Slowly decaying quasistationary electron states in spherical heavy quantum dots

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The energy spectrum of an electron in a spherical potential-hump heteroinclusion with a large effective mass is shown to be characterized by a set of quasidiscrete levels with large values of the angular momentum l. The lifetimes of quasistationary states in the hump increase with increasing l, i.e., with increasing excitation of the state. Energies and lifetimes of the quasistationary states are calculated numerically on the basis of selected parameter values. © *1994 American Institute of Physics.*

1. Quantum dots, which are usually heteroinclusions of a relatively narrow-gap material in a relatively wide-gap semiconducting medium, have been rather fashionable topics in recent physics research. The discontinuity in the electron band gives rise to an energy profile which localizes the motion of an electron within the quantum dot, where its effective mass is usually smaller than in the external medium.

In the present letter we consider a quantum entity constructed by interchanging the properties of the heteroinclusion and the surrounding medium. In other words, we consider a wide-gap inclusion in a narrow-gap medium. The original energy profile—a "potential hump" in the words of Landau and Lifshitz—does not initially localize an electron; it simply scatters the electron. We also assume that the electrons of the heteroinclusion are considerably heavier than the electrons of the narrow-gap medium. We assume that at a certain finite value $k=k_0$ of the wave vector there is a crossing of electron terms of the heteroinclusion, $\epsilon_1(k)$, and of the medium, $\epsilon_2(k)$:

$$\epsilon_1(k_0)=\epsilon_2(k_0). \tag{1}$$

[For simplicity we are assuming that the dispersion relations $\epsilon_{1,2}(k)$ are isotropic.] All these assumptions are illustrated in Fig. 1; we will refer to our entity as a "heavy quantum dot."

The model entity discussed below is a spherical heavy quantum dot of radius r_0. We assume that there is a sharp heterojunction at $r=r_0$ with a discontinuity U_0 in the electron band (Fig. 1). Shown for comparison in Fig. 1, by the dashed lines, is the potential profile of an ordinary quantum dot (spherical) with an inner narrow-gap material. Since the analysis is being carried out in terms of a model, we restrict the discussion to the single-band approximation:

$$\epsilon_1(k)=U_0+\frac{\hbar^2k^2}{2m_1},\ \epsilon_2(k)=\frac{\hbar^2k^2}{2m_2},\ m_1>m_2, \tag{2}$$

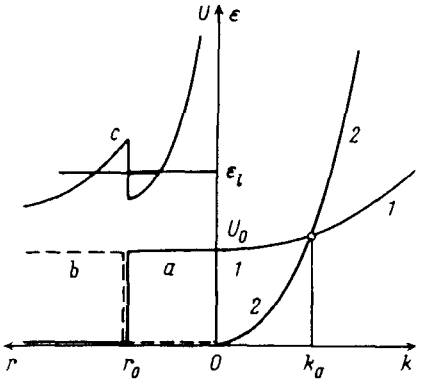

FIG. 1. Dispersion $\epsilon(k)$ and potential profiles $U(r)$. 1) $\epsilon_1(k)$; 2) $\epsilon_2(k)$. a—Heavy quantum dot; b—ordinary quantum dot; c—effective potential profile for an electron in a heavy quantum dot at a large value of l. Here U_0 is the discontinuity of the electron band at the heterojunction.

with $k_0^2=(2U_0/\hbar^2)m_1m_2/(m_1-m_2)$.

2. Writing the electron wave function $\psi(\mathbf{r})$ in the form

$$\psi(\mathbf{r})=Y_{lm}(\theta,\varphi)X_l(r,\epsilon)/r, \tag{3}$$

we find the following equations[1,2] for X:

$$X_l''+\frac{2m_1}{\hbar^2}\left(\epsilon-U_0-\frac{\hbar^2l(l+1)}{2m_1r^2}\right)X_l=0,\ r<r_0, \tag{4}$$

$$X_l''+\frac{2m_2}{\hbar^2}\left(\epsilon-\frac{\hbar^2l(l+1)}{2m_2r^2}\right)X_l=0,\ r>r_0, \tag{5}$$

where $Y_{lm}(\theta,\varphi)$ is the spherical harmonic, l is the azimuthal quantum number (angular momentum) of the electron, the prime means the derivative with respect to r, and $\epsilon>0$ is the energy of the electron. This energy has a continuous spectrum of values. It can be seen from (4) and (5) that under the condition

$$l(l+1)>2U_0r^2/\hbar^2(m_2^{-1}-m_1^{-1}) \tag{6}$$

the effective potential profile in which the electron is moving acquires an "inner" potential well (Fig. 1), in which the electron is quasilocalized.

The exact function $X_l(r,\epsilon)$ must satisfy standard conditions at $r=0$ and $r=\infty$, as well as the conditions

$$X(r_0-0)=X(r_0+0);\ \frac{1}{m_1}X'(r_0-0)=\frac{1}{m_2}X'(r_0+0). \tag{7}$$

The function we are seeking is of the form

$$X_l(r)=p_1rj_l(p_1r),\ r<r_0, \tag{8}$$

$$X_l(r)=p_2r[\beta_lh_l^{(1)}(p_2r)+\gamma_lh_l^{(2)}(p_2r)],\ r>r_0, \tag{9}$$

where

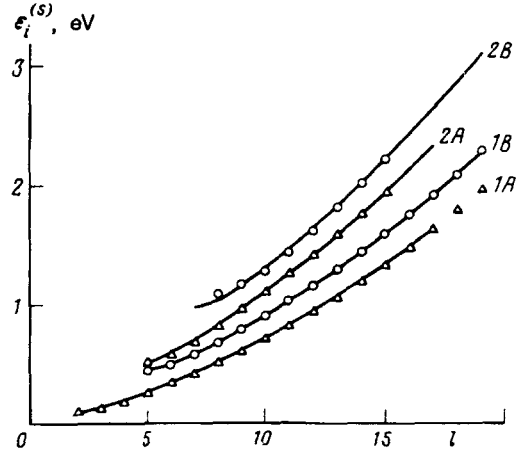

FIG. 2. Energies of the quasidiscrete levels, $\epsilon_l^{(s)}$, versus the angular momentum l for the two values $s=1,2$ and for the two sets of parameters (A and B) given in the text proper. Solid curves—Accurate numerical calculation; points—results of the first iteration.

$$p_1=\left(\frac{2m_1}{\hbar^2}(\epsilon-U_0)\right)^{1/2},\quad p_2=\left(\frac{2m_2\epsilon}{\hbar^2}\right)^{1/2},$$

$j_l(x)$ is the spherical Bessel function of the first kind, $h_l^{(1,2)}(x)$ are spherical Bessel functions of the third kind,[3] and β_l, and γ_l are arbitrary constants. The condition for the existence of a quasidiscrete level[1,2] is that there be no outgoing wave at $r\to\infty$, i.e., the condition $\gamma_l=0$. From (7) we then find

$$\frac{p_2}{m_2}\frac{h_l^{(1)'}(p_2r_0)}{h_l^{(1)}(p_2r_0)}=\frac{p_1}{m_1}\frac{j_l'(p_1r_0)}{j_l(p_1r_0)}-\frac{(m_2^{-1}-m_1^{-1})}{r_0}. \tag{10}$$

Equation (10) has only complex roots ϵ_l. We are interested in only those roots which lie in the lower half-plane and which have small imaginary components. These roots lie near zeros of the Bessel function: $J_{l+1/2}(p_1r_0)=0$, i.e.,

$$\epsilon_l^{(s)}\simeq U_0+\frac{\hbar^2}{2m_1r_0^2}(\sigma_{l+1/2}^{(s)})^2, \tag{11}$$

where $s=1$ corresponds to smallest zero of the function $\sigma^{-(l+1/2)}J_{l+1/2}(\sigma)$, $s=2$ corresponds to the next zero, etc. Approximation (11) is satisfactory under the condition $lm_1/m_2\gg 1/2$. Figure 2 shows approximate values of the real components $\epsilon_l^{(s)}$ found from (10) with the help of (11) as a zeroth approximation. They are plotted as a function of l. Also shown here are exact values of the real components $\epsilon_l^{(s)}$ found through direct calculation from (10). We used the following two sets of parameter values:

A) $m_2=0.041m_0$, $m_1=5m_2$, $U_0=0.01$ eV;

B) $m_2=0.047m_0$, $m_1=4m_2$, $U_0=0.16$ eV

(m_0 is the mass of a free electron). The radius of the inclusion is chosen to be the same: $r_0=75$ Å. Along with the "ground" quasidiscrete level $s=1$, a "first excited level" $s=2$ has been constructed in each case. For large values of l (>5), the zeroth approximation in (11) works well enough if we use as $\sigma_{l+1/2}^{(s)}$ the asymptotic values of the zeros calculated

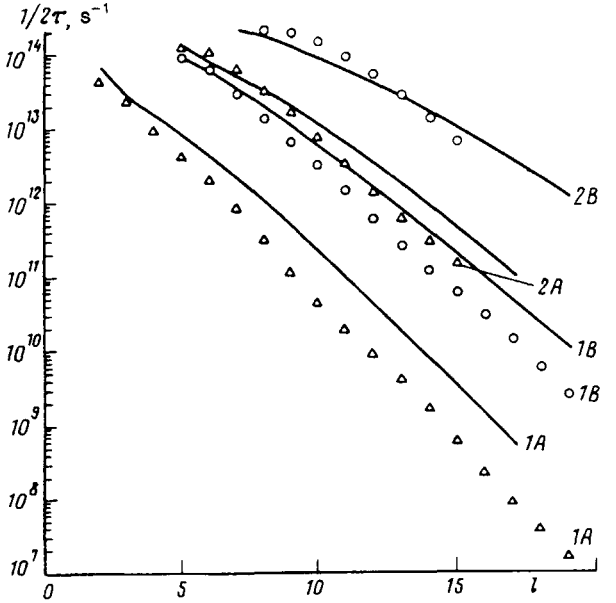

FIG. 3. Reciprocal of twice the lifetime, $1/(2\tau_l^{(s)})$, versus the angular momentum l for the same states ($s=1,2$) and for the same sets of parameter values (A and B) as in Fig. 2.

from the standard formulas.[3] Figure 3 shows the reciprocal of twice the electron lifetime in the quasidiscrete level, $1/(2\tau)$, versus the angular momentum l for the same sets of parameter values, A and B, and for the values $s=1,2$. Here we used the formula

$$\frac{1}{2\tau_l^{(s)}} = -\frac{1}{\hbar}\mathrm{Im}\epsilon_l^{(s)}. \tag{12}$$

Shown along with the results of the accurate calculations are the results of the first iteration. It can be seen from Fig. 3 that at large values of l we have a behavior $\tau_l^{(s)} \sim \exp(\alpha l)$. The constant α is slightly different for the two sets of parameter values used in the calculations: $\alpha_A > \alpha_B$. For $s=1$ and $s=2$, however, these constants are approximately the same, according to Fig. 3. The state lifetimes $\tau_l^{(1)}$ are roughly 10^2 times the lifetime $\tau_l^{(2)}$, so the ground states are much stabler than the first excited states.

It can also be seen from Fig. 3 that the results calculated by the iterative procedure are noticeably different from the exact results, although they do contain all the qualitative aspects of the behavior. With decreasing radius of the heavy quantum dot, r_0, the energies $\epsilon_l^{(s)}$ increase as r_0^{-2} at large values of l, while the lifetimes of the quasistationary states, $\tau_l^{(s)}$, fall off as r_0^2.

At sufficiently large values of l and r_0 (as can be seen from Fig. 3), the lifetimes $\tau_l^{(s)}$ in the heavy quantum dot are greater than plausible values of the momentum and energy relaxation times of an electron in a semiconductor. In other words, such states become essentially indistinguishable from "stationary" states. (Since the spectrum is discrete, most transitions involving the emission or absorption of phonons inside the heavy quantum dot are forbidden.) These states are similar to the stationary states discussed in Ref. 4. Those other states arise in thin quantum barriers with a large electron

mass at large values of the longitudinal wave vector. In "heavy" quantum wires of the same nature, there can be both stationary states (analogous to those studied in Ref. 4) and quasistationary states, like those discussed above.

For which heteropairs could the model adopted above be successfully realized? This model is based on the assumption that the discontinuity (U_0) of the electron bands is comparatively small, that the wave vector k_0 is comparatively small, and that the ratio of effective masses m_1/m_2 is comparatively large. If we adhere to the standard Kane models of the spectrum, we would be interested in heteropairs with a large difference between energy gaps: $\epsilon_{g1} \gg \epsilon_{g2}$. A large part of the change in the gap, $\epsilon_{g1} - \epsilon_{g2}$, should occur at the discontinuity in the valence band. In particular, this condition does not hold in such standard isomorphic heteropairs as $Al_xGa_{1-x}As/GaAs$ and $In_xGa_{1-x}As/In_yAl_{1-y}As$ [here we have $y = y(x)$ from the condition for an isomorphic case], in which a large part of the discontinuity lies in the electron bands. The condition which we need holds in the isomorphic heteropair[5] $In_{0.53}Ga_{0.47}As/InP$, but the mass ratio $m_1/m_2 \simeq 2$ is not large enough. Better combinations of parameter values are found in heterojunctions which include wide-gap II –VI semiconductors. In the pseudomorphic heteropair CdS/Ge, for example, which was studied in Ref. 6, we have $U_0 \simeq 0.01$ eV and $m_1/m_2 \simeq 5$, as in parameter set A discussed above. The parameters in set B are reproduced approximately in the pseudomorphic pair CdS/GaSb. We might also mention the pairs CdSe/GaSb, CdSe/InSb, etc. (see the parameter values of these pairs in Refs. 6 and 7).

Another group of entities to which the arguments above apply (at a qualitative level) are insulating precipitates in semiconductors (or gaseous or vacuum voids in semiconductors). The sizes of these inclusions span a very broad range (including nanometer values). In this case we would need a difference on the order of 3–4 eV between the electron affinities (in the case of Si/SiO_2, for example, this difference is[8] ~ 3.2 eV). This requirement rules out the use of the single-band or Kane analysis, and it shows that we can speak in only qualitative terms.

A trapping of electrons by high-lying, quasidiscrete, slowly decaying levels of a heavy quantum dot can have a strong influence on high-field (hot) electron transport in the material of a matrix if the concentration of these heavy dots is sufficiently high, and the trapped electrons are taken out of play completely (as in the case of conventional electron traps). At the same time, the transient trapping and return processes would be completely different here and would be described by short times.

Since our analysis is only at a model level, we have not included the image potential in the Hamiltonian. The contribution of image forces to the level shift is (according to the estimates of Ref. 9) small for the parameter values adopted here.

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