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Energy spectrum of ideal quantum dots controlled by an external electric field

A.M. Mandel, V.B. Oshurko

Abstract. **We have constructed a theoretical model describing the energy spectrum and autoionisation probability for an ideal quantum dot in the external DC and AC electric fields, free of using the delta-potential approximation and perturbation theory. The wave functions of the electron quasi-stationary states under these conditions are calculated. To this end, we have elaborated a new method for regularising the Gamov wave function used to calculate the complex electron energy, describing both the energy spectrum of the system and the probability of the state decay (autoionisation). The oscillations of the Stark shift and the energy level width due to the DC electric field are found. It is shown that these oscillations essentially affect the energy spectrum of the quantum dot and principally cannot be described within the frameworks of perturbative approaches.**

Keywords: *ideal quantum dots, external electric field, regularisation of Gamov wave function, oscillations of Stark shift and energy level width.*

1. Introduction

At present the problems of interaction between intense electromagnetic fields (in particular, laser fields) and various nanostructures are a subject of considerable interest [1–6]. It is due to the prospects of development and application of different types of nanostructures, which stimulated a variety of theoretical and experimental publications on the interaction of intense electromagnetic fields with nanoobjects. In particular, of significant interest is the known problem of theoretical description of the process of quantum dot ionisation by an intense electromagnetic field. Below we mainly consider DC fields, but the effect of the AC component will be also described.

Such a problem was solved, for example, in Refs [3–5]. The closest formulation of the problem was presented in Ref. [3], where the explicit analytical expressions for the 2D quantum dot ionisation probability in DC and AC electric fields were derived without using the perturbation theory. To describe a finite-size quantum dot a 2D quadratic potential was used. However, the main result was obtained on the basis of the Green function, which is a solution of the Schrödinger equation only in the exterior domain of the quantum dot. It is well known that this solution is fundamentally based on the approximation of the potential by a Dirac delta-function. As a result, the authors of Ref. [3] actually could not consider the effect of the dot final dimensions and reproduced the known results for the ionisation probability in the attractive delta-function potential. This obviously restricts the applicability of the model to the description of real experimental results.

In the description of a finite-dimension potential well in an external electric field, we encounter two serious problems. First, in the Schrödinger equation the axial symmetry imposed on the system by the field 'conflicts' with the symmetry of the boundary conditions caused by the shape of the quantum dot (in our case it is spherical). As a result, the analytical solution is expressed as a double series of special functions (see, e.g., [7]). It is extremely difficult to find eigenvalues for such solutions. Second, the rather old problem of regularising the so-called Gamov wave function still remains not completely solved [8, 9].

This problem was first formulated and actively studied in alpha-decay theory [8]. Strictly speaking, the wave function here is not a solution of the steady-state Schrödinger equation because of the finite lifetime of the state. Nevertheless, the steady-state Schrödinger equation still can be used, if the probability of the state decay is small. To this end, an imaginary term proportional to the decay rate should be introduced into the Hamiltonian eigenvalues. However, the normalisation integrals and a number of other physical quantities containing integrals of the wave function diverge, as could be expected for a 'dissociable' system [10]. This fact significantly complicates the manipulation with the quasi-stationary states and makes the correctness of the obtained results doubtful. In the DC electric field, the situation is even more complex. Here the Gamov wave function itself has the form of an exponentially diverging integral (see, e.g., [11]).

We know only two ways to solve this problem, and both have been formulated only in the approximation of the attractive delta-function potential. The first one [12] is based on the transformation of the single-fold (already rather cumbersome) integral expressing the Green function in the electric field into a two-fold integral. We were not able to repeat the authors' calculations and thoroughly discussed the issue in Ref. [13]. In the second approach, Mur et al. [14] apply the Zeldovich's idea [9] to introduce a regularising factor, $\exp(-\alpha r^2)$, $\alpha \to 0$, into the integrand, where r is the radial variable of the spherical system. This method is obviously simpler than the first one. However, as noted by the authors themselves [14], the domain of its applicability is restricted to the

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situation when the real part of the energy is greater than the imaginary one. Moreover, here the integrand is complicated with not quite clear consequences, which, in our opinion, requires an independent way of the correctness checking.

The combination of two above problems makes the description of a quantum dot (i.e., a potential well of finite size and depth) in an external electric field a rather difficult problem to solve*. At present two approaches to its solution have been outlined. In the first approach (see, e.g., [5]) the boundary conditions that determine the spherically symmetric structure of the solution are considered exactly, but the electric field is described within the framework of the perturbation theory, which allows one to avoid the problem of the Gamov function divergence. However, the calculations within this approach are extremely cumbersome and hardly reproducible, so that it is difficult to evaluate the physical picture and the domain of the model applicability. To simplify the situation, the authors had to assume equal the electron and hole effective masses, which undoubtedly restricted the model**. Finally, the description reduced to the common 'tunnel exponent' approximation for the energy level width {Eqns (16) and (20) from Ref. [5]}, in which the electric field is taken into account only within the frameworks of the perturbation theory. However, the authors found an effect unexpected for problems of this sort, namely, the sign of the electric field-induced correction to the energy level width was found to change depending on the coupling energy. In our opinion, this result has the same origin as the oscillations of the energy level width in the DC electric field found by us.

The second approach to the description of quantum dots in the electric field is somewhat opposite to the first one. Here the effect of the electric field is considered exactly, and the quantum dot is modelled by a delta-function well. An example is paper [3], already mentioned above. The comparison of its result with our ones is of particular significance, since we use an analogous representation for the attractive potential of the quantum dot and the similar continuity condition for the logarithmic derivative on the spherical boundary of the dot to determine the energy level. The difference in the geometry of the problems (in Ref. [3] they consider ionisation from 2D dots) is absolutely inessential for understanding the physical meaning of the present model. The key point is that for the solution the authors use the Green function that is a solution of the equation only in the exterior domain of the quantum dot {Eqns (7), (9) from Ref. [3]}. The origin of this solution is also clear from the character of the presented reference. Moreover, performing the saddle-point evaluation of the obtained integral, the authors of [3] use the contribution of only one saddle point, which is also typical for the delta-function potential approximation. If the radius of the potential well does not tend to zero, there must be two saddle points [see Eqn (7) of the present paper]. One of them conserved in the approximation of the delta-function well makes the major contribution to the energy level width, while the other one that vanishes in this approximation determines its oscillations. Thus, in our opinion, the authors of Ref. [3] only declare the finite-size quantum well problem. Hence, it is not surprising that the final result for the ionisation probability (level width) in the DC electric field {Eqn (29) from Ref. [3]} reproduces the old and well known result for the delta-function potential well [11] with a certain correction for the problem geometry.

In the present paper, we construct a model that combines the advantages of the two above approaches. We describe ideal quantum dots, i.e., zero-dimensional semiconductor heterostructures, the potential wells of which admit only one bound-state energy level [15]. To avoid the hole localisation in the well with further exciton formation, the energy structure of the dot should be 'covariant' [16] with respect to the matrix, i.e., both the bottom of the conduction band and the top of the valence band should be lower than those in the matrix.

From the practical point of view, the simple spectrum of ideal quantum dots and the sensitivity of the spectrum to the effect of external magnetic and electric fields provide a base for multiple applications in nanoelectronics, spintronics, laser physics, etc. A number of characteristics of ideal 3D spherical quantum dots in the magnetic field has been calculated in our papers [17–20]. The aim of the present paper is to propose a more correct theoretical description of an ideal quantum dot in the external DC and AC electric fields. For this purpose, we elaborate a method for the regularisation of the wave function, simple in computations and having no limitations on the ratio of the real and imaginary parts of energy. The method based on introducing a small negative imaginary addition to the field strength is used to calculate the complex-valued energy of the electron, localised in an ideal quantum dot. One of consequences of the found solution is the effect of oscillations of the Stark shift and energy level width in the DC electric field. As far as we know, this effect has not been previously described. Thus, we study the capabilities of using the electric field to control the energy spectrum of an ideal quantum dot.

2. Wave function of a bound electron in the electric field

As a potential well, let us consider a semiconductor heterostructure, such as a spherical quantum dot with a radius R in an external matrix. Similar to [17] and other papers, we define the attractive potential in the form

$$U(r) = \begin{cases} -|U_0|, & r < R, \\ 0, & r > R, \end{cases} \tag{1}$$

where the depth of the potential well $|U_0|$ is the difference of energies of the conduction band bottom of the matrix and the dot; and r is the radial coordinate of the spherical system.

For $r > R$ the Schrödinger equation in the presence of an electric field has the standard form

$$\frac{\hbar^2}{2m_{\text{ex}}^2}\Delta\psi_{\text{ex}}(\boldsymbol{r}) + (W - eEz)\psi_{\text{ex}}(\boldsymbol{r}) = 0\,. \tag{2}$$

The real part of the complex-valued energy is $\mathrm{Re}(W) < 0$, since this is the binding energy of the state. The rest notations are as follows: m_{ex}^* is the effective mass of an electron in the matrix material; Δ is the Laplace operator in spherical coordinates; e is the absolute value of the electron charge; and E is the modulus of the electric field strength directed along the z axis. The only bound state in the well is an s-state.

* The situation with magnetic field is simpler in this sense, since the state of the electron remains a steady-state one. Therefore, only the problem of two 'conflicting' symmetry species remains.

** The authors of Ref. [5] consider an open quantum dot of 'core–shell' type, from which the tunnelling of electrons is possible even without any external field; see also the analogous paper [6].

In this case, for the solution it is convenient to use the Green function in the electric field (see, e.g., [11, 21, 22]). The solution of this problem for the general case is well known {[22], Eqn (5) on page 844}:

$$\psi(\boldsymbol{r}) = \frac{1}{4\pi}\Big(\frac{m}{2\pi \mathrm{i}\hbar}\Big)^{1/2}\int_0^\infty \frac{\mathrm{d}t}{t^{3/2}}$$

$$\times \exp\frac{\mathrm{i}}{\hbar}\Big[Wt + \frac{mr^2}{2t} + \frac{eEy}{\omega}\Big(\frac{\sin(\omega t)}{\omega t} - 1\Big)$$

$$-\frac{2eEz}{\omega^2 t}\sin^2\frac{\omega t}{2} - \frac{e^2E^2}{2m\omega^2}\Big(t - \frac{4}{\omega^2 t}\sin^2\frac{\omega t}{2}\Big)\Big].$$

Here m is the mass of a free electron; t is the time; x and y are the Cartesian coordinates (the wave propagates along the z axis); and ω is the wave frequency. In the limiting case $\omega \to 0$, the above expression yields the formula for the DC electric field

$$\psi_{\mathrm{ex}}(\boldsymbol{r}) = A\int_0^\infty \frac{\mathrm{d}t}{t^{3/2}}\exp(\mathrm{i}\varphi),$$

$$\varphi = \frac{\mathrm{i}}{\hbar}\Big[\frac{mr^2}{2t} + \Big(W - \frac{1}{2}eEz\Big)t - \frac{(eE)^2}{24m}t^3\Big]$$

where A is a normalisation constant.

It is convenient to make the integration variable dimensionless by the replacement $t \to \tau|U_0|/\hbar$.

After these transformations we arrive at the final expression for the Green function in the electric field in the external matrix (with m replaced with $m \to m^*_{\mathrm{ex}}$)

$$\psi_{\mathrm{ex}}(\boldsymbol{r}) = A\int_0^\infty \mathrm{d}\tau\tau^{-3/2}\exp(\mathrm{i}\varphi^0_{\mathrm{ex}}), \tag{3}$$

where

$$\varphi^0_{\mathrm{ex}} = \frac{m^*_{\mathrm{ex}}|U_0|r^2}{2\hbar^2\tau} + \frac{\tau}{|U_0|}\Big[W - \frac{1}{2}eEz - \frac{(eE\hbar\tau)^2}{24m^*_{\mathrm{ex}}|U_0|^2}\Big].$$

This solution can be essentially simplified based on the following considerations. Obviously, it is axially symmetric. At the same time, condition (1) that determines the shape of the potential well has a spherical symmetry. Thus, a certain 'conflict of symmetries' arises in the problem. The external field 'imposes' a certain symmetry species, and the shape of the well corresponds to a different one. In this situation, it is rather difficult to derive a qualitatively clear analytical solution. Note that the symmetry conflict of this sort is generally typical for processes in external fields [17–20]. The simplest solution is possible in relatively weak fields*. Here the field is considered to be weak in the sense of its critical influence on the situation, if it satisfies the condition

$$E \ll 2|\mathrm{Re}(W)|/(eR). \tag{4}$$

The physical meaning of this condition is rather simple: the work of the field force on the particle that moves along a well should not critically change the binding energy, i.e., should not cause ionisation. In other words, the geometric z region is considered for which expression (4) is valid. This means that the point $z_0 = -2|\mathrm{Re}(W)|/(eE)$, where the available region of common over-barrier motion begins for an electron, should be separated from the well boundaries. In the course of ionisation, the electron is tunnelling into this point at the expense of the electric field work. The electron state will be quasi-stationary if the potential barrier between the points $z = -R$ and $z = z_0$ is broad enough. To calculate the binding energy, we need the Green function only in the vicinity of the potential well. Therefore, in Eqn (3) one can omit the term $eEz/2$ keeping, however, the next term quadratic with respect to the field. This immediately makes the situation spherically symmetric, which essentially simplifies the problem. Let us explain this idea once again. The linear term is 'discarded' because of the validity of inequality (4) rather than because of the absolute smallness of the field E, and this does not mean at all that the next term quadratic with respect to the field weakly affects the situation.

As already mentioned above, the integral in Eqn (3) diverges at the upper limit due to the negative imaginary part of the complex energy W. The simplest and most natural way to suppress this divergence is to introduce a small negative imaginary addition into the field strength, i.e., to replace E with $E - \mathrm{i}\alpha$, where $\alpha \to 0$. After this replacement, the integral in Eqn (3) obviously converges, and its value rather quickly becomes independent of the upper integration limit. No restrictions on the convergence related to the condition $\mathrm{Re}(W) \geqslant \mathrm{Im}(W)$ mentioned in Ref. [14] arise in our case. The integral perfectly converges even when $\mathrm{Re}(W) = 0$ and $\mathrm{Im}(W) \neq 0$. Moreover, the calculations are additionally substantiated by the fact that in weak fields integral (3) is close to its saddle-point estimate.

This estimate dramatically differs from that in the delta-function well case. The condition $\mathrm{d}\varphi^0_{\mathrm{ex}}/\mathrm{d}\tau = 0$ yields the biquadratic equation that determines the saddle points

$$\frac{(eE\hbar)^2}{2m^*_{\mathrm{ex}}}\tau^4 - 4W|U_0|^2\tau^2 + \frac{2m^*_{\mathrm{ex}}|U_0|^4r^2}{\hbar^2} = 0. \tag{5}$$

It has two roots in the lower half-plane* of the complex τ plane near the imaginary axis:

$$\tau_0^{(1,2)} = -2\mathrm{i}\frac{|U_0|}{eE\hbar}(-m^*_{\mathrm{ex}}W)^{1/2}[1 \mp (1-\beta)^{1/2}]^{1/2}, \tag{6}$$

where

$$\beta = \Big(\frac{eEr}{2W}\Big)^2.$$

We see that the first root 'survives' in the limiting case $E \to 0$,

$$\tau_0^{(1)} \underset{E\to 0}{\to} -\mathrm{i}\frac{r|U_0|}{\hbar}\Big(\frac{m^*_{\mathrm{ex}}}{-2W}\Big)^{1/2} + O(E^2),$$

with the corrections proportional to the field powers. The second root in this limiting case does not exist at all. Thus, it describes a principally nonperturbative contribution of the field to solution (3). On the contrary, in the limiting case $r \to 0$

* For bound states the notions of 'weak' and 'strong' fields are much more conventional than for the free ones. In particular, for a free electron in vacuum the field is strong if it can produce an electron–positron pair at the Compton wavelength [7]. In a semiconductor, the field is considered to be strong if it can produce an electron–hole pair [23]. For an electron localised by a delta-function potential, any field is weak near the delta-function well and strong otherwise [24].

* The fact that the roots lie in the lower half-plane of the 'intrinsic time' τ is due to the causality principle [25].

only the second root 'survives', also with the corrections regular in r:

$$\tau_0^{(2)} \underset{r\to 0}{\to} -\mathrm{i}\frac{2|U_0|}{eE\hbar}(-m_{\mathrm{ex}}^* W)^{1/2} + O(r^2). \tag{7}$$

It is clear that only this root has an analogue in the delta-function potential approximation.

In this model the shift of the real part of the energy level in the field (the Stark shift) is usually calculated in the form of an asymptotic series in powers of E^2 (see, e.g., [22]). Its coefficients can be obtained by expanding the contribution of the last term of Eqn (3) in the vicinity of the point $\tau = 0$. In this case the dependence $W(E)$ is also to be taken into account. The energy level width in this approximation is determined by the contribution of the saddle point $\tau_0^{(2)}$ in the limiting case (7). The introduction of a small but finite radius of the force centre (in our case it is the radius of the quantum dot) can be considered as a certain 'regularisation' of the delta-function potential at small distances. It is easy to see that the procedure considerably improves the analytic properties of the theory*. It is clear that this regularisation is somewhat contradicting the logics of the method itself. The main attractive feature of the delta-function potential approximation is due just to the simplicity, caused by the reduction of the interaction radius to zero [26]. The backside of this simplicity is the loss of relation between the initial energy level characteristics and the properties of the potential well, as well as the additional nonanaliticity.

The saddle-point estimate of integral (3) takes the form

$$\psi_{\mathrm{ex}}(r) = \frac{A}{(2m_{\mathrm{ex}}^*|U_0|)^{1/2}}\frac{eE\hbar}{(-2W)} \times\left\{\frac{\exp\varphi_3}{[(1-\beta)^{1/2}-1+\beta]^{1/2}} - \frac{\mathrm{i}\exp\varphi_4}{[(1-\beta)^{1/2}+1-\beta]^{1/2}}\right\}, \tag{8}$$

where

$$\varphi_{3,4} = -\frac{4}{3}\frac{(-m_{\mathrm{ex}}^* W^3)^{1/2}}{eE\hbar}\frac{1\mp(1-\beta)^{1/2}+\beta}{[1\mp(1-\beta)^{1/2}]^{1/2}}. \tag{9}$$

We see that when $E \to 0$, the first term yields an exponential decrease, typical for bound states:

$$\psi_{\mathrm{ex}}(r_{\mathrm{ex}}) \sim \exp\left[-\frac{1}{\hbar}(-2m_{\mathrm{ex}}^* W)^{1/2} r\right]/r,$$

and the second term vanishes as an essentially singular point.

To formulate the condition for the electron binding energy, one has to construct the solution of the Schrödinger equation in space inside a quantum dot. Previously we have shown [17–20] how it can be done for potential (1) in the presence of a magnetic field. In the electric field, the situation is quite analogous after the simplification of the Green function under the condition (4). Let us analytically continue the solution from the exterior domain into the domain $r < R$, replacing the appropriate constants. One should keep in mind that the wave function must be limited at $r = 0$. Inside the well the Schrödinger equation reads

$$\frac{\hbar^2}{2m_{\mathrm{in}}^*}\Delta\psi_{\mathrm{in}}(\boldsymbol{r}) + (|U_0| + W - eE'z)\psi_{\mathrm{in}}(\boldsymbol{r}) = 0, \tag{10}$$

where the field strength inside the spherical quantum dot is $E' = 3E/(\mathcal{E}+2)$ [27]; m_{in}^* is the electron effective mass in the material of the dot; and $\mathcal{E}$ is the relative permittivity of the dot material in the matrix. Correspondingly, two linear-independent simplified solutions for this domain are

$$\psi_{\mathrm{in}}(\boldsymbol{r}) = B\int_0^\infty \mathrm{d}\tau\tau^{-3/2}\exp(\pm\mathrm{i}\varphi_{\mathrm{in}}^0), \tag{11}$$

where B is a normalising constant and

$$\varphi_{\mathrm{in}}^0 = \frac{m_{\mathrm{in}}^*|U_0|r^2}{2\hbar^2\tau} + \frac{\tau}{|U_0|}\left[|U_0| + W - \frac{(eE'\hbar\tau)^2}{24m_{\mathrm{in}}^*|U_0|^2}\right].$$

It is easy to show that the boundary condition at the zero point is satisfied by the following linear combination of these solutions:

$$\psi_{\mathrm{in}}(\boldsymbol{r}) = B\int_0^\infty \mathrm{d}\tau\tau^{-3/2}[\exp(\mathrm{i}\varphi_{\mathrm{in}}^0) - \mathrm{i}\exp(-\mathrm{i}\varphi_{\mathrm{in}}^0)]. \tag{12}$$

Then, following Ref. [9], we construct the function $\chi(\boldsymbol{r}) = r\psi(\boldsymbol{r})$ and require its logarithmic derivative to be continuous at the boundary of the quantum dot. As a result, we obtain the closed equation that after regularisation allows the calculation of the bound state energy level

$$m_{\mathrm{in}}^*\frac{\int_0^\infty \mathrm{d}\tau\tau^{-5/2}[\exp(\mathrm{i}\varphi_{\mathrm{in}}^0) + \mathrm{i}\exp(-\mathrm{i}\varphi_{\mathrm{in}}^0)]}{\int_0^\infty \mathrm{d}\tau\tau^{-3/2}[\exp(\mathrm{i}\varphi_{\mathrm{in}}^0) - \mathrm{i}\exp(-\mathrm{i}\varphi_{\mathrm{in}}^0)]} = m_{\mathrm{ex}}^*\frac{\int_0^\infty \mathrm{d}\tau\tau^{-5/2}\exp(\mathrm{i}\varphi_{\mathrm{ex}}^0)}{\int_0^\infty \mathrm{d}\tau\tau^{-3/2}\exp(\mathrm{i}\varphi_{\mathrm{ex}}^0)}. \tag{13}$$

3. Complex bound electron energy. Stark shift and autoionisation probability. Distinctions from the delta-function potential model

Even after the described regularisation procedure, two circumstances hamper the use of Eqn (13). First, the integrals in the left-hand side of (13) strongly oscillate at $E' \to 0$. These oscillations are due to the contribution of the second saddle point in the considered domain [in contrast to Eqn (6), these points lie near the real axis]:

$$\tau_0^{(1,2)} = 2\frac{|U_0|}{eE\hbar}[m_{\mathrm{in}}^*(|U_0| + W)]^{1/2}[1\mp(1-\gamma)^{1/2}]^{1/2}, \tag{14}$$

where

$$\gamma = \left[\frac{eE'r}{2(|U_0| + W)}\right]^2.$$

The corresponding saddle-point estimate of Eqn (11) has the form

$$\psi_{\mathrm{in}}(\boldsymbol{r}) = \frac{B}{(2m_{\mathrm{ex}}^*|U_0|)^{1/2}}\frac{eE\hbar}{2(|U_0| + W)}$$

* The property of the electric field to improve the analytic properties of the functions that describe threshold reactions in the quantum field theory and quantum mechanics at the expense of 'removing' the singularities such as branching points near the threshold was analysed in detail in Ref. [13].

$$\times\left\{\frac{\exp\varphi_1}{[(1-\beta)^{1/2}-1+\beta]^{1/2}}-\frac{\mathrm{i}\exp\varphi_2}{[(1-\beta)^{1/2}+1-\beta]^{1/2}}\right\}, \quad (15)$$

where

$$\varphi_{1,2}=\frac{4}{3}\frac{[m_{\mathrm{in}}^{*}(|U_0|+W)^3]^{1/2}}{eE'\hbar}\frac{1\mp(1-\gamma)^{1/2}+\gamma}{[1\mp(1-\gamma)^{1/2}]^{1/2}}.$$

As will be seen below, the above oscillations give rise to strong 'noisiness' of the general trend of the appropriate curves. It is reasonable to extract this trend by removing the oscillatory contribution. This can be done both analytically and using the software means. It is important to note that for the considered purpose one cannot merely omit the contribution of the second saddle point. Replacing all integrals in Eqn (13) with their saddle-point estimates and omitting the terms with $\sin\varphi_2$ and $\cos\varphi_2$, we arrive at the 'smoothed' equation for the bound state energy level

$$m_{\mathrm{in}}^{*1/2}\left[\frac{|U_0|+W}{-W}\frac{1+(1-\gamma)^{1/2}}{1+(1-\beta)^{1/2}}\right]^{1/2}\cot\varphi_1=$$
$$-m_{\mathrm{ex}}^{*1/2}\left\{1+\mathrm{i}\left[\frac{1-(1-\beta)^{1/2}}{1+(1-\beta)^{1/2}}\right]^{1/2}\exp(\varphi_4-\varphi_3)\right\}. \quad (16)$$

All calculations below are performed using either this expression, or Eqn (13), in which the values of the integrals are replaced with saddle-point estimates (8) and (15).

The second 'technical' circumstance that complicated the calculations is limitation (4) on the field magnitude. If the real part of energy is small, then even a small electric field can be sufficient to eliminate the potential barrier between the potential well in the quantum dot and the surrounding matrix. In other words, in this case the value of β can exceed unity, and this is beyond the frameworks of the used approximation. Therefore, we terminate the calculations at the field magnitude restricted by Eqn (4).

The size of an ideal quantum dot should lie in the strictly determined interval between the 'lower' and 'upper' critical radii [9]. The limitation from below is due to the following reason. In the centre of the potential well, the electron density [the function $\chi(r)$, joined at the boundary of the quantum dot] has a node. Outside the well, the electron density of the 1s state exponentially decreases. Therefore, inside the well the electron density must have a maximum. In this connection, the minimal possible radius of the ideal quantum dot is $R_{\min}=\pi\hbar/[2(2m_{\mathrm{in}}^{*}|U_0|)]^{1/2}$ [17, 19, 20]. The maximal possible radius is $R_{\max}=3R_{\min}$, in this case the second energy level of the 2s state appears in the well. As easily seen from Eqn (16), a weak external field somewhat increases both radii, practically conserving their ratio.

It is worth paying attention to a circumstance, which in our opinion is very important. The delta-function potential is commonly considered as a limit of a 'sequence' of wells becoming more and more narrow and deep. If so, solutions (8), (12), and, above all, conditions (13) for the energy level must continuously transit into the delta-function well solution. However, there is no such transition, which follows already from the existence of the minimal radius, and the fact that $R_{\min}\underset{|U_0|\to\infty}{\to}0$ does not change anything. For this reason, in the delta-function potential method the energy of the bound state is an arbitrary external parameter. In this method the known transcendental equation for the complex energy (see, e.g., [11], [25], etc.) is an analogue of condition (16). It can be easily obtained from Eqn (3) requiring the scattering length to be independent of the external field. However, this equation offers no possibility to select particular values of the binding energy and describes only the behaviour of the energy level known in advance in the external field.

4. Discussion of results and conclusions

Now we can proceed to the discussion of the results obtained. Figure 1 presents the dependences of the Stark shift on the field strength for ideal quantum dots of different size. The field strength itself here and in other Figures is normalised to the field

$$E_0=(2m_{\mathrm{in}}^{*})^{1/2}|U_0|^{3/2}/(e\hbar),$$

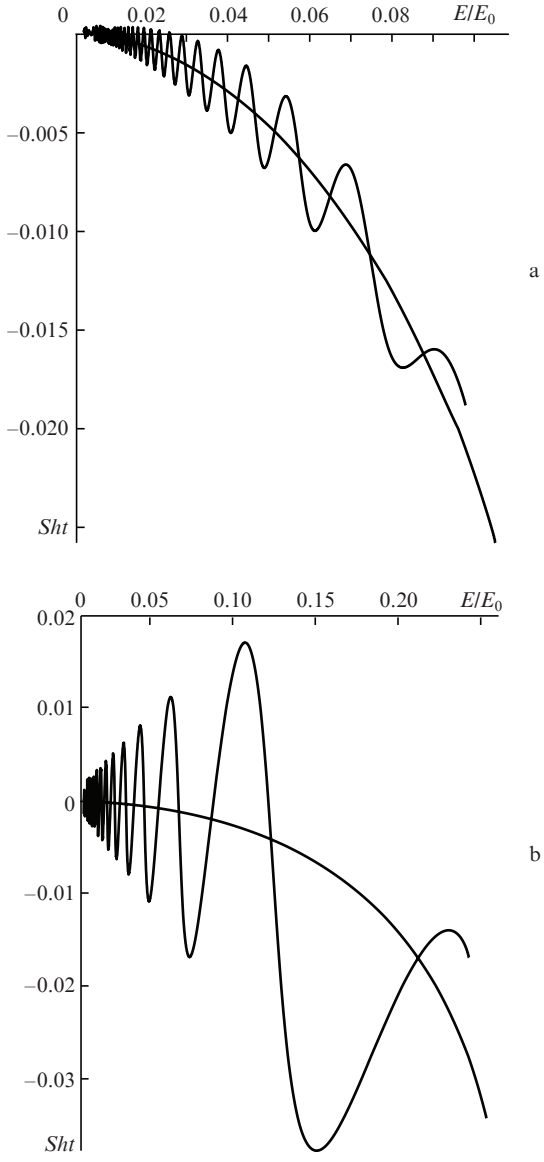

Figure 1. Dependences of the Stark shift value on the electric field for the quantum dots with the radius (a) 2.5 and (b) 3.5 nm. Here and in Figs 2–4 the monotonic curves are calculated using Eqn (16), the oscillating curves are calculated using the exact formula (13). The electron masses in the interior and exterior domains are $m_{\mathrm{in}}^{*}=0.05m$ and $m_{\mathrm{ex}}^{*}=0.1m$, respectively, and the relative permittivity of the quantum dot material is $\mathcal{E}=2$.

and the shift of the real part of the level is normalised to the potential well depth $|U_0|$:

$$Sht = (\mathrm{Re}\, W - W_0)/|U_0|,$$

where W_0 is the binding energy of the level in the absence of the external field, i.e., in the limiting case $E \to 0$. The monotonic curves are computed using the approximate 'smoothed' formula (16), and for the oscillating ones the exact expression (13) was used. The calculation was carried out for the following set of model (but quite realistic) parameters: $m^*_{\mathrm{in}} = 0.05m$, $m^*_{\mathrm{ex}} = 0.1m$, $\mathcal{E} = 2$. One can see that the field dependence of the Stark shift is much more complex and interesting than that in the delta-function potential approximation (the latter is close to the monotonic curves). The oscillations considerably affect the shift. As seen from Eqn (15), these oscillations are related to the contribution from those saddle points that vanish in the delta-function well approximation. Overall, their frequency is inversely proportional to the field strength, and the amplitude depends on the field in a complex way. Roughly speaking, it is proportional to the field and inversely proportional to the binding energy, which, in turn, depends on the field. Therefore, the relative value of the oscillation amplitude at first increases with the field growth and then begins to fall so that finally the envelopes of the oscillating curves converge to the monotonic ones. We recall that the limitation $\beta < 1$ restricts the domain of reliable calculations. We also note that with the growth of the well size even the sign of the Stark shift may change.

Figure 2 presents the dependences of the Stark shift on the electric field for different values of the relative permittivity of the quantum dot material. In our opinion, the dependences are rather curious. The calculation is carried out at the same mass ratios as in Fig. 1 and at the fixed radius of the quantum dot $R = 3$ nm. The following values of permittivity were chosen: $\mathcal{E} = 0.25$, 1 and 4. It is seen that the smoothed values of the shift rather weakly response to the change in relative permittivity. In other words, the averaged value of the shift weakly depends on the field inside the potential well. This independence is enhanced by our approximation (4). On the contrary, the oscillating part of the Stark shift is rather sensitive to the interior field. Generally, this fact agrees with the logics of the known pseudopotential approximation [9]. It is clear that exactly the interference effects that determine the shift oscillations are most sensitive to the local variations of the wave function.

Now let us proceed to the consideration of the electric field dependence of the energy level width (the imaginary part of the complex energy). We recall that the imaginary part of the complex energy is related to the probability of the state decay, and in our case (one bound energy level in the well) the only possible decay channel is the transition of electron into the conduction band of the matrix (conditionally referred to as ionisation). Thus, the imaginary part of the energy is the ionisation probability per unit time. In Fig. 3, this dependence is presented for three different diameters of the quantum dot. We use the same field and energy units and the same values of constants as in Fig. 1. As above, we use the approximate formula (16) for the monotonic curves and Eqn (13) for the oscillating ones. One can easily see that the oscillations here are less significant than in the case of the Stark shift. Their behaviour depending on the field has generally the same character as in the case of the Stark shift. Naturally, the probability of electron extraction from the potential well for the fixed field

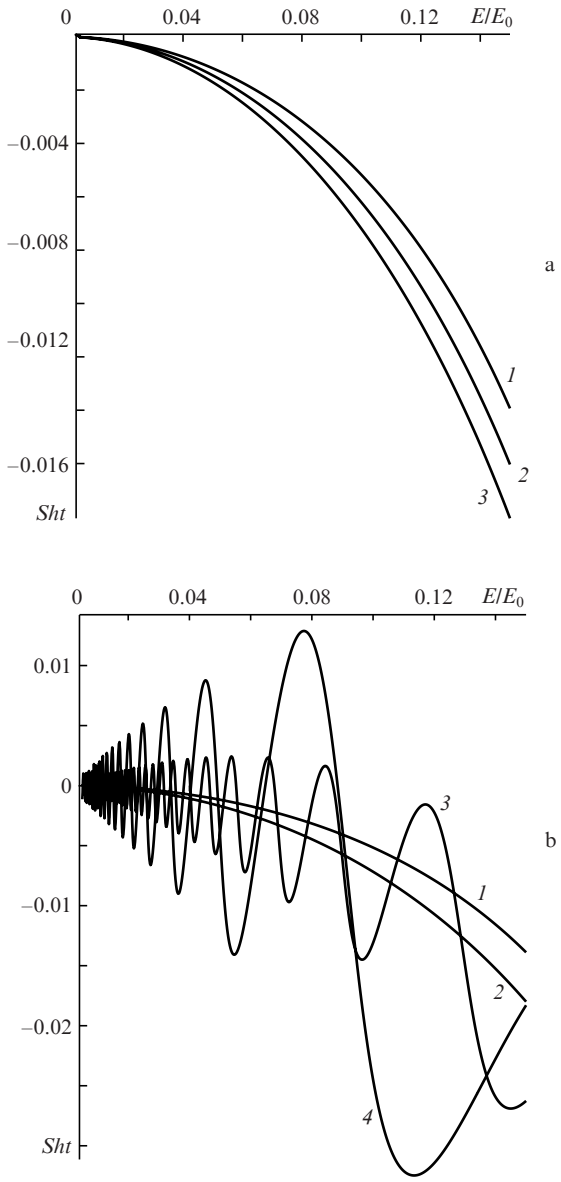

Figure 2. Dependence of the Stark shift value on the electric field strength for the quantum dots with the radius 3 nm (a) for $\mathcal{E} = (1)$ 0.25, (*2*) 1 and (*3*) 4, as well as (b) for $\mathcal{E} = (1, 4)$ 0.25 and (*2*, *3*) 4. The units of the field strength and the energy, as well as the electron masses are the same as in Fig. 1.

decreases with increasing well width. As above, the domain of calculations is restricted by the condition $\beta < 1$.

The field dependences of the energy level width in quantum dots of similar size for different values of permittivity are presented in Fig 4. The same trends as in Fig. 2 are observed. The monotonic curves are practically undistinguishable, in spite of the considerable range of $\mathcal{E}$ variation. The oscillations in some sense manifest the difference of permittivity, hidden in the averaged curves. The frequency of oscillations increases with increasing $\mathcal{E}$, i.e., with a decrease in the electric field strength within the volume of the potential well, since it is inversely proportional to the fields strength inside the quantum dot, too.

Finally, let us briefly discuss the role of the AC component of the field. Equations (13) and (16) that determine the value of the complex energy for the DC field have the general form

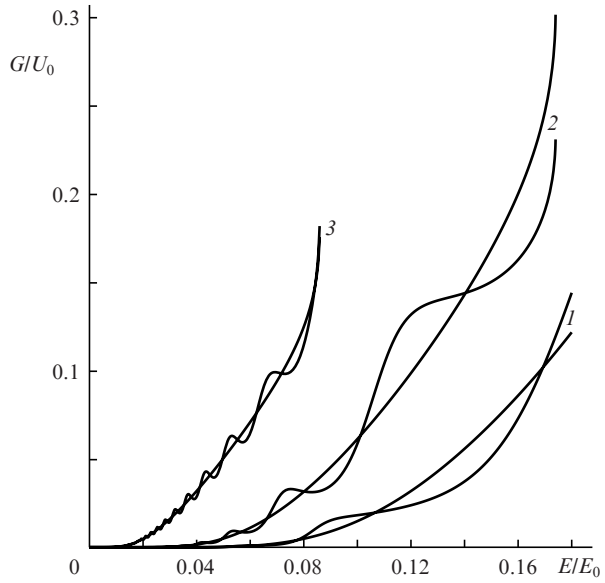

Figure 3. Dependences of the energy level width on the electric field strength for the quantum dots with the radius (*1*) 2.5, (*2*) 3 and (*3*) 3.5 nm, the electron effective masses $m_{in}^* = 0.05m$, $m_{ex}^* = 0.1m$, and $\mathcal{E} = 2$.

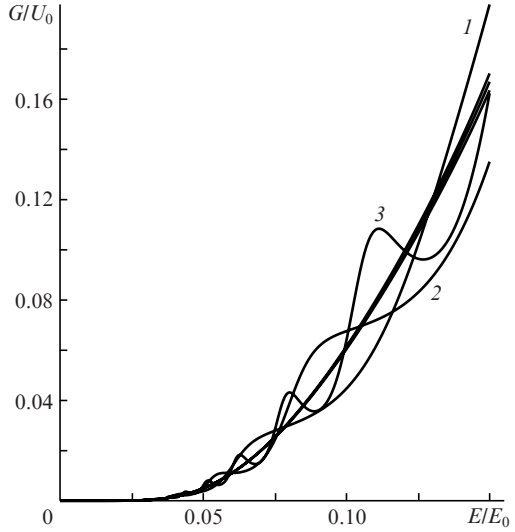

Figure 4. Dependences of the energy level width on the electric field strength for the quantum dots with the radius 3 nm at $\mathcal{E} =$ (*1*) 0.25, (*2*) 1 and (*3*) 4; the monotonic curves virtually coincide. The effective masses are the same as in Fig. 3.

$$f_1(E) = f_2(E). \tag{17}$$

To estimate roughly the effect of the AC light wave field, we replace $E \to E_0 + \Delta E\sin(\omega t)$ and assume that the constants satisfy the relation $E_0 \gg \Delta E$. Since the boundary conditions (13) and (16) are satisfied at any moment of time, the values of complex energy should oscillate in time with the frequency ω. These oscillations superpose with the intrinsic oscillations in the DC field, related to the finite size of the quantum dot (see Figs 1–4). This superposition can give rise to interesting resonance phenomena, the detailed study of which is far beyond the scope of the present paper.

Here we restrict ourselves to the simplest version of the adiabatic approximation. Let us average over the period the previous relation,

$$\frac{1}{T}\int_0^T f_1(E,t) = \frac{1}{T}\int_0^T f_2(E,t), \tag{18}$$

and take into account the fact that the amplitude of the periodic perturbation is small against the background of the direct component of the field:

$$f_{1,2}(E,t) \approx f_{1,2}(E_0) + \frac{\mathrm{d}f_{1,2}(E_0)}{\mathrm{d}E}\Delta E\sin(\omega t) + \frac{1}{2}\frac{\mathrm{d}^2 f_{1,2}(E_0)}{\mathrm{d}E^2}\Delta E^2\sin^2(\omega t).$$

After averaging over the period, relation (18) that determines the complex energy of the level transforms in the following way:

$$f_1(E_0) + \frac{1}{4}\frac{\mathrm{d}^2 f_1(E_0)}{\mathrm{d}E^2}\Delta E^2 = f_2(E_0) + \frac{1}{4}\frac{\mathrm{d}^2 f_2(E_0)}{\mathrm{d}E^2}\Delta E^2.$$

One can easily see that even in this primitive version the situation with the effect of the wave field is ambiguous. From Figs 1–4 it is seen that for the monotonic dependences resulting from Eqn (16) the contribution from the AC field in the adiabatic approximation is rather small, as it could be expected. At the same time, according to the exact formula (13), the resonance phenomena in the superposition of the DC field and the light wave field are quite possible, and this possibility is due to exactly the finite size of the potential well. In the delta-potential approximation, they vanish in a similar way, as the oscillations of the Stark shift and the energy level width.

From the obtained results, it is worth making two remarks.

1. The regularisation method of Gamov quasi-stationary states is not as universal as the Zel'dovich method. However, in the situations when the divergences are due to the effect of the electric field it may be useful. Our method yields simpler and better converging expressions.

2. The effect of the electric field on the behaviour of bound single-electron states in the wells of finite depth and size (like quantum dots) is much more complex and diverse than predicted by the delta-function potential approximation. The main cause of this additional complexity is the oscillations of both real and imaginary parts of the complex energy of the bound particle in the DC field. These oscillations exist only in the finite-size potential well and are principally irreproducible using either the delta-potential approximation or the perturbation theory.

Thus, we have constructed the theoretical model describing the energy spectrum of a 3D quantum dot in the external DC and weak AC electric fields, using neither the delta-function potential approximation, nor the perturbation theory. For this purpose, we have proposed a simple method of regularising the Gamov wave function and applied it to the calculation of the complex-valued energy of the electron that describe both the optical spectrum of the system and the probability of the state decay (autoionisation). The effect of oscillation of the Stark shift and the energy level width in the

DC electric field, which is possible only in a potential well having finite depth and size, was found.

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