ENERGY SPECTRA AND LIFETIMES OF QUASIPARTICLES IN AN OPEN CYLINDRICAL QUANTUM WIRE

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The energies and lifetimes of the quasistationary states of quasiparticles in an open cylindrical quantum wire have been calculated numerically in the effective mass approximation making use of the scattering matrix method. The calculations have been performed for a $GaAs/Al_xGa_{1-x}As/GaAs$ nanoheterosystem. The dependences of the quasiparticle lifetimes in quasistationary resonance states on the geometrical sizes of nanosystems and the quasiparticle's longitudinal quasimomentum have been obtained. The lifetime of quasiparticles in the system concerned has been shown to decrease exponentially with increase in their longitudinal quasimomenta. For energies above the potential barrier, a repulsion of energy levels, which manifests itself through a nonmonotonic lifetime behavior, is observed.

1. Introduction

The first advances in the creation of lasers based upon semiconductor quantum wires and semiconductor quantum dots [1–3], as well as the promising prospects in the development of essentially new semiconductor devices, which are based on quantum-mechanical phenomena, have attracted the efforts of many researchers to the study of physical processes that occur in one- and zero-dimensional nanosystems. At present, a plenty of scientists, both theorists and experimenters, works in this branch. Modern technological methods allow complex multilayered nanoheterostructures of various dimensions to be created [4,5], which stimulates the intense theoretical studies of physical phenomena in such nanosystems.

The theory of electron, hole, and exciton spectra, as well as the theory of the interaction between those quasiparticles and phonons in closed spherical multilayered nanosystems in the framework of the effective mass approximation, has been developed in works [4–8].

For closed nanosystems, the environment represents the highest potential barrier with respect to the potentials of internal layers. Therefore, the wave functions of quasiparticles, whose energies are lower than the height of this barrier in the environment, quickly tend to zero. In closed nanoheterosystems, the quasiparticle states are stationary, and the quasiparticle spectrum generally consists of discrete and continuous parts.

In open nanosystems, where a quasiparticle can penetrate, owing to the tunnel effect, into the environment, where its potential energy is smaller than that in internal layers, the lifetimes of quantum states are finite. Such states are called quasistationary. In works [9–13], the researches concerning the quasistationary states of quasiparticles of the Breit–Wigner type in open spherical nanoheterosystems in the energy range below the potential barrier height and weakly coupled resonance states in the continuous spectrum range have been carried out. Cylindrical open nanosystems, which attract a special interest owing to the opportunity to be the basis for creating a quantum transistor [14], turned out less studied [15, 16]. At the same time, the lifetimes of excitons and the resonance states in the continuous spectrum range have not been studied at all.

This work aims at studying theoretically the quasistationary states of electrons, holes, and excitons in an open complex cylindrical quantum wire (CCQW) which involves a single potential barrier; in particular, in a $GaAs/Al_xGa_{1-x}As/GaAs$ nanosystem.

2. Hamiltonian and the Wave Functions of an Electron and a Hole in an open CCQW

We study the electron and hole spectra of an open CCQW. The construction of the CCQW and the schemes of the potential energies of an electron and a hole in it are shown in Fig. 1. The open CCQW is composed of a GaAs kernel (potential well *0*) and an $Al_xGa_{1-x}As$ layer (potential barrier *1*), both being embedded into the infinite medium of GaAs (potential well *2*). In the effective mass approximation and in the approximation of the independent bands of light and heavy holes in the CCQW $GaAs/Al_xGa_{1-x}As/GaAs$

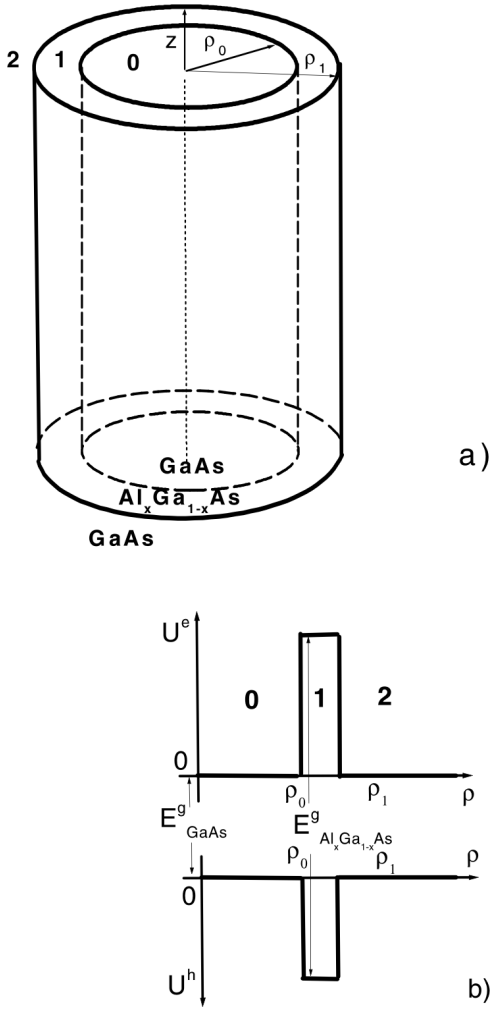


Fig. 1. CCQW scheme (a) and the diagrams of the electron and hole potential energies in a CCWQ (b)

within the concentration range of $0 < x < 0.43$, where $Al_xGa_{1-x}As$ is a direct-band-gap semiconductor, the theories for electrons and light and heavy holes become equivalent. A difference between the spectral properties of electrons and holes arises only at the stage of numerical calculations because of the different effective masses of quasiparticles and the different potential fields acting on them.

In the cylindrical coordinate system with the origin at the center of the heterostructure, the electron is characterized by the effective mass $\mu(\rho)$ and the potential energy $U(\rho)$, which are the functions of the distance from the CCQW axis, because they have different values in different media:

$$\mu(\rho) = \begin{cases} \mu_0, & \rho < \rho_0, \\ \mu_1, & \rho_0 \le \rho \le \rho_1, \\ \mu_0, & \rho > \rho_1, \end{cases}$$

$$U(\rho) = \begin{cases} 0, & \rho < \rho_0, \\ U, & \rho_0 \le \rho \le \rho_1, \\ 0, & \rho > \rho_1. \end{cases} \tag{1}$$

Since the effective mass depends on ρ, the stationary Schrödinger equation looks like [14]

$$\left(-\frac{\hbar^2}{2}\vec{\nabla}\frac{1}{\mu(\rho)}\vec{\nabla} + U(\rho)\right)\Psi(\vec{r}) = E\Psi(\vec{r}). \tag{2}$$

Taking the axial symmetry of the problem into account, the solution of Eq. (2) is tried in the form

$$\Psi(\rho, \varphi, z) = \frac{1}{\sqrt{L}} R(\rho)\ e^{im\varphi}\, e^{ikz}, \quad m = 0, \pm1, \pm2, ..., \tag{3}$$

where $R(\rho)$ is the radial wave function.

Substituting Eq. (3) into Eq. (2), we obtain the equation for the radial wave function

$$\left\{-\frac{\hbar^2}{2}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\frac{\rho}{\mu(\rho)}\frac{\partial}{\partial\rho}\right) - \frac{m^2}{\rho^2\mu(\rho)} - \frac{k^2}{\mu(\rho)}\right] + \right.$$

$$\left. + U(\rho) - E\right\} R_{m,k}(\rho) = 0. \tag{4}$$

One can see that both the magnetic quantum number m and the quasimomentum of the longitudinal motion of a quasiparticle k are the parameters of Eq. (4) and, hence, of the required function $R_{m,k}(\rho)$ which is sought in the form

$$R_{m,k}(\rho) = \begin{cases} R^0_{mk}(\rho), & \rho < \rho_0, \\ R^1_{mk}(\rho), & \rho_0 \le \rho \le \rho_1, \\ R^2_{mk}(\rho), & \rho > \rho_1. \end{cases} \tag{5}$$

Substituting Eq. (5) into Eq. (4) brings about three equations of the same type:

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2} + \frac{2\mu_i}{\hbar^2}\times\right.$$

$$\left.\times\left(E - U_i - \frac{\hbar^2k^2}{2\mu_i}\right)\right] R^i_{mk}(\rho) = 0, \quad (i = 0, 1, 2), \tag{6}$$

the solutions of which are the linear combinations of Hankel functions of different arguments:

$$R_{mk}(\rho) = \begin{cases} R^0_{mk}(\rho) = \mathrm{A}^{(0)}_m [H^-_m(\chi_0\rho) + H^+_m(\chi_0\rho)], & \rho < \rho_0, \\ R^1_{mk}(\rho) = \mathrm{A}^{(1)}_m \left[H^-_m(i\chi_1\rho) + S^1_{mk}(E)\ H^+_m(i\chi_1\rho)\right], & \rho_0 \le \rho \le \rho_1, \\ R^2_{mk}(\rho) = \mathrm{A}^{(2)}_m [H^-_m(\chi_0\rho) + S_{mk}(E)\ H^+_m(\chi_0\rho)], & \rho > \rho_1, \end{cases} \quad (7)$$

where

$$\chi_0 = \sqrt{\frac{2\mu_0}{\hbar^2}E - k^2}, \quad i\chi_1 = \sqrt{\frac{2\mu_1}{\hbar^2}(E-U) - k^2}. \quad (8)$$

All coefficients A and the scattering matrix $S_{mk}(E)$ are determined unequivocally from the normalization condition and the continuity conditions for the wave function and the probability density flux at both interfaces.

Now, according to the scattering theory [17], we continue analytically the S-matrix into the complex energy plane ($E \to \tilde{E} = E - i\Gamma/2$). The positions of poles of the real and imaginary parts of the S-matrix coincide and determine the energy spectrum and the band widths of the open nanosystem. In so doing, the real part of a certain position of a pole of the S-matrix is equal to the energy E of a resonance quasistationary state, while the imaginary one determines its width Γ which is connected with the probability for a quasiparticle to tunnel through the barrier and with the lifetime of the quasiparticle in this state.

In contrast to the case of the S-matrix for an open spherical nanoheterosystem [10, 11], where, provided that the orbital quantum number l equals 0 or 1, one succeeded in obtaining the analytical solutions of the relevant dispersion equation. A similar problem for the investigated case of a cylindrical nanosystem can be solved only by numerical methods. We also note that a new fundamental issue arises in this problem: if the problem is one-dimensional, the S-matrix depends on both the energy and longitudinal quasimomentum, contrary to the zero-dimensional case. This results in that both the energy E and the lifetime τ of quasiparticles in quasistationary states turn out to be functions of the longitudinal quasimomentum k.

3. Analysis and Discussion of Results

The numerical calculations of the S-matrix and the positions of its poles in the complex energy plane allow the dependences of the resonance energies $E$and the lifetimes τ of both the quasistationary and resonance states of electrons and holes on the quasiparticle quasimomentum and the CCQW's geometrical sizes to be studied.

Fig. 2 shows the results of calculations of the resonance energies $E^e_{nm}(k)$ and the lifetimes $\tau^e_{nm}(k)$ of electrons in the quasistationary states of a CCQW GaAs/Al_xGa_{1-x}As/GaAs as functions of the longitudinal quasimomentum k at $\rho_0 = 15\,a_{\mathrm{GaAs}}$, $\Delta\rho = \rho_1 - \rho_0 = 5a_{\mathrm{GaAs}}$, $m = 0$ or 1, and for the fixed Al content $x = 0.4$. This figure also includes the plots of the dispersion laws for electrons — $E^e_0(k) = \frac{\hbar^2k^2}{2\mu^e_0}$ and $E^e_1(k) = U^e + \frac{\hbar^2k^2}{2\mu^e_1}$ — in massive semiconducting crystals $Al_xGa_{1-x}As$ and GaAs, respectively, which the corresponding layers of the investigated CCQW are made up of.

From Fig. 2, one can see that the dispersion curves $E^e_0(k)$ and $E^e_1(k)$ divide the plane (E, k) into three regions: (I) the region, where $E < E^e_0(k)$; here, the S-matrix has no poles, and, accordingly, there are no quasiparticle bound states; (II) the region, where $E^e_0(k) < E < E^e_1(k)$; here, the S-matrix has poles in the complex energy plane which determine the energy and the lifetime $\tau \sim \Gamma^{-1}$ of quasiparticles in the quasistationary states of the Breit—Wigner type; and (III) the region, where $E > E^e_1(k)$; here, quasiparticles are in weakly bound resonance states above the potential barrier.

Let us analyze the electron states in regions II and III in detail. As is obvious from Fig. 2, every fixed k-value in region II is connected with a certain finite number of resonance quasistationary states; as k varies, these states form resonance quasistationary bands. The number of bands is determined by geometrical sizes of the CCQW, as well as by the effective masses and the potential energies of a quasiparticle in various media of the system. In region III, the number of resonance quasistationary states is unlimited, and all of them are characterized by short lifetimes.

The main features of the electron resonance bands are as follows. The k-dependence of the quasiparticle energy

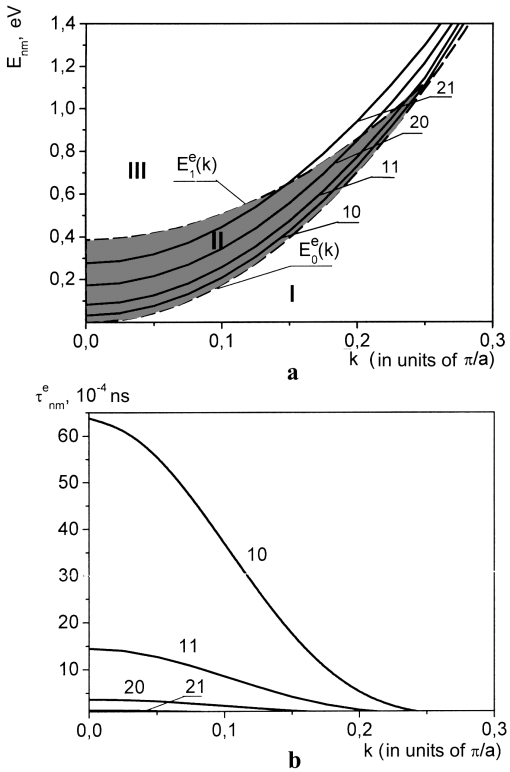


Fig. 2. Dependences $E_{nm}(k)$ (a) and $\tau_{nm}(k)$ (b) for nm-states $(n = 1, 2;\ m = 0, 1)$ for $\rho_0 = 15a_{\mathrm{GaAs}}$ and $x = 0.4$

is approximated very well in all resonance states by the quadratic law $E^e_{nm}(k) = E^e_{nm} + \frac{\hbar^2 k^2}{2\mu^e_{nm}}$, where E^e_{nm} is determined by the solution of Eq. (6) at $k = 0$; and the values of the averaged effective electron mass μ^e_{nm} are very close to the corresponding effective electron masses in GaAs. Notice that we use the term "the averaged effective mass" to emphasize the fact that a quasiparticle moves in a longitudinal direction simultaneously in all the CCQW layers as an entire quantum-mechanical object possessing the quasimomentum k, although it dwells in different layers with different probabilities. Since the particle is located in GaAs with the highest probability, it is natural that its averaged mass is rather close to μ_{GaAs}. As the band number N increases, the averaged effective mass of the quasiparticle grows a little, because the "effective height" of the potential barrier (a distance from the resonance level to the potential-barrier top) decreases, and the quasiparticle penetrates into $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$, where its effective mass is larger than that in GaAs, with higher probability. All the bands of the resonance energies $E^e_{nm}(k)$ of quasiparticles are characterized by the maximal value of the longitudinal quasimomentum $\bar{k}^e_{nm}$, at which the

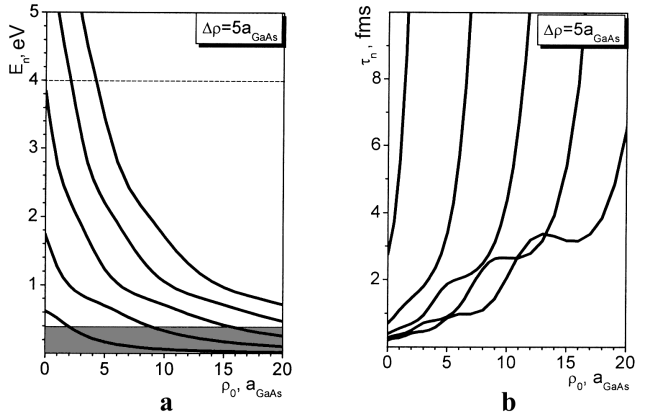
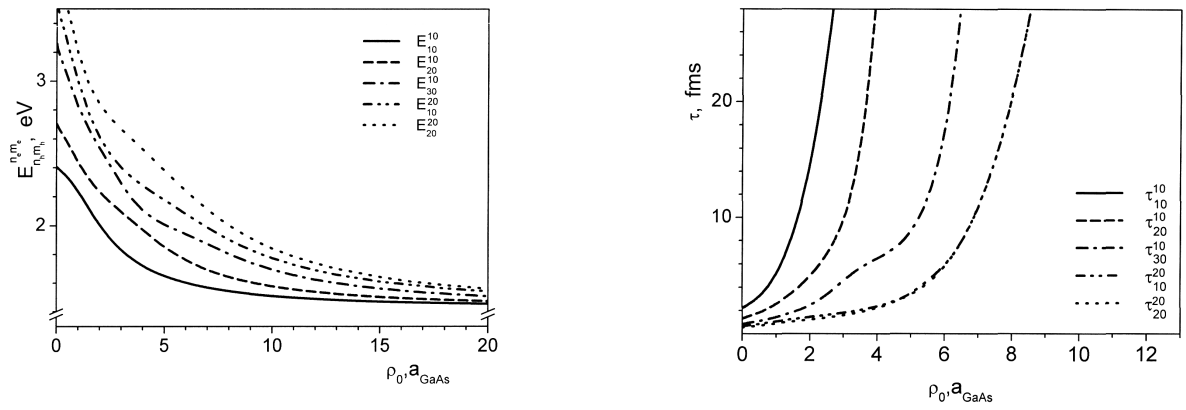


Fig. 3. Dependences of the electron energy spectrum E_n (a) and the electron lifetime τ_n (b) on ρ_0 for $\Delta\rho = 5a_{\mathrm{GaAs}}$ and $x = 0.4$

energy of the quasiparticle is lower than the potential barrier height. In quantum-mechanical states with $k > \bar{k}^e_{nm}$, quasiparticles are characterized by short lifetimes (Fig. 2,b); therefore, we call such states "weakly bound resonance states".

In Fig. 3, the dependences of the energy spectrum and the lifetime of an electron on the dimension of the inner conductor of the quantum wire at $k = 0$ are depicted. The shadowed region in panel a marks the energy range below the potential barrier height. In this region, the energy spectrum falls down monotonously, while the lifetime grows exponentially. In the energy range above the potential barrier height, a poorly pronounced effect of level repulsion is observed. Such an effect is explained as follows. For an electron with energy higher than the potential barrier height, semiconducting media *0* and *1* are nothing else but the potential wells of various widths. Were these wells independent, each of them would possess an own system of quantum-mechanical levels. The widening of well *0* makes the dimensional quantization weaker, which is accompanied by a decrease of the corresponding level energies. In the case where quantum wells *0* and *1* form a single quantum-mechanical system for the electron, the energy levels which correspond to states with identical symmetry repulse one another. The wider the quantum well *1*, the more is the number of quantum-mechanical levels in it, and the more pronounced is the effect of level repulsion. As a result, the energy spectrum of the electron in the range above the potential barrier height includes quickly and slowly descending sections. In the range of the energy level repulsion, the quasiparticle changes its localization in the nanosystem. The slowly descending sections of the energy spectrum correspond



a **b**

Fig. 4. Dependences of the excitation energy $E^{n_h m_h}_{n_e m_e}$ (a) and the lifetime (b) of the exciton on ρ_0 for $\Delta\rho = 5a_{\rm GaAs}$ and $x = 0.4$

to energies, at which the electron is located in medium *1* with higher probability. The lifetime of such states weakly depends on the size of well *0*, which is illustrated by the dependences $\tau(\rho_0)$ in Fig. 3,*b*. The quickly descending sections of the energy spectrum in Fig. 3,*a* correspond to the states, where the electron is located in medium *0* with higher probability. In this case, the lifetime of such states grows exponentially, as their energy diminishes.

The energy and lifetime dependences for heavy and light holes in an open quantum wire are qualitatively the same as those for electrons. Quantitative discrepancies are connected with a lower potential barrier height U^h and different values of the effective mass of quasiparticles.

On the basis of the dependences of the electron and heavy hole energies in the lowest energy bands at $k = 0$, the numerical calculations of the dependence of the exciton excitation energy on the radius of inner conductor *0* of the open quantum wire were carried out by the formula

$$E^{n_h m_h}_{n_e m_e} = E^e_{n_e m_e} + E^h_{n_h m_h} + E_g - E^{eh}, \tag{9}$$

where $E^e_{n_e m_e}$ and $E^h_{n_h m_h}$ are the electron and hole energies, respectively; E_g is the energy gap width; and E^{eh} is the energy of electron–hole coupling, which is determined by the formula

$$E^{eh} = \int \Psi^{e^*}_{n_e m_e} \Psi^{h^*}_{n_h m_h} \frac{e^2}{|\vec{r}_e - \vec{r}_h|} \Psi^e_{n_e m_e} \Psi^h_{n_h m_h} d\vec{r}_e d\vec{r}_h. \tag{10}$$

Since the lifetime of an exciton in the inner conductor of the quantum wire depends on the electron and hole lifetimes in states $n_e m_e$ and $n_h m_h$, respectively, and the quasiparticle coupling energy is considerably lower than the energy of their dimensional quantization, the estimation of $\tau^{n_h m_h}_{n_e m_e}$ can be performed using the formula

$$\frac{1}{\tau^{n_h m_h}_{n_e m_e}} = \frac{1}{\tau^e_{n_e m_e}} + \frac{1}{\tau^h_{n_h m_h}}. \tag{11}$$

The results of calculations of $E^{n_h m_h}_{n_e m_e}$ and $\tau^{n_h m_h}_{n_e m_e}$ for the lowest five energy levels are shown in Fig. 4. Since the binding energy for an exciton E^{eh} is low, as compared to the energy $E^e_{n_e m_e} + E^h_{n_h m_h} + E_g$, the behavior of the curves $E^{n_h m_h}_{n_e m_e}(\rho_0)$ is governed by the dependences of the dimensional quantization energies of electrons and holes. Therefore, if the inner conductor of the quantum wire is narrow, a nonmonotonic behavior of the exciton excitation energy is observed, which is also reflected on the corresponding lifetimes $\tau^{n_h m_h}_{n_e m_e}$ of the exciton inside the nanosystem.

The general conclusions are as follows. The method of the S-matrix, which is mainly used for spherically symmetric problems [10–13], allows the spectral characteristics of open complex cylindrical quantum nanoheterosystems with resonance quasistationary states to be calculated. The variation of the barrier thickness weakly affects the position of electron energy levels in the range below the potential barrier height and drastically changes the energies of the weakly bound resonance states in the range above it. The dependence of the lifetime of quasiparticles in the resonance states with energies above the potential barrier height on the barrier thickness has a nonmonotonic character connected with the variation of the localization of quasiparticles. The dependences of the exciton excitation

energy and the exciton lifetime on the nanosystem's sizes reproduce the characteristic properties of electrons and holes.

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ЕНЕРГЕТИЧНИЙ
СПЕКТР ТА ЧАСИ ЖИТТЯ
КВАЗІЧАСТИНОК У ВІДКРИТОМУ
ЦИЛІНДРИЧНОМУ КВАНТОВОМУ ДРОТІ

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Р е з ю м е

У наближенні ефективної маси, використовуючи теорію S-матриці, чисельними методами отримано енергії та часи життя квазістаціонарних станів квазічастинок у відкритому складному циліндричному квантовому дроті. Конкретний розрахунок виконано для системи $GaAs/Al_xGa_{1-x}As/GaAs$. Отримано залежності часів життя квазічастинок у квазістаціонарних резонансних станах від геометричних розмірів наносистеми і від поздовжнього квазіімпульсу. Показано, що в резонансних станах досліджуваної наносистеми часи життя квазічастинок експоненціально зменшуються зі збільшенням поздовжнього квазіімпульсу. В області енергій, вищих за висоту потенціального бар'єра, спостерігається розштовхування енергетичних рівнів, яке проявляється в немонотонній поведінці часів життя.