' \mathcal{E}(t')\right) \psi_0(x, t). \tag{50}$$

This result motivates us to introduce a new time variable \tilde{t} for a while. We require the fulfilment of the following relationship:

$$\partial/\partial\tilde{t} \dots = \exp\left(-\frac{i}{\hbar} \int_0^t dt' \mathcal{E}(t')\right) \partial/\partial t \left[\exp\left(\frac{i}{\hbar} \int_0^t dt'' \mathcal{E}(t'')\right) \dots \right]. \tag{51}$$

The direct use of this definition enables us to state that Eq. (48) is tantamount to the equation

$$i\hbar \frac{\partial \tilde{\psi}(x, t)}{\partial \tilde{t}} = H_0(x) \tilde{\psi}(x, t). \tag{52}$$

Being cognizant of the fact that $i\hbar\partial/\partial t$ is the energy operator in the Schrödinger picture, we may state that $i\hbar\partial/\partial\tilde{t}$ has also the meaning of the energy operator, although in another picture. We may speak of a picture that is complementary to what used to be called the interaction (Dirac) picture in the quantum field theory.

5.2. Formulation adapted for the context with QDs

As long as we attribute an *external* origin to the random function $\mathcal{E}(t)$, we have to say that the presence of the relaxation time τ in the Liouville equation is due to *internal* stochastic processes, such as the electron–phonon scattering. To emphasize the internal nature of the relaxation time, let us write the relaxation time as τ_{in} . So, when the delta-wells stand for the QDs in the structure presented schematically in Fig. 4, we write the Liouville equation as

$$i\hbar [\partial\rho(x, x_0, t)/\partial\tilde{t} + \rho_1(x, x_0, t)/\tau_{\text{in}}] = [H_0(x) - H(x_0)]\rho(x, x_0, t). \tag{53}$$

In the Schrödinger picture, Eq. (53) reads

$$\partial\rho(x, x_0, t)/\partial t + \rho_1(x, x_0, t)/\tau_{\text{in}} = -(i/\hbar)\mathcal{E}(t)\rho(x, x_0, t) + \Lambda(x, x_0)\rho(x, x_0, t), \tag{54}$$

or

$$\begin{aligned} &\partial\rho(x, x_0, t)/\partial t + \rho(x, x_0, t)/\tau_{\text{in}} + [(i/\hbar)\mathcal{E}(t) - \Lambda(x, x_0)]\rho(x, x_0, t) \\ &= \rho_{\text{eq}}(x, x_0)/\tau_{\text{in}}. \end{aligned} \tag{55}$$

Here, $\Lambda(x, x_0)$ is the time-independent function given by Eq. (36). In the previous section, we have prescribed the initial function $\rho_0(x, x_0)$ in the case when $\mathcal{E}(t) \equiv 0$. Now, we consider the same initial function even for the density matrix $\rho(x, x_0, t)$, *i.e.* $\rho_0(x, x_0) = \rho(x, x_0)$. The direct comparison of Eq. (55) with Eq. (37) gives us the equality

$$\rho(x, x_0, t) = P(t)\rho_0(x, x_0, t) \quad (56)$$

with the prefactor

$$P(t) = \exp \left(-\frac{i}{\hbar} \int_0^t dt' \mathcal{E}(t') \right). \quad (57)$$

6. The density matrix $\rho(x, x_0, t)$ as a stochastic function

6.1. General setting

In the previous section, we have defined $\mathcal{E}(t)$ as a stationary stochastic process. Since the function $\rho_0(x, x_0, t)$ is deterministic (we have calculated it in Sec. 4), the stochastic behavior of the density matrix $\rho(x, x_0, t)$ is fully determined by the function $P(t)$.

From now on, the angular brackets $\langle \rangle$ will signify the averaging with respect to $\mathcal{E}(t)$. We define the autocorrelation function $W_{\mathcal{E}}$ of the stochastic process $\mathcal{E}(t)$ as an even function of $\Delta_t = t_2 - t_1$

$$W_{\mathcal{E}}(\Delta_t) = W_{\mathcal{E}}(-\Delta_t) = \langle [\mathcal{E}(t_1) - \bar{\mathcal{E}}] [\mathcal{E}(t_2) - \bar{\mathcal{E}}] \rangle. \quad (58)$$

The zero value of Δ_t defines the variance of \mathcal{E}

$$\sigma_{\mathcal{E}}^2 = W_{\mathcal{E}}(0) = \langle [\mathcal{E}(t) - \bar{\mathcal{E}}]^2 \rangle. \quad (59)$$

The stationarity of $\mathcal{E}(t)$ means that $\bar{\mathcal{E}}$ and $\sigma_{\mathcal{E}}^2$ are time-independent parameters. We require that $W_{\mathcal{E}}(\infty) = 0$. There are several scenarios underlying a plausible use of the random function $\mathcal{E}(t)$. Our choice is a Gaussian model that we define as memoryless. The memorylessness means that $\mathcal{E}(t)$ is a Markovian process.

6.2. Noise as a Gaussian memoryless stochastic process

Obviously, $P(t)$, being a functional of $\mathcal{E}(\tau)$, is a random function of the time variable $t > 0$. We write

$$P(t) = \exp[-i\bar{\mathcal{E}}t/\hbar] X(t),$$

$$\langle P(t) \rangle = \exp \left[-i\bar{\mathcal{E}}t/\hbar \right] \langle X(t) \rangle, \tag{60}$$

$$X(t) = \exp \left[- (i/\hbar) \int_0^t d\tau \left[\mathcal{E}(\tau) - \bar{\mathcal{E}} \right] \right]. \tag{61}$$

We can prove (see, *e.g.*, [13]) that

$$\langle X(t) \rangle = \exp \left[- \frac{1}{2\hbar^2} \int_0^t \int_0^t d\tau_1 d\tau_2 W_{\mathcal{E}}(|\tau_1 - \tau_2|) \right]. \tag{62}$$

Since the Gaussian process $\mathcal{E}(t)$ is Markovian, we have to respect Doob’s theorem [14] according to which the autocorrelation function has the form of

$$W_{\mathcal{E}}(|\tau_1 - \tau_2|) = \sigma_{\mathcal{E}}^2 \exp(-\Gamma|\tau_1 - \tau_2|). \tag{63}$$

The inverse value of the quantity $\Gamma > 0$ may be interpreted as a correlation time. The symbol $\sigma_{\mathcal{E}}^2 = W(0)$ denotes the variance of $\mathcal{E}(\tau)$. The calculation of the double integral in Eq. (62) can easily be carried out. We prefer to use the dimensionless variable $u = \Gamma t$ and write

$$F(u) \equiv \langle X(t) \rangle. \tag{64}$$

We define the constant

$$D = \sigma_{\mathcal{E}}^2 / (\hbar^2 \Gamma^2). \tag{65}$$

Then function (64) can be written as

$$F(u) = \exp[-Df(u)], \tag{66}$$

with

$$f(u) = u + \exp(-u) - 1. \tag{67}$$

The function $f(u)$ is plotted in the part (a) of Fig. 3. The asymptote of $f(u)$ is the straight line $f_{\text{as}}(u) = u - 1$. The part (b) of Fig. 3 shows the function $F(u)$ for some values of the parameter D .

Using formula (56), we obtain promptly the averaged density matrix

$$\langle \rho(x, x_0, t) \rangle = \langle P(t) \rangle \rho_0(x, x_0, t). \tag{68}$$

Since the function $\langle P(t) \rangle$ is real, we can directly subject formula (44) to the averaging with respect to $\mathcal{E}(t)$

$$\langle v_{-}(x, t) \rangle = \frac{\hbar}{m} \langle P(t) \rangle \text{Im} \left. \frac{\partial \rho_0(x, x_0, t)}{\partial x} \right|_{x_0=x}. \tag{69}$$

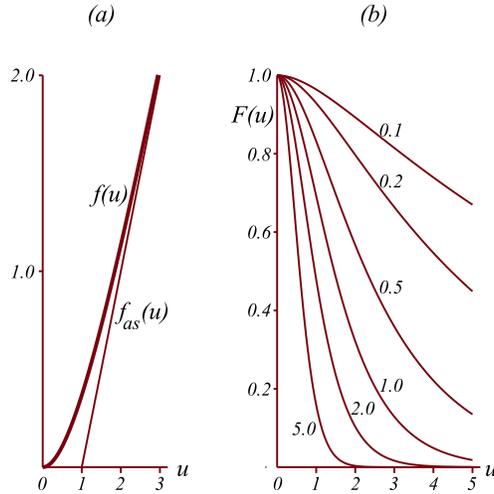


Fig. 3. Function $F(u)$ ($u = \Gamma t$) for some values of the parameter $D = \sigma_{\mathcal{E}}^2 \tau_{\text{cor}}^2 / \hbar^2$. (Numerals at the curves denote the values of D .)

Then the averaged current density in the point $x = 0$ reads

$$\begin{aligned} \langle v_-(0, t) \rangle &= A(a) \sin \{ [E_2(a) - E_1(a)] t / \hbar \} \exp[-Df(\Gamma t)] e^{-t/\tau}, \\ c_1(0) &= -c_2(0) = 1/\sqrt{2} \end{aligned} \quad (70)$$

with the constants D and $A(a)$ defined above. We deem it adequate to formally redefine amplitude

$$\tilde{A}(a, t) = A(a) \exp \left\{ \frac{\sigma_{\mathcal{E}}^2}{\hbar^2 \Gamma^2} [1 - \exp(-\Gamma t)] \right\}. \quad (71)$$

Then expression (70) attains the more convenient form

$$\langle v_-(0, t) \rangle = \tilde{A}(a, t) \sin \{ [E_2(a) - E_1(a)] t / \hbar \} e^{-t/\tau}. \quad (72)$$

Here, τ means the total relaxation time defined by the equation

$$\frac{1}{\tau} = \frac{1}{\tau_{\text{ex}}} + \frac{1}{\tau_{\text{in}}}, \quad \tau_{\text{ex}} = \frac{\hbar^2 \Gamma}{\sigma_{\mathcal{E}}^2}. \quad (73)$$

For $t \gg 1/\Gamma$, the prefactor $\tilde{A}(a, t)$ is practically constant and the damping of the oscillational transfer of the electron between the wells is essentially given by the exponential function in formula (72).

7. Discussion

7.1. A realistic model related to the problem with two delta-wells

The potential energy with two equal delta-wells can be emulated in a quantum wire which we can imagine as a very thin parallelepiped embedded in a dielectric environment. To imitate the quantum wells, we consider the quantum wire as a heterogeneous block presented schematically as ABABA, where A, B are two lattice-matched direct-gap semiconductors, such as AlGaAs and GaAs, encapsulated in a sapphire matrix. Sapphire (Al_2O_3) is a particularly convenient substrate for the epitaxial deposition of single-crystalline GaAs (and lattice-matched AlGaAs) patterns (*cf. e.g.* [15, 16]). In the flat-band approximation, the profile of the ABABA structure in the wire direction (x -direction) is shown in Fig. 4. Accepting the effective-mass theory, we may interpret the function $E_c(x)$ (the thick black piecewise segmented line in Fig. 4) as the potential energy for a conduction electron. The two wells in Fig. 4, corresponding to the semiconductor B, represent two equal quantum dots. Similarly, the function $E_v(x)$ (the thick grey piecewise segmented line in Fig. 4) corresponds to the potential energy of holes. The energy scale for holes is defined oppositely to the energy scale for electrons. This means that the energy of a hole grows downwards. So we can imagine a hole located in a well whose width is equal to $a - d_{\text{dot}}$, and the QDs, flanking this well, as barriers for the hole.

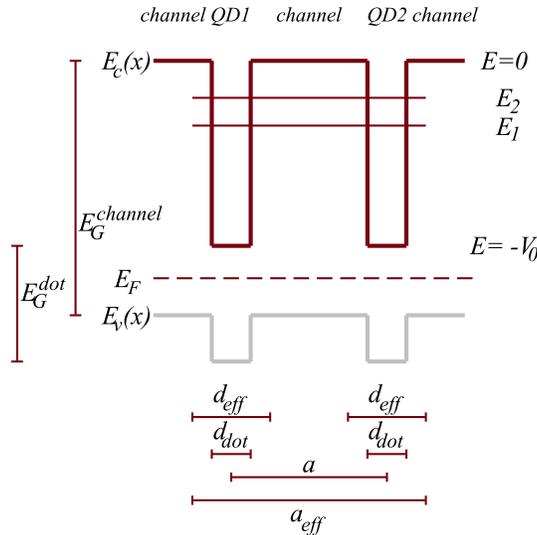


Fig. 4. Scheme of two deep wells inside a semiconductor structure.

Let us suppose that the temperature is sufficiently low, such that $k_B T \ll |E_2|$. Then we may neglect the presence of conduction electrons in the quantum wire under consideration. If the quantum wire hosts one *excess* electron, then, according to Appendix B, we may use the Schrödinger-type equation for this electron

$$\hat{H}_{\text{eff}}(x)\phi_\mu(x) = E_\mu\phi_\mu(x), \quad \mu = 1, 2, \quad (74)$$

$$\hat{H}_{\text{eff}}(x) = -[(\hbar^2/(2m_A)]d^2/dx^2 - (m_A/m_B)^{1/2}V_0d_{\text{dot}}[\delta(x+a/2) + \delta(x-a/2)]. \quad (75)$$

$\phi_1(x)$, $\phi_2(x)$ are the envelope wave functions corresponding, respectively, to the negative eigenenergies E_1 , E_2 of Hamiltonian (75), and m_A (m_B) is the electron effective mass defined for the semiconductor A (B). With

$$\Omega = \left(\frac{m_A}{m_B}\right)^{1/2} V_0 d_{\text{dot}}, \quad (76)$$

Eq. (74) is identical with Eq. (3) which was the starting point for the computations presented in this paper. If

$$0 < m_A a \Omega / \hbar^2 < 1, \quad (77)$$

i.e. if the distance a between the delta-wells is shorter than

$$a_{\text{crit}} = \frac{\hbar^2}{m_A \Omega}, \quad (78)$$

it is irrelevant to speak of the tunnelling between the QDs. On the other hand, if the distance a is sufficiently longer than a_{crit} , the wells are distinguishably separated. We postulate the possibility to use the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H}_{\text{eff}}(x)\psi(x, t) \quad (79)$$

for the envelope function $\psi(x, t)$. Let us define the initial wave function $\psi_0(x) = [\phi_1(x) - \phi_2(x)]/\sqrt{2}$. This choice means, as we have shown in Sec. 3.1, that we consider the initial insertion (at $t_0 = 0$) of the excess electron in the QD1. The wave function $[\phi_1(x) - \phi_2(x)]/\sqrt{2}$ is not stable and the electron begins swinging between two locations (QD1 and QD2). This swinging is a pure tunnelling process since there is no participation of electrons with positive energies.

7.2. Estimates of the critical distance a_{crit} and of the pulsation period t_{per}

The effective mass of the conduction electrons in the Γ -point of the Brillouin zone is $0.067m_0$ for GaAs and $0.15m_0$ for AlAs [18]. For the ternary alloy $\text{Al}_\xi\text{Ga}_{1-\xi}\text{As}$ with the fraction $\xi = 0.4$ of Al, the linear interpolation gives the effective mass equal to $0.1m_0$. So we choose $m_A = 0.1m_0$ and $m_B = 0.067m_0$. Then $(m_A/m_B)^{1/2} = 1.2217$. The width d_{dot} of the QD should not be less than 1.5 nm. Indeed, let us assume that the plane $\{111\}$ is perpendicular to the x -direction. Then the interval $(0, d_{\text{dot}})$ contains about five $\{111\}$ planes and this may be enough for the concept of the effective mass m_B . When $d_{\text{dot}} = 1.5$ nm and $V_0 = 0.1$ eV, formula (76) gives us the value $\Omega = 2.936 \times 10^{-29}$ Jm. The calculation of the eigenenergy E_0 becomes simple (*cf.* inequality (B.12) in Appendix B) if the quantity $\zeta = [2m_B V_0]^{1/2} d_{\text{dot}} / (2\hbar)$ is small, allowing the replacement of $\tan \zeta$ by ζ . With $m_B = 0.67m_A$, $V_0 = 0.1$ eV, we have got $\zeta \approx 0.3145$ and $\tan \zeta \approx 0.3253$. Thus, we can state that with the accuracy of about five percent the calculations of the eigenenergies E_1 and E_2 for the potential energy with rectangular wells as in Fig. 4 give the same values as the calculations in the delta-well model. With the values of the parameters used in this discussion, we obtain $|E_{00}| = 0.088$ eV and the critical distance $a_{\text{crit}} = 4.16$ nm. For $a \approx a_{\text{crit}}$, we estimate that t_{per} is roughly equal to 2×10^{-12} s. So, if the distance a is shorter than 20 nm, the swinging of the electron between the two QDs should be measured on a picosecond (or even finer) scale.

7.3. Decoherence length ℓ_{decoh} and domination of the electron-phonon scattering for $a \gg \ell_{\text{decoh}}$

Intuitively, we take it for granted that the tunnelling between two QDs is negligible if the distance a between them is much higher than a_{crit} . In this case, the difference $E_2 - E_1$ is small and we may use the equation

$$E_2 - E_1 \approx |E_{00}| \exp(-a/a_{\text{crit}}) \quad (80)$$

(*cf.* formulae (10)). If $k_B T \gg E_2 - E_1$, we expect that the tunnelling between the QDs should be to a great extent suppressed. We define the *decoherence length* ℓ_{decoh} by the equation

$$k_B T = |E_{00}| \exp(-\ell_{\text{decoh}}/a_{\text{crit}}). \quad (81)$$

With $T = 30$ K, we have got $k_B T = 2.6 \times 10^{-3}$ eV; then with values of $|E_{00}|$ and a_{crit} given in the previous subsection, we obtain the decoherence length $\ell_{\text{decoh}} \approx 15$ nm.

Let us choose $a = 40$ nm. Then Eq. (80) gives the energy difference $E_2 - E_1 \sim 6 \times 10^{-6}$ eV. Correspondingly, the period of the oscillations (if there were no damping effect) would be $t_{\text{per}} = 2\pi\hbar/(E_2 - E_1) \sim 7 \times 10^{-10}$ s.

Let us now discuss the situation when only the intrinsic field $\mathcal{E}_{\text{in}}(t)$, due to thermodynamic fluctuations, is present. Recalling formulae (43), (44), we have still to estimate the value of τ in the damping factor $\exp(-t/\tau)$. In the volume with the diameter about 40 nm, involving a single pair of the QDs, the number of defects is small. Despite the irregularity of positions of these defects, they must be considered as a *deterministic* perturbation to the motion of the electron between the QDs. (The stochasticity in the probabilistic sense would be relevant, if we were not considering a single pair, but a statistical ensemble of a huge amount of the QDs defined with the same distance a between them.) Nevertheless, we can put forward an argument that if $a \gg a_{\text{crit}}$, then τ is essentially related to the interaction of the electron with phonons and this is a stochastic process running in time. We denote the relaxation time τ in this case as τ_{eph} . Experiments with ultrapure crystals of GaAs [17] proved that $\tau_{\text{eph}} \sim 3 \times 10^{-11}$ s. (We suppose that a value not much differing from this holds also for AlGaAs.) Then we obtain the factor $\exp(-t_{\text{per}}/\tau_{\text{eph}}) \sim \exp(-70/3) \sim 10^{-10}$. Thus, if $a > 40$ nm, the tunnelling between the QDs is negligible. This, of course, means that an electron injected into one of the two QDs under consideration can dwell in this QD for a time that is many orders of magnitude longer than the ideal tunnelling period t_{per} .

7.4. *The scattering of the electron with phonons approximated as a Gaussian random process*

When the electron undergoes the scattering with phonons, we may say that this process is stochastic and, moreover, that it is Markovian, since there are no obvious reasons to expect memory effects as a result of the electron–phonon interaction. Therefore, respecting Eq. (73), we propose to employ the formulae

$$\tau_{\text{ex}} = \frac{\hbar^2 \Gamma_{\text{ex}}}{\sigma_{\mathcal{E}_{\text{ex}}}^2}, \quad \tau_{\text{in}} = \frac{\hbar^2 \Gamma_{\text{in}}}{\sigma_{\mathcal{E}_{\text{in}}}^2}. \quad (82)$$

If the externally induced noise is absent, we take $\sigma_{\mathcal{E}_{\text{ex}}} = 0$, *i.e.* $\tau_{\text{ex}} \rightarrow \infty$. The meaning of the parameters Γ_{in} , $\sigma_{\mathcal{E}_{\text{in}}}$ is the same as of the parameters Γ , $\sigma_{\mathcal{E}}$ introduced in Subsec. 6.2. We assume that $\langle \mathcal{E}_{\text{in}}(t) \rangle = 0$, $\sigma_{\mathcal{E}_{\text{in}}}^2 = \langle \mathcal{E}_{\text{in}}^2(t) \rangle$.

Undoubtedly, to calculate the parameters Γ_{in} , $\sigma_{\mathcal{E}_{\text{in}}}$ within the framework of a rigorous kinetic theory would be very challenging. To estimate the order of magnitude of the parameter Γ_{in} , we propose a simplified approach as follows. We presume that if $a < \ell_{\text{decoh}}$, then the thermal fluctuations cannot efficiently bring about transitions between the energies E_1 , E_2 . Only when a reaches the value of ℓ_{decoh} , the thermal energy $k_{\text{B}}T$ is sufficient for the transition from E_1 to E_2 , and this may be interpreted as the phonon

absorption. In other words, we argue that the motion of the electron between the QDs is influenced by the electron–phonon interaction only if $a > \ell_{\text{decoh}}$, since then $k_{\text{B}}T > E_2 - E_1$. As the thermal excitation propagates with the sound speed, we posit (although admitting that this might be a very crude estimate) the Ansatz

$$\Gamma_{\text{in}} \sim v_{\text{s}}/\ell_{\text{decoh}}. \tag{83}$$

We consider Γ_{in} as the rate with which at least one phonon can be absorbed during the motion of the electron from QD1 to QD2. Taking $v_{\text{s}} \approx 5 \times 10^4$ m/s (the sound speed of sapphire is 5050 m/s) and $\ell_{\text{decoh}} \approx 15$ nm, we obtain the correlation time $1/\Gamma_{\text{in}} \sim 3 \times 10^{-13}$ s. This value is much lower than $\tau_{\text{in}} = \hbar^2 \Gamma_{\text{in}}/\sigma_{\mathcal{E}_{\text{in}}}^2$. For $\tau_{\text{in}} \approx \tau_{\text{eph}} \sim 3 \times 10^{-11}$ s and $\Gamma_{\text{in}} \sim 3 \times 10^{12}$ s⁻¹, we obtain $\sigma_{\mathcal{E}_{\text{in}}} \sim (1/3) \times 10^{-22}$ J. This value is practically of the order of magnitude of the thermal energy. (For $T = 30$ K, we obtain $k_{\text{B}}T \sim 4 \times 10^{-22}$ J. In view of the crude estimates that we have used, we may still say that the factors 1/3 and 4 are comparable.)

7.5. Possible extension of the theory

Our discussion can be extended to the case when delta-wells are ordered in a periodic array. Then we may speak of a Kronig–Penney model related to a superlattice formed by quantum dots. If there were no fluctuations, an electron should travel freely from dot to dot in a Bloch-type manner. When this Bloch-type motion concerns the lowest energy band of the superlattice, this is actually a tunnelling problem. According to our results, the thermodynamic fluctuations can effectively impede the Bloch-type motion, provided that the lattice constant a of the superlattice is not too small. We refrain from quantifying this problem here pointing only to the relevance of a time t_{jump} during which a jump of the electron from one QD to the neighboring one should be realized. We expect that the probability of such a tunnelling jump is proportional to the exponential factor $\exp(-t_{\text{jump}}/t_{\text{eph}})$.

7.6. Interference of externally induced noise with the tunnelling as a low-temperature possibility

It remains to discuss the efficacy with which a simulated noise can interfere with the tunnelling. We think of a computer simulation of the Gaussian process $\mathcal{E}_{\text{ex}}(t)$. If the CPU speed of the computer is defined as 2GHz, this means that the time necessary for one operation of the CPU is not less than $t_{\text{oper}} \sim 5 \times 10^{-10}$ s. To realize the simulation of $\mathcal{E}_{\text{ex}}(t)$, we have to choose the value of the correlation time $1/\Gamma_{\text{ex}}$ sufficiently higher than t_{oper} . A realistic option may be $1/\Gamma_{\text{ex}} = 2 \times 10^{-9}$ s. We take $|E_{00}| = 0.088$ eV, $a_{\text{crit}} = 4.16$ nm as in Subsec. 7.2, and choose $a = 50$ nm. Then Eq. (80) gives the energy

difference $E_2 - E_1 \sim 5 \times 10^{-8}$ eV. Correspondingly, $t_{\text{per}} = 2\pi\hbar/(E_2 - E_1) \sim 10^{-8}$ s. To eliminate the thermal noise, we ought to consider the temperature less than one millikelvin. Indeed, $k_{\text{B}}T$ is about 9×10^{-9} eV at $T = 10^{-4}$ K, so that thermal excitations from E_1 to E_2 may surely be excluded from consideration. The choice of $\sigma_{\mathcal{E}_{\text{ex}}} \sim 5 \times 10^{-7}$ eV in the simulation experiment would give the relaxation time $\tau_{\text{ex}} = \hbar^2\Gamma_{\text{ex}}/\sigma_{\mathcal{E}_{\text{ex}}}^2 \sim 10^{-9}$ s. The smallness of the factor $\exp(-t_{\text{per}}/\tau_{\text{ex}}) \sim \exp(-10)$ implies that the noise may indeed effectively influence upon the tunnelling of the electron between the QDs.

This proposed possibility to *decelerate* the tunnelling process by employing an artificially induced noise is contrasting to the *acceleration* of the diffusion of ions when a randomly oscillating electric field is applied to a sample exhibiting electromigration [19].

8. Conclusion

In this paper, we have dealt with the low-energy solution(s) of the 1D Schrödinger equation with the potential energy defined as a pair of equal delta-wells. We have shown that the delta-wells may be considered as a good model of quantum dots in a quantum wire inside a semiconductor structure. In this case, for a qualified comprehension of the motion of an electron along the quantum wire, it was adequate to employ a density-matrix theory and to solve the Liouville equation. We focused attention on the motion of electron with a negative energy E . This possibility is realizable at low temperatures substantiating to exclude, as we did, positive electron energies from consideration. We have solved the Liouville equation in the approximation of a constant relaxation time.

We considered two quantum dots, QD1 and QD2, as points with a given distance a between them. Our intent was to analyze the problem of passing the electron from QD1 to QD2. Since $E < 0$, this was a genuine tunnelling problem. We have emphasized that there exists a critical distance a_{crit} . If $a > a_{\text{crit}}$, there exist two negative eigenenergies, E_1 , E_2 . We have proved that the tunnelling between QD1 and QD2 represents a periodically repeated process: the electron changes its location from QD1 to QD2, afterwards to QD1, again to QD2, *etc.* We have also discussed why this pulsation process should undergo a damping. This damping is mainly due to thermodynamic fluctuations. We suggested, however, that the damping can also be effected by applying an external source of noise and that this should necessitate a computer simulation.

I thank P. Markoš for critical comments to this article.

Appendix A

As is seen in Fig. 1, $E_1 < E_2$. The eigenfunction $\phi_1(x)$ corresponding to E_1 is an even function of x defined for $x > 0$ and the eigenfunction $\phi_2(x)$ corresponding to E_2 is an odd function of x defined for $x > a_{\text{crit}} = 2/\gamma$. Recall that $\gamma = 2m\Omega/\hbar^2 > 0$. We take $\phi_1(x), \phi_2(x)$ as real functions. We define them normalized

$$\int_0^\infty dx [\phi_\mu(x)]^2 = 1/2, \quad \mu = 1, 2. \tag{A.1}$$

Explicitly,

$$\phi_1(x) = \begin{cases} N_1 \cosh(\kappa_1 x) / \cosh(\kappa_1 a/2), & 0 < x < a/2, \\ N_1 \exp[-\kappa_1(x - a/2)], & a/2 < x. \end{cases} \tag{A.2}$$

$$\begin{aligned} N_1 &= \sqrt{\kappa_1} \left[1 + \tanh(\kappa_1 a/2) + \frac{\kappa_1 a/2}{\cosh^2(\kappa_1 a/2)} \right]^{-1/2}, \\ \kappa_1 &= \sqrt{-2mE_1(a)/\hbar^2} > 0. \end{aligned} \tag{A.3}$$

$$\phi_2(x) = \begin{cases} N_2 \sinh(\kappa_2 x) / \sinh(\kappa_2 a/2), & 0 < x < a/2, \\ N_2 \exp[-\kappa_2(x - a/2)], & a/2 < x. \end{cases} \tag{A.4}$$

$$\begin{aligned} N_2 &= \sqrt{\kappa_2} \left[1 + \coth(\kappa_2 a/2) - \frac{\kappa_2 a/2}{\sinh^2(\kappa_2 a/2)} \right]^{-1/2}, \\ \kappa_2 &= \sqrt{-2mE_2(a)/\hbar^2} > 0. \end{aligned} \tag{A.5}$$

Appendix B

We will now calculate the eigenenergy E_0 corresponding to the discrete eigenfunction $\Phi_0(x)$ in a very narrow symmetric rectangular well. For the width and depth of the well, we use, respectively, the symbols d_{dot} and V_0 . Having in mind a conduction electron in the ABA structure, we consider the effective mass m_A for $|x| > d_{\text{dot}}/2$ and the effective mass m_B for $-d_{\text{dot}}/2 < x < d_{\text{dot}}/2$. Thus, the x -dependence of the effective mass is defined by the function

$$\begin{aligned} m^*(x) &= [1 - \Theta(x + d_{\text{dot}}/2)]m_A + [\Theta(x - d_{\text{dot}}/2) - \Theta(x + d_{\text{dot}}/2)]m_B \\ &\quad + \Theta(x - d_{\text{dot}}/2)m_A, \end{aligned} \tag{B.1}$$

where $\Theta(x)$ is the Heaviside step function. Let us first use the energy scale in which the zero energy corresponds to the bottom of the well. In this case, we write the discrete eigenenergy that we want to calculate with the tilde: the energy \tilde{E}_0 lies in the interval $(0, V_0)$. However, when the same energy is written without the tilde, it means that we consider the energy scale shifted by the constant V_0 . The energy E_0 is negative: $E_0 = \tilde{E}_0 - V_0 < 0$.

If the width of the well d_{dot} tends to zero, there exists only one discrete eigenenergy and it lies near the top of the well, *i.e.*

$$\frac{V_0 - \tilde{E}_0}{V_0} \ll 1. \quad (\text{B.2})$$

The eigenfunction corresponding to \tilde{E}_0 is symmetric

$$\tilde{\Phi}_0(-x) = \tilde{\Phi}_0(x), \quad (\text{B.3})$$

$$\begin{aligned} \tilde{\Phi}(x) = & [1 - \Theta(x + d_{\text{dot}}/2)]\tilde{\Phi}_L(x) + [\Theta(x - d_{\text{dot}}/2) - \Theta(x + d_{\text{dot}}/2)] \\ & \times \tilde{\Phi}_M(x) + \Theta(x - d_{\text{dot}}/2)\tilde{\Phi}_R(x). \end{aligned} \quad (\text{B.4})$$

With the quantities

$$k = \left[2m_B \tilde{E}_0\right]^{1/2} / \hbar, \quad \kappa = \left[2m_A (V_0 - \tilde{E}_0)\right]^{1/2} / \hbar, \quad (\text{B.5})$$

$$\begin{aligned} \tilde{\Phi}_L(x) &= A \exp(\kappa x), & x < -d_{\text{dot}}/2, \\ \tilde{\Phi}_M &= \cos(kx), & -d_{\text{dot}}/2 < x < d_{\text{dot}}/2, \\ \tilde{\Phi}_R(x) &= A \exp(-\kappa x), & d_{\text{dot}}/2 < x. \end{aligned} \quad (\text{B.6})$$

Owing to the symmetry of $\tilde{\Phi}_0(x)$, we may confine ourselves to formulating the boundary conditions for the interface $x = -d_{\text{dot}}/2$

$$\tilde{\Phi}_L(-d_{\text{dot}}/2) = \tilde{\Phi}_M(-d_{\text{dot}}/2), \quad (\text{B.7})$$

$$\frac{1}{m_A} \left. \frac{d\tilde{\Phi}_L(x)}{dx} \right|_{x=-d_{\text{dot}}/2-0} = \frac{1}{m_B} \left. \frac{d\tilde{\Phi}_M(x)}{dx} \right|_{x=-d_{\text{dot}}/2+0}. \quad (\text{B.8})$$

Condition (B.8) has resulted from the equation

$$-\frac{\hbar^2}{2} \frac{d}{dx} \left[\frac{1}{m^*(x)} \frac{d\tilde{\Phi}(x)}{dx} \right] + V(x)\tilde{\Phi}(x) = E\tilde{\Phi}(x) \quad (\text{B.9})$$

which was proposed in [20] for envelope wave functions in the one-band approximation, if the effective mass m^* is x -dependent. Conditions (B.7), (B.8) give us the equation

$$\tan\left(\frac{k d_{\text{dot}}}{2}\right) = \frac{m_B}{m_A} \frac{\kappa}{k}. \tag{B.10}$$

After inserting here expressions (B.5), we obtain the transcendental equation for \tilde{E}_0

$$\frac{m_A}{m_B} \left(\frac{\tilde{E}_0}{V_0}\right)^{1/2} \tan\left(\frac{[2m_B \tilde{E}_0]^{1/2} d_{\text{dot}}}{2\hbar}\right) = \left(\frac{V_0 - \tilde{E}_0}{V_0}\right)^{1/2}. \tag{B.11}$$

The smallness of the right-hand side of Eq. (B.11) (which has been stipulated by condition (B.2)) presumes the possibility to replace \tilde{E}_0 in the left-hand side by V_0 , when we require the fulfilment of the condition

$$\frac{[2m_B V_0]^{1/2} d_{\text{dot}}}{2\hbar} \ll 1. \tag{B.12}$$

Then the tangent may be replaced by its argument and Eq. (B.11) is reduced to an algebraic equation for \tilde{E}_0 , from which we obtain the result

$$\tilde{E}_0 \approx V_0 - \left(\frac{m_A}{m_B}\right) \frac{m_A V_0^2 d_{\text{dot}}^2}{2\hbar^2}, \tag{B.13}$$

or, if we shift the scale of energies,

$$E_0 = - \left(\frac{m_A}{m_B}\right) \frac{m_A V_0^2 d_{\text{dot}}^2}{2\hbar^2}. \tag{B.14}$$

When comparing this result with the expression for the negative eigenenergy in the case of a single delta-well (with $m_A = m$), we observe that

$$\Omega \approx \left(\frac{m_A}{m_B}\right)^{1/2} V_0 d_{\text{dot}}. \tag{B.15}$$

Thus, the fraction m_A/m_B has been absorbed in Ω .

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