Diamagnetic impurity centers in thin semiconducting layers

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We investigate states of an electron or hole captured by a diamagnetic impurity center in a semiconductor layer of finite thickness. By a diamagnetic impurity center (DIC) we mean an impurity center in a strong magnetic field whose effect on the electron states greatly exceeds that of the Coulomb interaction between the electron and the center. The magnetic field is directed perpendicular to the plane of the layer. Analytic expressions for the energy levels are obtained in which the dependence on the layer width, impurity position relative to the edges of the layer, and the magnitude of the magnetic field, is explicit. We show that as the width of the layer decreases, the levels shift towards shorter wavelengths, from the range of the discrete Coulomb spectrum to the range of size-quantized energies. The levels shift in the same direction when the impurity center is displaced from the symmetry plane of the layer. A special discussion is given of states of a DIC located at one of the boundaries of the semiconductor layer. Our results can also be used as an approximate solution to the problem of a diamagnetic exciton in a quantum well if the constituent electron and hole of the latter have very different masses.

The energy spectrum and optical properties of multilayer structures and single quasi-two-dimensional quantum wells with sizes on the order of 10^{-7}–10^{-6} cm are to a considerable degree determined by exciton states and states of current carriers that are trapped by impurity centers. A clear example of such a structure is the heterostructure that exists between layers of the semiconductors GaAs and $Al_xGa_{1-x}As$ (with $x = 0.3$), where the latter has a larger band gap width. In papers by a number of authors[1–4] it was observed that excitons and impurity states play an important role in the formation of the absorption and luminescence spectra of these systems.

The subject of this paper is the theoretical investigation of states of electrons (or holes) that are trapped by Coulombic impurity centers in a single quantum well in the presence of a very strong magnetic field, i.e., a field whose effect on the states of the electron considerably exceeds that of the Coulomb interaction of the electron with the center. By analogy with a Wannier-Mott exciton in a strong magnetic field (i.e., the diamagnetic exciton[5]), we will refer to such a center as a diamagnetic impurity center (DIC). In this paper, primary consideration is given to the investigation of the spectrum of hydrogenic states of the DIC. For the energy levels we obtain analytic expressions, which contain dependence on the layer thickness, the position of the impurity relative to the edges of the layer, and magnetic field, in various approximations. In the calculations we use the effective-mass approximation with a simple parabolic dispersion law, together with zero boundary conditions at the layer edges (i.e., a quantum well); we do not include the so-called "self-action" (see, e.g., Ref. 6) of the charges of the electron and center, assuming that the dielectric permittivity of the layer and the surrounding medium are close to one another.

The results we obtain can also be used as an approximate solution of the problem of a diamagnetic exciton in a quantum well, if the masses of the electron and hole are very different (i.e., $m_h \gg m_e$). In this case, by solving for the energy eigenvalues of the problem of an impurity center with a light particle as a function of the position of the center within the well, we obtain adiabatic potentials for the states of the heavy particle. Our conclusions also form a basis for the theoretical investigation of magneto-optic properties of semiconductor heterostructures with specified spatial distributions of impurity centers. In particular, we investigate states of the DIC located at the edges of the semiconductor layer.

Let us consider a semiconductor layer of width d bounded by the planes $z = \pm d/2$, containing a Coulomb center with position satisfying $-d/2 \leqslant z = b \leqslant +d/2$. In the effective-mass approximation, the equation that determines the states of this impurity center in a magnetic field $\mathbf{H}$ parallel to the z-axis in a medium with dielectric permittivity ε_1 surrounded by a medium with dielectric permittivity ε_2 has the form[3]

$$\left\{\frac{1}{2\mu}\left(-i\hbar\nabla+\frac{e}{2c}[\mathbf{Hr}]\right)^2-\frac{e^2}{\varepsilon[\rho^2+(z-b)^2]^{1/2}}\right\}\Psi(\mathbf{r})$$

$$=E\Psi(\mathbf{r}). \qquad (1)$$

$$\varepsilon=(\varepsilon_1\varepsilon_2)^{1/2}$$

By solving this equation we determine the total energy of the particle E and the wave function $\Psi(\boldsymbol{\rho},z)$, which satisfies the boundary conditions

$$\Psi(\boldsymbol{\rho},\ \pm d/2)=0. \qquad (2)$$

The characteristic dimensional parameters of the problem are the impurity radius $a_0=\varepsilon\hbar^2/\mu e^2$, the magnetic length $a_H=(\hbar c/eH)^{1/2}$, and the layer width d. In what follows, we will consider DIC for which the following inequality holds:

$$a_H \ll a_0, \qquad (3)$$

indicating that the effect of the magnetic field is much larger than that of the Coulomb field of the impurity. Rather than formulating a general approach to the solution of Eq. (1) under conditions (2) and (3), we discuss only the special cases listed below.

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1. PERTURBATION THEORY: $a_H \ll a_0, d \ll a_0$

The first of the conditions of this section [condition (3)] implies that the binding energy of the particle at the impurity center $\propto \hbar^2/\mu a_0^2$ is small compared to the distance between Landau levels $\propto \hbar^2/\mu a_H^2$ (the energy of motion of the particle in the plane of the layer). The second condition implies that this binding energy is, however, much smaller than the distance between the size-quantized levels $\propto \hbar^2/\mu d^2$ for motion of the particle perpendicular to the layer, i.e., along the direction of the magnetic field. The solution to Eq. (1) that is unperturbed by the impurity potential and which satisfies condition (2) is well-known, and for the chosen orientation of the magnetic field is written in the form

$$\Psi^{(0)}(\mathbf{r}) = X_{\perp N,m}(\boldsymbol{\rho})\,\psi_n^{(0)}(z), \tag{4}$$

where

$$\psi_n^{(0)}(z) = \left(\frac{2}{d}\right)^{1/2} \sin\frac{n\pi}{d}\left(z+\frac{d}{2}\right), \qquad n=1,2,3,\ldots; \tag{5}$$

here $X_{\perp N,m}(\boldsymbol{\rho})$, $N, |m| = 0,1,2,\ldots$ is a function that describes the motion of the particles in the magnetic field in the plane x,y (see Ref. 7).

The unperturbed energy has the form

$$E^{(0)} = E_{\perp N,m} + \mathscr{E}_n^{(0)},$$

where

$$E_{\perp N,m} = \frac{\hbar eH}{2\mu c}(2N+|m|-m+1) \pm \beta H. \tag{6}$$

Here β is the effective magnetic moment of an electron, and

$$\mathscr{E}_n^{(0)} = \frac{\hbar^2\pi^2 n^2}{2\mu d^2}, \qquad n=1,2,3,\ldots \tag{7}$$

From this we see that the unperturbed energy spectrum is a combination of the equidistant Landau levels (6) and the size-quantized level (7).

Let us calculate the impurity-induced energy shift of those states of (5) that are odd with respect to the operation $z \to -z$, i.e., those for which $n = 2p+1$, $p = 0,1,2,\ldots$. These states form the lowest series belonging to the Landau level with $N = m = 0$. The shift is determined by the diagonal matrix elements of the Coulomb attraction energy calculated for the functions (4) with $N = m = 0$, $n = 2p+1$. After integration over the coordinates ρ, φ, the correction to the energy $4E^{(0)}_n$ acquires the form

$$\Delta\mathscr{E}_p = -\frac{(2\pi)^{1/2}e^2}{\varepsilon d}\int_{t_-}^{t_+}\cos^2 q(a_H t+b)\,e^{t^2/2}\left\{1-\Phi\left[\left(\frac{t^2}{2}\right)^{1/2}\right]\right\}dt, \tag{8}$$

where

$$t_\pm = \frac{-b\pm d/2}{a_H}, \qquad q = \frac{(2p+1)\pi}{d};$$

here $\Phi(x)$ is the probability integral.[8]

In the region of very small values of the parameter d/a_H, the correction $\Delta\mathscr{E}_p$ (8) can be written in explicit form. If the layer is thin enough that the condition $d \ll a_H$ holds, then in Eq. (8) we can assume that $\Phi(x) \simeq 2\pi^{-1/2}x$; then

$$\Delta\mathscr{E}_p = -\left(\frac{\pi}{2}\right)^{1/2}\frac{e^2}{\varepsilon a_H}\left\{1-\frac{1}{4}\left(\frac{2}{\pi}\right)^{1/2}\frac{d}{a_H} \times\left[1+4\frac{b^2}{d^2}-\frac{2}{(qd)^2}(1+\cos 2qb)\right]\right\}. \tag{9}$$

For the case where the layer width considerably exceeds the magnetic length ($d \gg a_H$) while remaining much smaller than the radius a_0, the asymptotic value of the integral[8] entering into (8) leads to

$$\Delta\mathscr{E}_p = -\frac{e^2}{\varepsilon d}\left[-C+\ln\frac{d^2}{2a_H^2}\left(1-4\frac{b^2}{d^2}\right) -(C+\ln 2q^2a_H^2)\cos 2qb\right], \tag{10}$$

where $C = 0.577$ is the Euler constant.

Expression (10) was obtained by us under the condition $|t_{+,-}| \gg 1$, i.e., relatively large distances compared to a_H, which does not allow the impurity center to approach the edges of the layer.

Both the limiting results (9) and (10) lead us to the general conclusions that an impurity center with an attractive potential causes the carrier energy to decrease ($\Delta\mathscr{E}_p < 0$), and that displacement of the impurity center ($b \neq 0$) from the plane of symmetry of the layer $z = 0$ decreases the magnitude of the impurity shift $|\Delta\mathscr{E}_p|$.

2. GENERAL METHOD, $a_H \ll a_0$

Let us write the solution to Eq. (1) in the form of an expansion with respect to the transverse functions $X_{\perp N,m}(\boldsymbol{\rho})$ (Ref. 7):

$$\Psi(\mathbf{r}) = \sum_{N,m=0}^{\infty} X_{\perp N,m}(\boldsymbol{\rho})\,f^{(N,m)}(z). \tag{11}$$

After substituting Eq. (11) into Eq. (1), we obtain a system of equations for the expansion coefficients $f^{(N,m)}(z)$:

$$-\frac{\hbar^2}{2\mu}f^{(N,m)\prime\prime}(z) + \sum_{N'=0}^{\infty} V_{N,N'}^{(m)}(z)\,f^{(N',m)}(z) = \mathscr{E}_{N,m}f^{(N,m)}(z), \tag{12}$$

where

$$V_{N,N'}^{(m)}(z) = -\frac{e^2}{\varepsilon}\int\frac{X_{\perp N,m}(\boldsymbol{\rho})X_{\perp N',m}(\boldsymbol{\rho})}{[\rho^2+(z-b)^2]^{1/2}}\,d\boldsymbol{\rho}, \tag{13}$$
$$\mathscr{E}_{N,m} = E - E_{\perp N,m}.$$

As was shown in detail in Ref. 9, for a DIC subject to condition (3) the system (12) can be solved in the single-band approximation (with respect to the Landau bands), in which we set $V_{N,N'}^{(m)} = V_N^{(m)}\delta_{NN'}$; we will use this result in what follows. We will limit ourselves to states with $m = 0$ and ground Landau level $N = 0$. Let us consider various regions of the energy spectrum $\mathscr{E}_{0,0}$.

2.1. Region of discrete Coulomb spectrum: $\mathscr{E}_{0,0} < 0$

Converting to a new notation in Eq. (12)

$$\mathscr{E}_{0,0}^{(\nu)} = \mathscr{E}_\nu = -\frac{e^2}{2\varepsilon a_0\nu^2}, \qquad t = \frac{2(z-b)}{a_0\nu},$$

we obtain the following equation for the function $f_\nu^{(0,0)} \equiv f_\nu$:

$$f_\nu''(t) + \nu \left\langle 0 \left| \frac{1}{(t^2+g^2)^{1/2}} \right| 0 \right\rangle f_\nu(t) - \frac{1}{4} f_\nu(t) = 0, \quad (14)$$

in which

$$g^2 = \frac{4\rho^2}{a_0^2 \nu^2}.$$

Here, ν is a quantum number that determines the states of motion along the z-axis, and $\langle 0|\cdots|0\rangle$ denotes an average with respect to the function $X_{10,0}(\boldsymbol{\rho})$.

From condition (2) for the function f_ν it follows that

$$f_\nu\left[\frac{2}{a_0\nu}\left(-b \mp \frac{d}{2}\right)\right] = 0. \quad (15)$$

For further investigation of Eq. (14) we use the Hasegawa-Howard method, which was described in detail in Ref. (10). In the region

$$|t| \gg \frac{2a_H}{a_0\nu} \approx \langle 0|g|0\rangle \quad (16)$$

the solution to Eq. (14) has the form

$$f_\nu(t) = A_+ W_{\nu,1/2}(t) + B_+ M_{\nu,1/2}(t), \quad t>0, \quad (17)$$

where $W_{\nu,1/2}$, $M_{\nu,1/2}$ are Whittaker functions (see Ref. 8, p. 1073).

For $t<0$, the function $f_\nu(t)$ can be obtained from (17) by the replacements $A_+ \to A_-$, $B_+ \to B_-$, and $t \to \tau$, where $\tau = -t$.

For $|t| \ll 1$ we construct the solution by double integration of Eq. (14), using the initial function

$$f_\nu^{(0)}(t) = c + \alpha t (t^2+g^2)^{1/2} \ln[t + (t^2+g^2)^{1/2}].$$

By virtue of condition (3), the inequality $|t| \ll 1$ and (16) are found to be compatible. For values of $|t| \gg 2a_H/a_0\nu$ we retain terms of lowest order in t in these integrals to obtain

$$f_\nu(t) = (-\nu c_+ - \nu\alpha_+ {}^1\!/_4 \langle 0|g^2|0\rangle) t \ln t + (\nu c_+ \lambda(\nu) + \alpha_+ \langle 0|g \ln g|0\rangle) t, \quad t>0, \quad (18)$$

where

$$\lambda(\nu) = 1 - \frac{1}{2}C + \frac{1}{2}\ln\frac{2a_H^2}{a_0^2\nu^2}.$$

The form of the function $f_\nu^0(t)$ for $t<0$ can be obtained from the expression (18) by the replacements $c_+ \to c_-$, $\alpha_+ \to \alpha_-$, $t \to \tau$, where $\tau = -t$.

The form of $f_\nu^{(0)}(t)$ implies that we can fulfill the requirements that $f_\nu(t)$ and its first derivative be continuous at $t=0$ by imposing the conditions $c_+ = c_- \equiv c$, $\alpha_+ = -\alpha_- = \alpha$, respectively. Using the expansions of the Whittaker functions given, e.g., in Ref. 8 for $|t| \ll 1$, and setting equal the coefficients of terms that are the same order in t in Eqs. (17) and (18), as well as in the analogous expressions which apply for $t<0$, we obtain

$$\frac{A_+}{\Gamma(-\nu)} = -\nu c - \frac{1}{4}\nu\alpha\langle 0|g^2|0\rangle, \quad (19)$$

$$\frac{A_+}{\Gamma(-\nu)}\varphi(\nu) + B_+ = \nu c\lambda(\nu) + \alpha\langle 0|g\ln g|0\rangle, \quad (20)$$

$$\frac{A_-}{\Gamma(-\nu)} = -\nu c + \frac{1}{4}\nu\alpha\langle 0|g^2|0\rangle, \quad (21)$$

$$\frac{A_-}{\Gamma(-\nu)}\varphi(\nu) + B_- = \nu c\lambda(\nu) - \alpha\langle 0|g\ln g|0\rangle, \quad (22)$$

where

$$\varphi(\nu) = 2C - 1 + \psi(1-\nu) + \frac{1}{2\nu},$$

Here $\Gamma(u)$ and $\psi(u)$ are the gamma-function and its logarithmic derivative, respectively.

The conditions (15) give

$$A_+ W_{\nu,1/2}(t_1) + B_+ M_{\nu,1/2}(t_1) = 0, \quad (23)$$

$$A_- W_{\nu,1/2}(t_2) + B_- M_{\nu,1/2}(t_2) = 0, \quad (24)$$

$$t_{1,2} = \frac{2}{a_0\nu}\left(\frac{d}{2} \mp b\right).$$

By requiring that the system of Eqs. (19)–(24) with respect to the unknowns c, α, $A_{+,-}$, $B_{+,-}$ be solvable, we obtain two transcendental equations determining the quantum number σ and the corresponding energy $\mathscr{E}_\nu$. By calculating the matrix elements $\langle 0|g^2|0\rangle$ and $\langle 0|g\ln g|0\rangle$, we then can derive explicit expressions for these equations

$$\varphi(\nu) + \lambda(\nu) = -\frac{Q(\nu)}{\nu} + \frac{\Gamma(-\nu)}{2}\left(\frac{W_2}{M_2} + \frac{W_1}{M_1}\right) \pm \left[\frac{Q^2(\nu)}{\nu^2} + \frac{\Gamma^2(-\nu)}{4}\left(\frac{W_2}{M_2} - \frac{W_1}{M_1}\right)^2\right]^{1/2}, \quad (25)$$

where

$$1 \ll Q(\nu) = \frac{2\langle 0|g\ln g|0\rangle}{\langle 0|g^2|0\rangle} = \frac{a_0\nu\pi^{1/2}}{2^{1/2}a_H}\left[\ln\frac{2^{1/2}a_H}{a_0\nu} + 1 - \frac{C}{2}\right],$$

$$W_{1,2} = W_{\nu,1/2}(t_{1,2}), \quad M_{1,2} = M_{\nu,1/2}(t_{1,2}).$$

The procedure leading up to Eq. (25) implies that these equations are correct under conditions $2a_H/a_0\nu \ll 1$, $t_{1,2} \gg 2a_H/a_0\nu$. The second inequality requires that the attractive center be separated from the edge of the layer by a distance that exceeds a_H. If the attractive center is located in the plane of symmetry of the layer ($b=0$), the states can be classified with respect to parity. In this case, $t_1 = t_2$, $W_1 = W_2$, $M_1 = M_2$, and the upper sign in (25) will correspond to even, the lower sign to odd, energy levels. For an unbounded crystal ($d \to \infty$, $t_{1,2} \to \infty$), the asymptotic behavior of the Whittaker functions[8] for large real values of the argument implies that $W_{1,2} \cdot M_{1,2}^{-1} \to 0$, and we are led to equations which describe even and odd energy levels of the DIC.[10]

Let us investigate the group of levels that transforms into the even series at $b=0$ or as $d \to \infty$ in somewhat more detail. We will restrict ourselves to special cases for which the effects of shifting the center b or changing the layer width d can be taken into account explicitly. For these cases the Whittaker functions under the radical in Eq. (25) can be neglected.

a) Wide layer, center far from the boundary: $t_1 \gg 1$, $t_2 \gg 1$. In this case, the solution of Eq. (25) is conveniently written in the form $\nu = \nu_0 + \delta$, where $\nu_0 \simeq 0,1,2,3,\cdots$, is a root of the equation that describes the unbounded crystal ($t_1 = t_2 = \infty$), and δ is a correction that takes into account

the finiteness of the layer width d. For the correction to the ground state $\nu_0 \simeq 0$, taking into account the asymptotic form of the Whittaker function,[8] we obtain

$$\delta = \nu_0 \left(\frac{d}{a_0\nu_0}\right)^{2\nu_0} \exp\left(-\frac{d}{a_0\nu_0}\right)\left[\left(1+\frac{2b}{d}\right)^{2\nu_0} \exp\left(-\frac{2b}{a_0\nu_0}\right) + \left(1-\frac{2b}{d}\right)^{2\nu_0} \exp\left(\frac{2b}{a_0\nu_0}\right)\right].$$

The correction δ to the excited states $\nu_0 \sim k = 1,2,3,\cdots$, differs from the corrections obtained above by replacing the first factor $\nu_0 \to k(2k!^2)^{-1}$.

For small displacements $b \ll a_0\nu_0$ we have

$$\delta \propto \exp\left(-\frac{d}{a_0\nu_0}\right)\left(1+\frac{2b^2}{a_0^2\nu_0^2}\right),$$

from which it follows that decreasing the layer width d and shifting the attractive center from the symmetry plane (increasing b) both increase the value of ν, and consequently decrease the binding energy $|\mathscr{E}_\nu|$.

b) Wide layer, center close to one of the boundaries: $t_2 \gg 1$, $a_H/a_0\nu \ll t_1 \ll 1$. Here we require not only the asymptotic forms of the Whittaker functions but also their expansions for small values of t_1. In this case Eq. (25) acquires the form

$$\varphi(\nu) + 2\lambda(\nu) + \frac{1}{\nu t_1} - \ln t_1 = 0. \tag{26}$$

Its solution for $\nu \ll 1$ can be found in analytic form. All the conclusions arrived at above regarding the effect of changing the layer width and shifting the attractive center on the binding energy $|\mathscr{E}_\nu|$ turn out to be correct here as well.

In both the situations investigated above, the energy spectrum $\mathscr{E}_\nu < 0$ is a quasi-Coulombic series of levels having the value $\mathscr{E}_\nu = 0$ as a point of accumulation.

In the general case $t_{1,2} \simeq 1$, we must solve (25) numerically in order to find $\mathscr{E}_\nu$. In this case, qualitative arguments suggest that as the width of the layer d decreases down to values $d \simeq a_0$, the increase in particle energy due to size quantization will balance the decrease in energy due to attraction toward the center. As a result, the energy $\mathscr{E}_\nu$ will pass through zero and shift into the region $\mathscr{E} > 0$.

2.2. Size-quantized region $\mathscr{E}_{0,0} > 0$

The approach to investigating this portion of the spectrum is completely analogous to that described in Sec. 2.1; therefore, we will pause only to point out some of its features and present the final results.

If in Eq. (12) we introduce the notation

$$\mathscr{E}_{0,0}^{(s)} = \mathscr{E}_s = \frac{e^2}{2\varepsilon a_0 s^2}, \qquad t = \frac{2(z-b)}{ia_0 s},$$

then in the region $|t| \gg 2a_H/a_0 s$, a solution can be chosen in the form

$$f_s(t) = A_+ \operatorname{Re} W_{is,1/2}(t) + B_+ \operatorname{Im} M_{is,1/2}(t), \quad it > 0. \tag{27}$$

For the region $it < 0$ we must make the following replacements in (26): $A_+ \to A_-$, $B_+ \to B_-$, and $t \to \tau$, where $\tau = -t$.

After double integration of Eq. (12) with the starting function

$$f_s^{(0)}(t) = c + \alpha t(t^2-\tilde{g}^2)^{1/2} \ln[t+(t^2-\tilde{g}^2)^{1/2}],$$
$$\tilde{g}^2 = \frac{4\rho^2}{a_0^2 s^2}$$

and isolation of the real part of the resulting expression for $f_s(t)$, we obtain an iterative solution for $2a_H/a_0 s \ll |t| \ll 1$ in the regions $it > 0$ and $it < 0$. By smoothly matching the first of these solutions with (27), analogous to the matching in the region $it < 0$, and using the conditions for continuity of $f_s(t)$ and $f_s'(t)$ at $t = 0$ along with the boundary conditions

$$f_s(\tau_1) = f_s(\tau_2) = 0, \quad \tau_{1,2} = \frac{2}{ia_0 s}\left(\frac{d}{2} \mp b\right)$$

we obtain a system of six algebraic homogeneous equations with respect to the unknowns $A_{+,-}$, $B_{+,-}$, c, and α. The requirement that this system be solvable leads to two transcendental equations for the quantum number:

$$\tilde{\varphi}(s) + \lambda(s) = \frac{Q(s)}{s} + \frac{\Gamma(s)}{2}\left(\frac{\tilde{W}_2}{\tilde{M}_2} + \frac{\tilde{W}_1}{\tilde{M}_1}\right) \pm \left[\frac{Q^2(s)}{s^2} + \frac{\Gamma^2(s)}{4}\left(\frac{\tilde{W}_2}{\tilde{M}_2} - \frac{\tilde{W}_1}{\tilde{M}_1}\right)^2\right]^{1/2}, \tag{28}$$

$$\tilde{\varphi}(s) = \frac{\Gamma(s)}{2i}\left\{\frac{1}{\Gamma(is)}\left[i\frac{\pi}{2} + 2C - 1 + \psi(1+is) - \frac{1}{2is}\right] - \text{c.c.}\right\},$$

$$\lambda(s) = 1 - \frac{1}{2}C + \frac{1}{2}\ln\frac{2a_H^2}{a_0^2 s^2},$$

$$\frac{1}{\Gamma(s)} = \frac{1}{2i}\left[\frac{1}{\Gamma(is)} - \frac{1}{\Gamma(-is)}\right],$$

$$\tilde{W}_{1,2} = \operatorname{Re} W_{is,1/2}(\tau_{1,2}), \quad \tilde{M}_{1,2} = \operatorname{Im} M_{is,1/2}(\tau_{1,2}),$$

where the quantity $Q(s)$ is the same as in (25).

Expression (28) is applicable under the conditions

$$\frac{2a_H}{a_0 s} \ll 1, \quad |\tau_{1,2}| \gg \frac{2a_H}{a_0 s}.$$

Let us pause to discuss several special cases. If the center lies in the midplane of the layer ($b = 0$), then the states are classifiable with respect to purity. In this case, $\tau_1 = \tau_2$, $\tilde{W}_1 = \tilde{W}_2$, and $\tilde{M}_1 = \tilde{M}_2$. For the even-parity levels we use Eq. (28) with the lower sign, while the upper sign applies to the odd-parity levels. Let us compute the position of these levels for $s \ll 1$, substituting the asymptotic forms of the Whittaker functions for $|\tau_{1,2}| \gg 1$ into Eq. (28). For the odd levels we obtain the equation

$$s\left(C + \ln\frac{2a_H^2}{a_0^2 s^2}\right) = -\operatorname{ctg}\left(\frac{d}{2a_0 s} + s\ln\frac{d}{a_0 s}\right).$$

If we solve this equation by the method of iteration, assuming that $s = 0$ on the left side in the zeroth approximation, we find that

$$s^{-1} = \frac{a_0}{d}(2p+1)\pi, \quad p = 0, 1, 2, \ldots, \tag{29}$$

and the value of $\mathscr{E}_s$ coincides with the levels of the even-parity state $\mathscr{E}_n^{(0)}$ [see (7) for $n = 2p+1$] from size-quantization. The energy levels of the odd-parity states are given by the equation

$$s\left(C+\ln\frac{2a_H^2}{a_0^2s^2}\right)=\frac{4Q(s)}{s}-\operatorname{ctg}\left(\frac{d}{2a_0s}+s\ln\frac{d}{a_0s}\right).$$

In the zero-order approximation $s=0(a_0=\infty)$, the unbounded increase of $Q\propto a_0$ is cancelled by the singularities of the cotangent at the points

$$s^{-1}=\frac{a_0}{d}2\pi p,\quad p=1,2,3,\ldots$$

This being the case, the values of $\mathscr{E}_s$ are the levels of the odd-parity states $\mathscr{E}_n^{(0)}$ from (7), with $n=2p$.

From the expressions for $s\ll 1$, and the conditions under which (28) is applicable, it follows that these equations are valid for $a_H\ll d$. Of course, in this approximation, the same values of the energy $\mathscr{E}_n^{(0)}$ from (7) would be obtained for any value of b.

Let us now consider the states which transform into even-parity states as $b\to 0$ in the next approximation, taking into account the influence of the impurity potential and its finite radius a_0. The quantum numbers s will be the roots of the equation

$$s\left(C+\ln\frac{2a_H^2}{a_0^2s^2}\right)=-\frac{1}{2}\left\{\operatorname{ctg}\left(s\ln|\tau_1|+\frac{|\tau_1|}{2}\right)+\operatorname{ctg}\left(s\ln|\tau_2|+\frac{|\tau_2|}{2}\right)\right\}.$$

In looking for the roots s of this equation under conditions where their initial values are given by Eq. (29), we find that

$$\mathscr{E}_s=\mathscr{E}_n^{(0)}+\Delta\mathscr{E}_p,$$

where $\mathscr{E}_n^{(0)}$ is the energy level (7) for $n=2p+1$, and $\Delta\mathscr{E}_p$ coincides exactly with the right side of Eq. (10). This also is not unexpected, since the inequality $s\ll 1$ is in fact equivalent to the condition under which perturbation theory is applicable, i.e., $d\ll a_0$. This agreement may be regarded as confirmation of the correctness of the more general expression (8), a special case of which is Eq. (10).

For the case $d\simeq a_0$, it is necessary to investigate the general form of Eq. (28). Based on qualitative considerations, we may expect that an increase in the parameter d/a_0 will cause an increase in the number s, and consequently a decrease in the energy $\mathscr{E}_s$ to low values $\mathscr{E}\simeq 0$.

If the center is close to the edge of the layer ($|\tau_2|\gg 1$, $a_H/a_0s\ll|\tau_1|\ll 1$), then from Eq. (28) it is not difficult to arrive at an equation for $s\ll 1$ by making the replacement $\nu\to s$, $t_1\to|\tau_1|$ in Eq. (26).

2.3. Thin layer, $d\ll a_H$

For this type of layer, the t-dependent matrix element in Eq. (14) is expressed in terms of the probability integral, whose argument always remains small in value. If we limit ourselves to the first term of an expression of the probability integral $\Phi(x)\propto 2\pi^{-1/2}x$, then Eq. (14) can be written in terms of the variable z in the form

$$-\frac{\hbar^2}{2\mu}f_\nu''(z)+eF|z-b|f_\nu(z)=\left[\mathscr{E}_\nu+\left(\frac{\pi}{2}\right)^{1/2}\frac{e^2}{\varepsilon a_H}\right]f_\nu(z),$$

where $F=e/\varepsilon a_H^2$.

The equation so obtained describes states of a particle in a uniform electric field F. For its general solution $f_\nu(z)$ we can obtain a linear combination of the Airy functions Ai and Bi (see Ref. 11), and from condition (15) the energy $\mathscr{E}_\nu$ can be determined. However, we should note here that for these relations between a_H, d, and a_0 the conditions for applicability of perturbation theory are satisfied, in particular the general expression (8). Turning to a special case (9), we obtain

$$\mathscr{E}_\nu=\mathscr{E}_n^{(0)}+\Delta\mathscr{E}_p,$$

where $\mathscr{E}_n^{(0)}$, $n=2p+1$ is energy level (7), and $\Delta\mathscr{E}_p$ has the form (9).

2.4. Center at edge of layer, $b=-2$

a) Region of the discrete Coulomb spectrum: $\mathscr{E}_\nu=-e^2/2\varepsilon a_0\nu^2<0$. In this case, we are required to find the solution to Eq. (16) that satisfies the boundary conditions $f_\nu(0)=f_\nu(t_0)=0$, $t_0=2d/a_0\nu$. In region (16) the general solution $f_\nu(t)$ takes the form (17), while for $2a_H/a_0\nu\ll t\ll 1$ it takes the form (18), in which we must take $c_+=0$ since $f_\nu(0)=0$. From the condition that the solution (17) reduce to zero at $t=t_0$, and that it match smoothly in the region $t\ll 1$ with the function (18), we obtain a system of three equations for the coefficients A_+, B_+, α_+. The condition that this equation be solvable leads to an equation for the quantum number ν. This equation can be obtained from the relation (25), in which we should formally set

$$\lambda(\nu)=0,\quad W_2=W_1=W_0,$$

$$M_2=M_1=M_0,\quad W_0=W_{\nu,1/2}(t_0),\quad M_0=M_{\nu,1/2}(t_0)$$

choosing the sign " $-$ " in front of the radical.

If the crystalline layer is sufficiently wide ($t_0\gg 1$), then in order to find the quantum number $\nu=k+\delta$, where $k=1,2,3,\cdots$, we must find the correction $\delta\ll 1$ by solving the equation

$$\frac{1}{\delta}+\frac{2Q(k)}{k}+\frac{k}{(k!)^2\delta^2}t_0^{2k}e^{-t_0}=0.$$

It is not difficult to see that the last term on the left side, which comes from the finiteness of the layer width, increases the correction δ, and consequently decreases the binding energy of the Coulomb DIC compared to its energy in an unbounded crystal. If we assume that in a wide layer it is possible to classify the states with respect to parity in the conventional way, the last equation applies to the odd-parity states [see the text below Eq. (25)]. In order to investigate the dynamics of levels of differing parity when the attractive center approaches the edges of the layer without constraint, we apparently must turn to a numerical investigation of Eq. (14), because the analytic method we are using to derive the general formula (25) does not allow the center to approach the layer boundary closer than a distance on the order of the magnetic length.

b) Region of size-quantized energies: $\mathscr{E}_s=e^2/2\varepsilon a^0s^2>0$. Proceeding in a way completely analogous to the case of negative energies, we are led to an equation for determining the quantum number s. This equation can be obtained from (28), in which we must formally assume

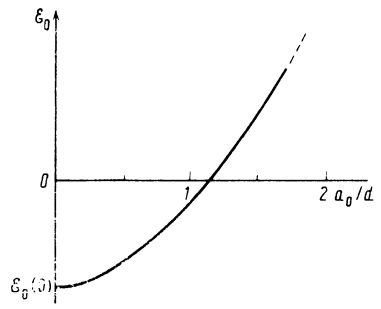

FIG. 1. Dependence of the position of the ground state of a DIC of radius a_0 on the layer width $d(\mathscr{E}_0(0) = -e^2/2\varepsilon a_0\nu^2, \nu<1)$.

$$\lambda(s)=0,\ \tilde{W}_2=\tilde{W}_1=\mathrm{Re}\,W_{is,1/2}(\tau_0),$$
$$\tilde{M}_2=\tilde{M}_1=\mathrm{Im}\,M_{is,1/2}(\tau_0),\quad \tau_0=\frac{2d}{ia_0s}$$

and take the sign " + " in front of the radical.

For $s\ll 1$, the equation for s takes the simple form

$$2s(C-1)=4Q(s)-\mathrm{ctg}\left(\frac{d}{a_0s}+s\ln\frac{2d}{a_0s}\right).$$

In the zeroth approximation $a_0=\infty$, $Q=\infty$, $s=0$, we find that $d/a_0s=n\pi$, $n=1,2,3,\cdots$, and as a result we obtain the full set of size-quantized energy levels $\mathscr{E}_n^{(0)}$ from (7).

In the next approximation,

$$\mathscr{E}_s=\mathscr{E}_n^{(0)}\left(1-\frac{2d}{a_0(n\pi)^2}\ln 2n\pi\right),\qquad \frac{d}{a_0n\pi}\ll 1.$$

The impurity potential causes a decrease in the particle energy. By further increasing the ratio d/a_0, we can decrease the particle's energy $\mathscr{E}_s$ down to small values $\mathscr{E}_s\cong 0$.

The investigation we have carried out allows us to isolate the dependence of the positions of the DIC energy levels on the width of the semiconductor layer d. In a wide layer $(d/a_0\gg 1)$, the position of the level $\mathscr{E}_\nu\ll 0$ coincides to exponential accuracy with its position in an unbounded crystal. As the parameter d/a_0 decreases, the energy increases, and for $d/a_0\approx 1$ it is found in the region $\mathscr{E}_\nu\approx 0$. As the parameter d/a_0 decreases, the energy level moves in the direction of positive values, and when $d/a_0\ll 1$, $d/a_H\ll 1$, it practically coincides with the system levels of an infinitely deep potential well of width d. The qualitative dependence of the position of the ground state level $\mathscr{E}_0$ on the layer width d is shown in Fig. 1.

The approximation used here of a single-band spectrum with respect to the Landau levels is entirely correct for the region of the discrete Coulomb spectrum that is adjacent to the bottom Landau level $N=m=0$ on the low-energy side. However, for the higher Landau levels we must keep in mind the following fact. The impurity quasi-Coulomb series that adjoins each higher Landau level may end up in the background of the spectrum of size-quantized energies that branch off of the previous Landau level. In order to take into account the interaction of the states of these overlapping energy spectra, it is necessary to use the two-band approximation developed in Ref. 9. In a wide layer $(d/a_0\gg 1)$, this interaction generally occurs all the time. In a narrow layer $(d/a_0\ll 1)$, two situations are possible. If the spacing between unperturbed impurity levels $\Delta E^{(0)}=E_{\perp N_1m_1}+\mathscr{E}_{n1}^{(0)}-E_{\perp N_2m_2}-\mathscr{E}_{n2}^{(0)}$ considerably exceeds the energy of a particle in the field of the impurity, then the one-band approximation is applicable as before. If, however, the spacing $\Delta E^{(0)}$ is comparable to the impurity interaction, then it is necessary to carry out a combined investigation of the Landau sublevels with N_1, m_1, and N_1, m_2.

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