

System of ideal quantum dots with Coulomb interaction

A.M. Mandel, V.B. Oshurko, S.M. Pershin

Abstract. The wave functions of single-electron states localised on a system of single-level ideal quantum dots in a semiconductor matrix are constructed. The standard Kane theory, which describes the renormalisation of the effective mass of electrons in bulk III–V semiconductors, is transformed, for the first time as far as we know, for small-size quantum dots. The renormalised electron mass in a quantum dot depends on its ground state energy, which, in turn, depends on this mass. Thus, a self-consistent problem is obtained for calculating the electron binding energy. The radius of the Debye screening of the Coulomb interaction in a system of quantum dots is calculated at room temperature. The Coulomb repulsion of electrons localised on dots limits from above the possible number of filled dots. The condition is formulated for the optimal concentration of quantum dots. A classical distribution function for the probability of quantum dot filling is constructed. It is found the state, where electrons fill exactly half the maximum possible number of filled dots, exhibits the minimal energy (and therefore the most stable), the condition being fairly universal. In particular, it can be used to estimate the limiting efficiency of quantum-dot diode lasers.

Keywords: system of single-level ideal quantum dots, Coulomb interaction, binding energy, transformation of Kane's theory for small quantum dots, critical size of ideal dots, Debye radius in the system of dots, distribution function over the number of filled dots, condition of optimal filling.

1. Introduction

The possibility of designing optical or optically controlled quantum computers, in particular, quantum-dot computers playing the role of qubits, has always been one of the most impressive problems of quantum electronics [1, 2]. Recently, however, it has become clear that the interaction in a system of quantum dots is more complicated than was previously

assumed [3]. This is especially important for a system of quantum dots immersed in a semiconductor matrix. In this case, the interaction with the environment can disturb the energy structure of the dot levels so much that the approximation of an isolated dot becomes unsuitable. On the other hand, the correct allowance for this interaction can make it possible to find new ways to increase the efficiency of electronic quantum-dot devices (in particular, lasers).

As is known, zero-dimensional heterostructures that can localise free charges in their potential wells are called quantum dots. They are considered ideal when they are able to localise only one electron [4]. In order for such dots to fail to bind holes, the energy structure of the heterosystem must be covariant [5], that is, both the bottom of the conduction band and the top of the valence band of the dot material must be lower than those in the matrix (in the barrier material). Due to its 'pure' spectrum, as well as the simplicity of its control by external fields, single-level ideal quantum dots will have many applications in nanoelectronics and spintronics, especially in connection with the problem of quantum information processing [6, 7].

In our previous papers [8–12], we calculated critical sizes, various characteristics of electronic states and their behaviour in external fields for single isolated quantum dots. In this case, we, following the overwhelming majority of other authors, used the tabular value characteristic of this medium as the effective mass of the bound electron in the material of the dot. However, as a more thorough analysis of the standard Kane (k, p)-model showed [13–15], the effective electron mass in a small quantum dot is renormalised not in the same way as in a bulk semiconductor. The main difference is that the mass depends on the energy of the ground state of an electron localised on the dot. This energy, in turn, itself depends on the effective mass of the electron and the size of the dot. The main goal of this paper is to propose an algorithm for determining the level energy and critical sizes in a system of single-level ideal quantum dots, taking into account the 'self-consistency' of the effective mass with the size of the dots, as well as to study the Coulomb interaction of such dots and their statistical distribution over filling probabilities at room temperature. We note right away that the obvious next (and, in our opinion, decisive) step in this direction is to take into account the exchange interaction of electrons in single-level ideal quantum dots. Physically it is clear what this will lead to. Therefore, in this work, we actually study the background, on which the spins of electrons localised on such dots will interact.

The paper has the following structure. In Section 2, we formulate and solve a transcendental equation for the energy of a single bound electron level in an ideal quantum dot. Its

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solution is determined by the size of the dot, by the depth of the potential well (jump in the energy of the bottom of the conduction band at the heterojunction), by the effective masses of electrons in the materials used and, to a lesser extent, by the average concentration of dots. To calculate the effective mass, the standard Kane model has been modified (for the first time, as far as we know) for small-size quantum dots (that is, it is actually brought into line with the dimensional quantization rules). It is shown that the critical size of a dot at which it remains single-level, and the level energy itself depend in a complex way on the average concentration of dots. It is fundamentally important that unlike the case of an isolated dot, a system of dots has no limit on the size of dots from below, at which the first bound level appears.

Section 3 deals with the screening of the Coulomb interaction of electrons localised on single-level ideal quantum dots by free charge carriers in the matrix. We confine ourselves to the case of semiconductors at room temperature. The screening under these conditions has a generally classical Debye character. We also calculated its effective radius in the system of dots.

In Section 4, we study the effect of the Coulomb repulsion of localised electrons on the probability of quantum dot filling. The energy of this repulsion (for a fixed size of dots) is proportional to the square of the total number of filled dots, and the total binding energy of electrons at points is proportional to the first power of this number. Therefore, from a certain moment of time the electron is forced out of the potential well. Consequently, the Coulomb interaction leads to a limitation from above on the possible number of single-level ideal dots filled with electrons. The maximum possible number of filled dots is proportional to the sample volume, dielectric constant of the matrix, electron binding energy, and is inversely proportional to the square of the Debye length. The most stable state of the system of such dots will be the state in which the number of filled dots will be exactly half the maximum possible number. This condition is universal in the sense that it does not depend on the properties of materials of the corresponding heterostructure and the concentration of dots. It is due only to the above-mentioned dependences on the number of filled dots of negative binding energy and positive Coulomb repulsion energy. Thus, it becomes meaningless to unnecessarily increase the concentration of single-level ideal quantum dots, because they will remain ‘empty’. This undoubtedly is directly related to the efficiency of semiconductor quantum dot lasers. In this section, we also construct a classical (Maxwellian) distribution function for the number of filled dots.

2. Transcendental equation for the energy of a single level of an ideal quantum dot and its solution. Critical size of a single-level ideal point

Monographs [16, 17] considered electronic states in the δ -potential system. Our situation is different only in the fact that we describe potential holes of finite size and depth. Nevertheless, both the Schrödinger equation for the single-electron state and its solution (essentially Green’s function) in the external matrix (in a space between the potential wells produced by the dots) are written exactly in the same manner as in the mentioned monographs:

$$-\frac{\hbar^2}{2m_{\text{ex}}^*}\Delta\psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad |\mathbf{r} - \mathbf{r}_i| > R, \quad (1)$$

$$\psi(\mathbf{r}) = A \sum_i [\exp(-\kappa |\mathbf{r} - \mathbf{r}_i|)] / |\mathbf{r} - \mathbf{r}_i|. \quad (2)$$

Here Δ is the three-dimensional Laplace operator; $E < 0$ is the electron binding energy in an ideal dot, which, as usual, is measured from the bottom of the conduction band of the barrier material; m_{ex}^* is the effective electron mass in the barrier material; R is the dot radius; $i = 1, \dots, N$ is the number of a specific quantum dot; $\kappa = \sqrt{-2m_{\text{ex}}^*E/\hbar^2}$ is the wave number of the bound electron in the material of the barrier; and A is the normalisation constant, which is insignificant.

In what follows, we will consider single-level ideal quantum dots as spheres of radius R and concentration n , the depth of the potential well being determined by the energy jump ΔE_c of the bottom of the conduction band at the heterojunction:

$$U(\mathbf{r}) = \begin{cases} -\Delta E_c, & r < R, \\ 0, & r > R. \end{cases} \quad (3)$$

Consequently, in the interior of the dot, the Schrödinger equation for single-particle states takes the form

$$-\frac{\hbar^2}{2m_{\text{in}}^*(R)}\Delta\psi(\mathbf{r}) - \Delta E_c\psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad |\mathbf{r} - \mathbf{r}_i| < R, \quad (4)$$

where the dependence $m_{\text{in}}^*(R)$ of the effective mass of an electron inside a single-level ideal dot on the size of the dot is introduced.

Below we will proceed from the condition

$$R \ll 1/\sqrt[3]{n}, \quad (5)$$

that is, the dots are not too densely packed, so that the average distance between neighbouring dots is much larger than their size. Then, following [16], in the vicinity of a dot with a specific number j , the electron radius vector \mathbf{r} can be ‘frozen’ in all terms (2), except for one relating to this dot. As a result, solution (2) transforms to

$$\psi(\mathbf{r}) = A \left[\frac{\exp(-\kappa\rho_j)}{\rho_j} + \sum_{i \neq j} \frac{\exp(-\kappa r_{ij})}{r_{ij}} \right], \quad (6)$$

where $\rho_j = |\mathbf{r} - \mathbf{r}_j|$, a $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between the centres of the dots. Following again [16], the sum in (6) can be estimated by replacing it with the integral:

$$\sum_{i \neq j} \frac{\exp(-\kappa r_{ij})}{r_{ij}} \rightarrow 4\pi n \int_0^\infty \exp(-\kappa r) r dr = \frac{4\pi n \hbar^2}{-2m_{\text{ex}}^*E}. \quad (7)$$

Now, similarly to [8, 10, 12], we write out solution (4) in the region inside the dot:

$$\psi(\mathbf{r}) = \frac{A \sin[\rho_j \sqrt{2m_{\text{in}}^*(R)(\Delta E_c + E)/\hbar^2}]}{\rho_j}. \quad (8)$$

In approximation (5), it is formally analogous to the solution inside an isolated dot.

For the closure of the problem, we only need to obtain an explicit dependence of the effective electron mass on the size

of the dot, $m_{\text{in}}^*(R)$. As is known, the process of mass renormalisation in a bulk II–V semiconductor (of type InAs, AlSb, GaAs, etc.) is described by the Kane (k, p) theory [13–15]. We should transform it in accordance with the rules of dimensional quantisation, that is, in fact, take into account the finite size of the quantum dot. We very briefly recall the main ideas of the Kane model, relating to our situation. The electron mass in the s-state in the vicinity of the minimum of the conduction band (doubly degenerate in spin) is renormalised due to the mixing of this state with the p-state of the hole in the vicinity of the maximum of the valence band (sixfold degenerate). Spin–orbit interaction splits this hole state into four-fold degenerate (heavy holes with a total angular momentum projection of 3/2 and light holes with a total angular momentum projection of 1/2) and doubly degenerate, separated from this maximum by the magnitude of the energy of the spin–orbit interaction Δ and also related with light holes (total momentum of 1/2). In the first order of the perturbation theory, the mixing energy – the Kane energy E_P – is proportional to the square of the matrix element of the momentum between the indicated states. Thus, the complete Kane equation is an equation for an eight-component ‘tetraspinor’ with the 8×8 Hamiltonian. As a result, for the effective mass of an electron in the vicinity of the minimum of the conduction band, Kane’s theory gives the expression:

$$\frac{m}{m_{\text{in}}^*} = 1 + \frac{E_P(3\varepsilon_g + 2\Delta)}{3\varepsilon_g(\varepsilon_g + \Delta)}, \quad (9)$$

where m is the free electron mass, and ε_g is the width of the forbidden zone; the coefficients in the right-hand side take into account the multiplicity of the degeneracy of the mixed states. [Formula (9) is the simplest expression, taking into account the contribution of only the valence band to the renormalisation of the electron mass at the bottom of the conduction band. Generally speaking, all zones contribute to the renormalisation, which is usually taken into account by introducing a small fitting parameter in (9).] The original equations (1), (4) with a renormalised mass are the coordinate part of the Pauli equation for the envelope of the electron wave function at the bottom of the conduction band, split from the original eight-component equation [13, 18].

How to bring this expression into line with the rules of dimensional quantization, that is, in fact, to take into account the ‘incompleteness’ of the band structure in a small size quantum dot? According to [15], the determining parameter in (9) is the band-gap energy ε_g . The type of the semiconductor – a narrow-gap or a wide-gap semiconductor – primarily determines the value of the effective mass (and, by the way, the Lande factor) of an electron at the bottom of the conduction band. It is well known that in narrow-gap materials electrons are most mobile. The energy of spin–orbit splitting is determined mainly by intra-atomic interactions, and the Kane energy is a parameter that is slightly different for different materials significantly exceeding the band-gap energy.

Thus, the incompleteness of the band structure in a quantum dot of small size should primarily affect the value of ε_g , that is, the actual distance (on an energy scale) between the top of the valence band and the bottom of the conduction band. But then the easiest way to take into account the size of a quantum dot is to replace ε_g with $\varepsilon_g + \Delta E_c - E$, which is the energy gap between the top of the valence band and the ground state of the electron in the quantum dot. (We do not

consider similar hole effects in the vicinity of the top of the valence band, because we assume the covariance of the heterostructure, which was discussed above.) As a result, for the effective mass we obtain (see also [19]) the equation

$$\frac{m}{m_{\text{in}}^*(R)} = 1 + \frac{E_P[3(\varepsilon_g + \Delta E_c - E) + 2\Delta]}{3\varepsilon_g(\varepsilon_g + \Delta E_c - E)(\varepsilon_g + \Delta E_c - E + \Delta)}. \quad (10)$$

Next, using the algorithm [16], we construct an auxiliary function $\rho_j \psi(\rho_j)$ in the vicinity of the j th dot, where $\psi(\rho_j)$ is determined from (6), (8), and set the continuity condition for the logarithmic derivative at the boundary of the dot, $\rho_j = R$. This leads to a transcendental equation for the electron binding energy

$$\begin{aligned} & \sqrt{2m_{\text{in}}^*(R)(\Delta E_c + E)} \cot(R\sqrt{2m_{\text{in}}^*(R)(\Delta E_c + E)}/\hbar) \\ &= \frac{-\sqrt{2m_{\text{ex}}^*E} \exp(-R\sqrt{-2m_{\text{ex}}^*E}/\hbar) + 4\pi n \hbar^3 / (-2m_{\text{ex}}^*E)}{\exp(-R\sqrt{-2m_{\text{ex}}^*E}/\hbar) + 4\pi n \hbar^2 / (-2m_{\text{ex}}^*E)}, \quad (11) \end{aligned}$$

which, together with equation (10), allows us to calculate it.

We can significantly simplify and clarify the physical meaning of the obtained equation by passing to more natural dimensionless units of length and energy:

$$R \rightarrow R/l_0 = R\hbar/\sqrt{2m_{\text{ex}}^*\Delta E_c}, \quad E \rightarrow \varepsilon = (-E)/\Delta E_c.$$

Here, l_0 is the de Broglie length for an electron with energy ΔE_c , and ε is the binding energy in fractions of the depth of the potential well. Equation (11) in the new units will take the form

$$\begin{aligned} & \sqrt{\frac{m_{\text{in}}^*}{m_{\text{ex}}^*}(1 - \varepsilon)} \cot\left[\frac{R}{l_0} \sqrt{\frac{m_{\text{in}}^*}{m_{\text{ex}}^*}(1 - \varepsilon)}\right] \\ &= \frac{-\varepsilon^{3/2} \exp(-R\sqrt{\varepsilon}/l_0) + 4\pi n l_0^3}{\varepsilon \exp(-R\sqrt{\varepsilon}/l_0) + 4\pi n l_0^2 R}. \quad (12) \end{aligned}$$

It is clear that mass renormalisation is in fact equivalent to a change in the scales of the electron localisation inside a dot.

The results of the calculation of the binding energy at various concentrations of quantum dots are shown in Fig. 1. In this case, we used the data for the covariant InAs/AlSb heterostructure from review [20]; the data are given in the figure caption. Figure 1 shows the starting concentration of quantum dots at which its influence on the binding energy becomes noticeable.

The most important question is in what range of sizes a quantum dot remains single-level, that is, ‘holds’ no more than one bound electronic state. For the exact answer it is necessary to solve numerically equation (12) in the limit $\varepsilon \rightarrow 0$, when it reduces to the equation

$$\sqrt{\frac{m_{\text{in}}^*(R)}{m_{\text{ex}}^*}} \cot\left[\frac{R}{l_0} \sqrt{\frac{m_{\text{in}}^*(R)}{m_{\text{ex}}^*}}\right] = \frac{l_0}{R}, \quad (13)$$

moreover, the value of n itself is not included directly in the formula. It immediately follows that the smallest critical size, that is, the minimum radius R_{min} at which the first bound level appears in a potential well, is equal to zero, unlike the case of single isolated dots. This is in complete agreement with the results of paper [16].

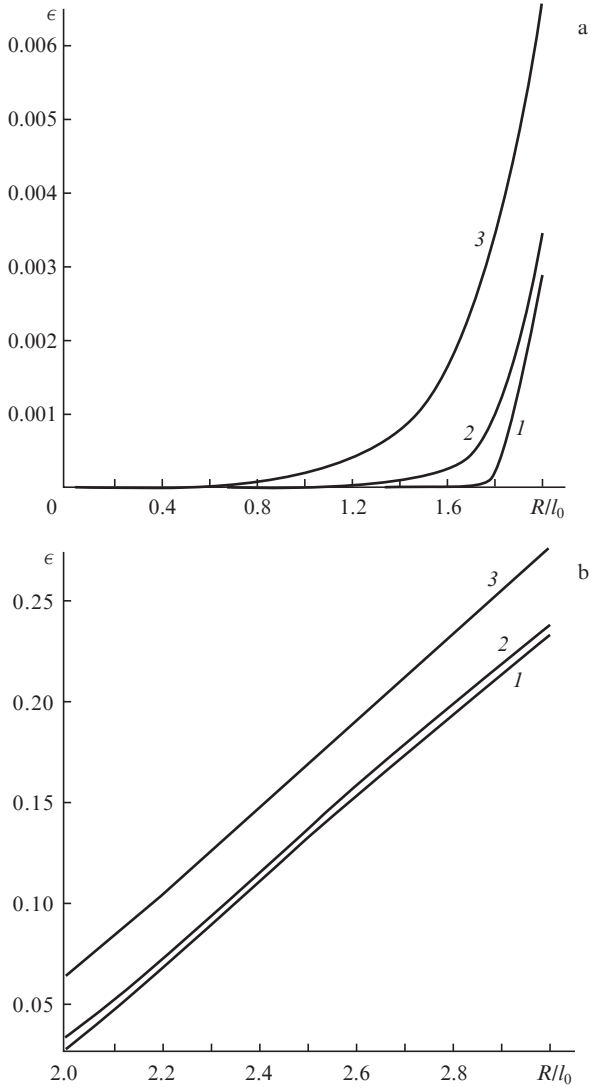


Figure 1. Binding energy ϵ of an electron localised on a single-level ideal quantum dot as a function of the dot radius for an InAs/AlSb heterostructure with the following parameters [20]: $\Delta E_c = 2.2$ eV, $\epsilon_g = 0.42$ eV, $\Delta = 0.39$ eV, $m_{in}^*(\infty) = 0.023m$ in InAs, and $m_{ex}^* = 0.14m$ in AlSb. Concentrations are as follows: $n = (1) 10^{16}$, $(2) 10^{17}$ and $(3) 10^{18}$ cm $^{-3}$; the length is $l_0 \approx 0.33$ nm.

The largest critical size of a quantum dot is determined by the condition for the appearance of the second bound level, after which the dot naturally ceases to be an ideal single-level one. The problem of finding it for single isolated dots in an external magnetic field was solved in [8, 10], and in an external electric field in [12], although in the approximation $m_{in}^*(R) = m_{in}^*(\infty)$. For a system of dots, by approximating $\cot x$ in the vicinity of the second zero ($x = 3\pi/2$) by the linear function*, from (13) we can obtain

$$R_{max} = \frac{3\pi}{4} \left(1 + \sqrt{1 - \frac{16}{9\pi^2}} \right) \sqrt{\frac{m_{ex}^*}{m_{in}^*(R_{max})}} l_0 \approx 4.5 \sqrt{\frac{m_{ex}^*}{m_{in}^*(R_{max})}} l_0. \quad (14)$$

*Such an approximation is possible with practically any realistic ratios of the effective masses. In review [20], for example, for a sufficiently large number of heterostructures considered there, we did not find any counterexamples.

The solution of this equation together with (12) and (10) determines the ideality range of spherical quantum dots. In particular, for the considered InAs/AlSb heterostructure, the radius $R_{max} \approx 4.976l_0 \approx 1.64$ nm and, again, practically does not depend on the concentration of dots.

Of interest are also the dependences of the energy of the bound level on the concentration of quantum dots. They are shown in Fig. 2. The concentration is given in dimensionless units nl_0^3 . Note that in this form it enters the equation for the binding energy (12). The upper limit of the concentration range corresponds to $n = 10^{18}$ cm $^{-3}$. It would seem to follow from Fig. 1 that with an increase in the radius of a quantum dot and, accordingly, the modulus of the ground-state energy, the sensitivity to changes in concentration also increases, but this is not quite the case. Electrons in small quantum dots are more sensitive to the presence of neighbouring dots (in fact, neighbouring potential wells) due to the large size of the electron cloud. This is most clearly illustrated by the following circumstance: single isolated dots with $R < R_{min}$ are not able to localise an electron at all, while in a system of dots (that is, for sufficiently large n), it is localised formally for arbitrarily small sizes of dots. In other words, the electron is ‘virtually present’ in a set of quantum dots. (It can be said this way: a set of dots forms a single ‘multi-cell’ potential well.) In our opinion, this is directly related to the possibility of implementing quantum computing in the system under consideration.

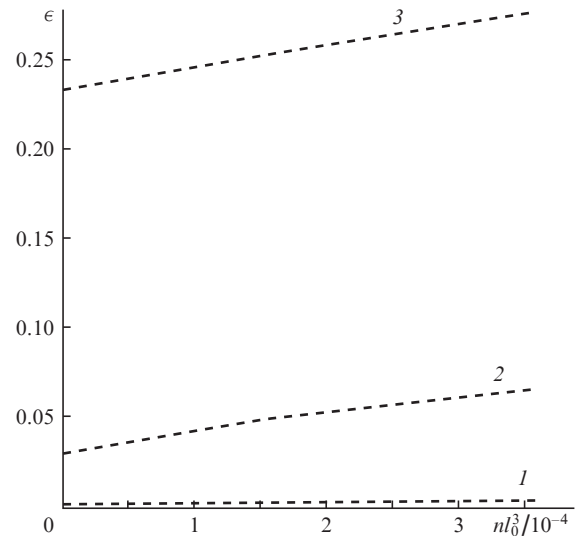


Figure 2. Binding energy ϵ of an electron localised on a single-level ideal quantum dot as a function of the concentration of dots for an InAs/AlSb heterostructure, the parameters of which are given in the caption to Fig. 1, at $R = (1) l_0$, $(2) 2l_0$ and $(3) 3l_0$.

3. Mechanisms for screening the charge of localised electrons

A quantum dot is, in essence, a potential well in which a negative charge can concentrate. There are two simplest mechanisms for screening this charge in a medium with free carriers. The first is the conventional Debye mechanism, that is, the formation of an external, sufficiently extended and mobile screening cloud around a charge localised on a dot. The sec-

ond is the embedment of holes into the vicinity of a potential barrier at the dot boundary. Clearly, the hole repulsive barrier potential* decreases under the action of a localised electron field, which distorts the structure of the barrier at the heterojunction. If the total potential in the vicinity of the dot boundary is above the top of the valence band in the matrix, this effect is classical, if below, we are dealing with quantum capture of holes into the potential barrier. A similar mechanism is characteristic of stronger (than Debye) Reed screenings and was considered in [21] for extended linear dislocations. As a result, the first of the described mechanisms exponentially cuts off the potential of a quantum dot filled with an electron at some distance, and the second one reduces the effective charge of a localised electron.

The criterion for the applicability of the weak-screening (Debye) approximation is the condition that the kinetic energy of the charge exceeds the potential energy [15]:

$$\frac{e\varphi_0(\rho_j)}{k_B T} < 1, \quad (15)$$

where $\varphi_0(\rho_j)$ is the potential produced by an electron localised on a single-level ideal dot. Possible violations of this condition in the neighbourhood of the dot boundary provide the conditions for the implementation of the second screening mechanism. Below, we will consider this condition fulfilled. It is clear that consistent consideration of the strong screening mechanism requires self-consistent consideration of the reverse effect of localised particles on the initial potential of the heterostructure and distorts the simple solutions (6) and (8) which we used. The rough action of the second screening mechanism can be taken into account, implying that the electron charge e is some effective charge, less than usual.

The Poisson equation describing the distribution of the potential in the vicinity of the j th dot with a filled electronic state has the form

$$\Delta\varphi = -\frac{q_e + q_i}{\varepsilon_0\varepsilon} = \frac{\varepsilon A^2 \exp(-2\kappa\rho_j)}{\varepsilon_0\varepsilon\rho_j^2} - \frac{2e^2 n_0 \varphi}{\varepsilon_0\varepsilon k_B T}. \quad (16)$$

Here q_e is the charge density produced by a localised electron; q_i is the induced charge density in the ‘Debye cloud’ of free carriers; n_0 is the concentration of free charge carriers in the barrier material; and ε is the dielectric constant of the barrier material. The expression for the induced charge density is linearised by the potential according to (15). In other words, in the dot of the medium with potential φ , the excess Δn of the concentration n_e of free electrons by the concentration n_h of free holes is estimated as

$$\begin{aligned} \Delta n &= n_h - n_e \\ &= n_0 \left[\exp\left(\frac{e\varphi}{k_B T}\right) - \exp\left(-\frac{e\varphi}{k_B T}\right) \right] \approx 2n_0 \frac{e\varphi}{k_B T}. \end{aligned} \quad (17)$$

Rewriting equation (16) in canonical form, we obtain

$$\frac{d^2\varphi}{d\rho_j^2} + \frac{2}{\rho_j} \frac{d\varphi}{d\rho_j} + \frac{\varphi}{L_D^2} = \frac{eA^2 \exp(-2\kappa\rho_j)}{\varepsilon_0\varepsilon\rho_j^2}, \quad (18)$$

where

$$L_D = \sqrt{\frac{\varepsilon_0\varepsilon k_B T}{2e^2 n_0}} \quad (19)$$

is the Debye screening length. The presence of 2 in the denominator is associated with the presence of two types of charge carriers in the intrinsic semiconductor producing a screening Debye cloud.

Equation (18) can be simplified if we take into account the fact that

$$1/\kappa \ll L_D. \quad (20)$$

In fact, at typical room temperature free-carrier concentrations of $n_0 \approx 10^8 - 10^{11} \text{ cm}^{-3}$, the screening length in intrinsic semiconductors is estimated to be $L_D \approx 3 - 300 \text{ }\mu\text{m}$. The $1/\kappa$ value can reach such values only at the binding energies of the localised electron, $\varepsilon \approx 10^{-8} - 10^{-10} \text{ eV}$. At such negligibly small energies, the bound state of an electron in a quantum dot, of course, will not be stable. Therefore, on the right-hand side of (18), one can make a replacement

$$A^2 \exp(-2\kappa\rho_j) / \rho_j^2 \rightarrow \delta(\rho_j). \quad (21)$$

In fact, this is a transition to the approximation of a point charge in equation (18), the possibility of which is due to relations (5) and (20). As a result, solution (18) takes on a more familiar form:

$$\varphi(\rho_j) = \frac{\exp(-\rho_j/L_D)}{4\pi\varepsilon_0\varepsilon\rho_j}. \quad (22)$$

4. Coulomb interaction of single-level ideal quantum dots. Optimal number of filled dots. Maxwell distribution for the number of filled dots

The electrons localised on dots, although screened by the Debye clouds, will interact with each other. It is clear that the energy of this Coulomb repulsion is positive and proportional to the square of the number of dots filled with electrons. Therefore, at a certain concentration of quantum dots, the Coulomb repulsion energy compensates for the total negative binding energy of electrons at single-level ideal dots, and the level will be ‘crowded out’ of the potential well. Naturally, this limits the number of quantum dots filled with electrons from above. Accordingly, the initial concentration of the considered dots is limited.

The energy of the Coulomb interaction per one filled dot can be estimated using the same algorithm as in (7), by replacing the sum with the integral:

$$\begin{aligned} \varepsilon_Q &= \frac{e^2 \tilde{n}}{\varepsilon_0\varepsilon} \int_R^L dr r \exp\left(-\frac{r}{L_D}\right) = \frac{e^2 \tilde{n}}{\varepsilon_0\varepsilon} \left[(R + L_D)^2 \exp\left(-\frac{R}{L_D}\right) \right. \\ &\quad \left. - (L + L_D)^2 \exp\left(-\frac{L}{L_D}\right) \right]. \end{aligned}$$

Given that the linear size of the sample is $L \approx 1 \text{ cm}$, the Debye length is $L_D \approx 3 - 300 \text{ }\mu\text{m}$ and the radius of the single-

* For the mentioned InAs/AlSb heterostructure, this barrier (the energy jump of the top of the valence band at the heterojunction) is 0.2 eV [20].

level ideal dot is $R \approx 1-3$ nm, for the energy of the Coulomb repulsion we obtain the estimate:

$$\epsilon_Q \approx \frac{e^2 \tilde{n} L_D^2}{\epsilon_0 \epsilon} = \frac{e^2 N L_D^2}{\epsilon_0 \epsilon \Omega}, \quad (23)$$

where \tilde{n} is the average concentration of the dots filled with electrons ($\tilde{n} \leq n$); $N = \tilde{n} \Omega$ is the total number of these dots; and $\Omega \approx 1$ cm³ is the characteristic sample volume.

It is clear that quantum dots will no longer be filled with electrons when it is energetically unfavourable, that is, under the condition

$$\epsilon_Q - \epsilon = 0.$$

Therefore, the maximum possible number of filled dots is

$$N_{\max} = \frac{\epsilon_0 \epsilon \Omega \epsilon}{e^2 L_D^2} = \frac{2n_0 \Omega \epsilon}{k_B T}. \quad (24)$$

Taking into account the above values of the constants characteristic of intrinsic semiconductors at room temperature, we have $N_{\max} \approx 10^8 - 10^{11}$.

Naturally, the question arises of how justified the initial one-particle approximation (6)–(11) is for determining the binding energy in the presence of neighbouring dots and the Coulomb interaction of localised electrons. Estimate (24) a posteriori justifies it. One can see from Figs 1 and 2 that for a tangible effect on the binding energy, a much larger concentration of single-level ideal quantum dots is needed than that given by the estimate of N_{\max} . As for the Coulomb interaction, the approaches used in obtaining estimates (23) and (24) are similar to the pseudopotential approximation [16].

The most stable state of a matrix with single-level ideal quantum dots will, of course, be a state with minimal energy. The total energy of a system of dots with the Coulomb interaction will be $N(\epsilon_Q - \epsilon)$, and the condition for its minimisation will determine the most probable number of dots filled with electrons:

$$N_0 = \frac{\epsilon_0 \epsilon \Omega \epsilon}{2e^2 L_D^2} = N_{\max}/2. \quad (25)$$

The latter condition is independent of the specific parameters of the heterostructure used and, in this sense, is universal. It is due, in essence, only to the fact that the total negative binding energy is proportional to the number of filled dots, and the positive Coulomb repulsion energy is proportional to the square of this number. This completely determines the position of the minimum energy. (A very interesting analogy with the energy of the ground state of a heavy nucleus is seen here. The total negative nuclear energy is proportional to the total number of nucleons, and the positive energy of the Coulomb repulsion is proportional to the square of the number of protons. Moreover, the strong interaction energy per one nucleon, as well as the localised electron binding energy, is considered to be independent of the Coulomb repulsion energy.)

Let us now construct the distribution function (of the Maxwell–Boltzmann–Gibbs type) with respect to the number of dots filled with electrons. It is easy to see that the minimum total energy of a system of dots is

$$E_{\min} = -\frac{\epsilon_0 \epsilon \Omega \epsilon^2}{4e^2 L_D^2},$$

and its fluctuations due to a change in the number of dots filled with electrons is

$$\Delta E = -\frac{e^2 L_D^2 (N - N_0)^2}{\epsilon_0 \epsilon \Omega}.$$

Thus, the distribution function for the number of filled single-level ideal quantum dots (or the probability of filling the dot with an electron) has the form:

$$p(N) \propto \exp\left[-\frac{e^2 L_D^2}{\epsilon_0 \epsilon \Omega k_B T} (N - N_0)^2\right].$$

Note in conclusion that in our work [8–12], we investigated some methods for controlling the wave function and spin states of electrons localised on single-level ideal quantum dots using external electric and magnetic fields. All this, in combination with the pure spectrum of single-level ideal dots, makes the systems described in the work extremely attractive for solving a whole range of microelectronics problems in general and spintronics and quantum information processing in particular. Regarding the evaluation of the maximum efficiency of diode quantum dot lasers, we intend to devote our next work to this issue.

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