Loosely bound particle with nonzero orbital angular momentum in an electric or magnetic field

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The effect of a magnetic or electric field on a loosely bound particle in a potential well with nonzero orbital angular momentum is investigated. A consistent analysis of the Schrödinger equation inside the well is replaced by a boundary condition for the wave function on the surface of a sphere. The radius of the sphere and the binding energy of the particle in the absence of a field are regarded as phenomenological parameters. Outside the bounding sphere, the wave function is constructed by differentiating the Green's function for a particle in an electric or magnetic field. The energy shift in weak and strong magnetic fields is calculated for the case of the p-state. The conditions for the appearance of a bound state under the influence of the magnetic field is ascertained in the case when there is no such state in the absence of a field, and the binding energy of this state is calculated. The energy shift and the level width in an electric field are calculated. The dependence of the polarizability on the binding energy at various values of the orbital momentum are also considered.

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1. INTRODUCTION

In our preceding papers[1,2] we considered the effect of an electric and magnetic fields on a particle with low binding energy in a potential well in the s-state. The Schrödinger equation within the well was replaced by a boundary condition for the wave function in the center, in analogy with the approach in which a zero-radius potential is used. However, this approach cannot be literally applied to the case of a nonzero orbital angular momentum. If the radius of a potential well capable of retaining the particle in a bound state with a given orbital angular momentum is allowed to tend to zero, and the depth is allowed to tend to infinity (with the position of the energy level unchanged), then the wave function everywhere outside the well vanishes. Therefore the boundary condition that replaces the Schrödinger equation inside the well must be imposed on a sphere of finite radius r_0.

Thus, in place of a single phenomenological parameter (the binding energy) used in the zero-radius potential model, in the case of a nonzero orbital angular momentum it is necessary to have to parameters: the binding energy and the radius r_0 of the bounding sphere. We set r_0 equal to the effective radius employed in the theory of slow-particle scattering.[3] The radius of the bounding sphere can be expressed in terms of the normalization coefficient in the asymptotic wave function. By virtue of the known connection between these coefficients and the residue of the scattering amplitude at its pole, both definitions turn out to be equivalent (see Appendix I).

We shall assume r_0 to be sufficiently small and take into account, wherever possible, only the values of the lowest order in r_0.

In Sec. 2 we formulate the boundary condition for an arbitrary angular momentum l. In Sec. 3, the boundary condition is used to consider the influence of the magnetic field on a weakly bound particle in the p-state, while in Sec. 4 it is used to consider the effect of the electric field. Certain calculations are relegated to the Appendix.

2. BOUNDARY CONDITION

We consider a particle with rectangular potential well of radius r_0, having an energy ε and orbital angular momentum l. We use a system of units with $\hbar = M = 1$ (for a charged particle we put also $e = 1$) and represent the energy in the form $e = -\alpha^{-2}/2$. We assume that $\alpha r_0 \ll 1$.

We write the wave function in the form

$$\psi = Y_{lm}(\theta, \varphi) R_l(r). \tag{2.1}$$

The radial wave function $R_l(r)$ outside the sphere of radius r_0 is proportional to the spherical Hankel function $h_l^{(1)}(i\alpha r)$. We put

$$R_l = a_l \alpha^{l+1} i^{l+2} h_l^{(1)}(i\alpha r). \tag{2.2}$$

The factor i^{l+2} is introduced to make the normalization factor a_l real. The factor α^{l+1} is introduced to obtain in the limit as $\alpha \to 0$ a finite wave function of zero energy (belonging to the discrete spectrum). The normalization factor a_l depends little on energy at small α. Since we are interested in a state with low binding energy, we can use the limiting value of a_l corresponding to $\alpha = 0$. This value is determined from the normalization condition and is equal to (see Appendix I)

$$a_l = \left[2\frac{(2l-1)}{(2l+1)}\right]^{1/2} \frac{r_0^{l-1/2}}{(2l-1)!!}. \tag{2.3}$$

At $\alpha r \gg 1$ we obtain from (2.2)

$$R_l \sim B_l r^{-1} \exp(-\alpha r),$$

where

$$B_l = \left[2\frac{(2l-1)}{(2l+1)}\right]^{1/2} \frac{r_0^{l-1/2} \alpha^l}{(2l-1)!!}. \tag{2.4}$$

We use relation (2.4) also in the case of a short-range potential well of arbitrary shape. Then (2.4) serves as a definition of r_0, according to which r_0 is expressed

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in terms of the coefficient B_l in the asymptotic form of the wave function. We consider now the value of R_l at $r=r_0$. Recognizing that $\alpha r_0 \gg 1$, we expand $h_l^{(1)}(i\alpha r_0)$ in a series and retain only the terms that matter most for the calculation, and neglect the small corrections to them.

To clarify the structure of this expansion, we use the relation

$$h_l^{(1)}(z)=j_l(z)+in_l(z).$$

The first two terms of the expansion of $n_l(z)$ take the form $-(2l-1)!![z^{-l-1}+z^{-l+1}/2(2l-1)]$. The third term is of order z^{-l+3}. The expansion of the function j_l begins with z^l. If we retain only two terms in the expansion of n_l, then we must discard j_l at all $l \geq 2$, inasmuch as in these cases z^l is of higher order of smallness than z^{-l+3}.

We therefore put at $l \geq 2$

$$R_l=a_l(2l-1)!!\left(\frac{1}{r_0^{l+1}}-\frac{\alpha^2}{2(2l-1)r_0^{l-1}}\right). \tag{2.5}$$

At $l=1$, allowance for the first term in the expansion of j_l is legitimate, for in this case z^{-l+3} is of higher or-order of smallness than z^l. Allowance for j_l leads in fact only to a small insignificant correction in many cases. However, for example in the calculation of the diamagnetic energy shift, we shall see that this term turns out to be significant. We therefore write out fully the limiting value of R_1, including the term $\sim r_0$:

$$R_1=a_1\left(\frac{1}{r_0^2}-\frac{\alpha^2}{2}+\frac{\alpha^3 r_0}{3}\right). \tag{2.6}$$

We shall find it convenient to change over to a different normalization, in which the coefficient of r_0^{-l-1} is equal to unity. Substituting (2.5) or (2.6) in (2.1), leaving out the factor $a_l(2l-1)!!$ and denoting the result by Φ, we obtain

$$\int \Phi Y_{lm}^* d\Omega=\frac{1}{r_0^{l+1}}-\frac{\alpha^2}{2(2l-1)r_0^{l-1}}, \quad l\geq 2; \tag{2.7}$$

$$\int \Phi Y_{1m}^* d\Omega=\frac{1}{r_0^2}-\frac{\alpha^2}{2}+\frac{\alpha^3}{3}r_0, \quad l=1. \tag{2.8}$$

Relations (2.7) and (2.8) will be regarded as the boundary condition that replaces the consistent analysis of the Schrödinger equation in the field of a short-range well of arbitrary shape. We shall use these conditions also in the case when a magnetic or electric field is present in addition to the short-range well. The function Φ is then a suitable exact solution of the Schrödinger equation for a particle in a homogeneous electric or magnetic field. Of course, the angle and radial variables do not separate in this solution.

3. EFFECT OF A MAGNETIC FIELD ON A LOOSELY BOUND PARTICLE IN THE p-STATE

The problem is to find a solution Φ_m, singular at $r=0$, of the Schrödinger equation for a charged particle in a homogeneous magnetic field directed along the z axis. The solution must satisfy on the surface of a sphere of small radius r_0 the boundary condition

$$\int \Phi_m Y_{1m}^* d\Omega=\frac{1}{r_0^2}-\frac{\alpha_0^2}{2}+\frac{\alpha_0^3}{3}r_0. \tag{3.1}$$

We denote by $\alpha_0^2/2$ the binding energy in the absence of the magnetic field. The sought solution is expressed in terms of the derivatives, with respect to the cylindrical coordinates, of the Green's function $G(\mathbf{r},\mathbf{r}')$ for a homogeneous magnetic field at $\mathbf{r}'=0$:

$$\Phi_0=(3\pi)^{1/2}\frac{\partial G}{\partial z}; \quad \Phi_{\pm1}=\left(\frac{3\pi}{2}\right)^{1/2}\left(\frac{\partial G}{\partial \rho}-\omega\rho G\right)e^{\pm i\varphi}. \tag{3.2}$$

Here ω is the Larmor frequency, equal in ordinary units to $e\mathscr{H}/2Mc$.

The function $\partial G/\partial z$ satisfied in obvious fashion the Schrödinger equation in a homogeneous field. The fact that $\Phi_{\pm1}$ (3.2) also satisfies the Schrödinger equation in a homogeneous field is somewhat less obvious, but can also be proved (see Appendix II). The function G can be represented in the form of the integral

$$G=\int_0^\infty K e^{i\epsilon t}dt.$$

The kernel K for a particle in a homogeneous electric or magnetic field was constructed by Feynman and Hibbs.[4]

In the case of a magnetic field, it is convenient to replace t by the integration variable $x=i\omega t$. Then $G(\mathbf{r},0)$ takes the form

$$G=-\frac{\omega^{1/2}}{(2\pi)^{3/2}}\int_0^\infty (1+\operatorname{cth} x)\exp\left(-\frac{\alpha^2 x}{2\omega}-\frac{\omega z^2}{2x}-\frac{\omega\rho^2}{2}\operatorname{cth} x\right)\frac{dx}{x^{1/2}}. \tag{3.3}$$

Here $\alpha^2/2$ is the binding energy reckoned from the boundary of the continuous spectrum. The position of this boundary at $m=0$ is equal to ω (Ref. 5). The position of the boundary of the continuous spectrum at $m=-1$ is also equal to ω, and at $m=1$ it is 3ω.[5]

Differentiating (3.3) with respect to ρ and z and substituting in (3.2), we obtain

$$\Phi_0=Y_{10}\frac{\omega^{3/2}r_0}{(2\pi)^{1/2}}\int_0^\infty (1+\operatorname{cth} x)\exp\left[-\frac{\alpha^2 x}{2\omega}-\frac{\omega r^2}{2x}-\frac{\omega\rho^2}{2}\left(\operatorname{cth} x-\frac{1}{x}\right)\right]\frac{dx}{x^{3/2}}; \tag{3.4}$$

$$\Phi_{\pm1}=Y_{1\pm1}\frac{\omega^{3/2}r_0}{(2\pi)^{1/2}}\int_0^\infty (1+\operatorname{cth} x)^2\exp\left[-\frac{\alpha^2 x}{2\omega}-\frac{\omega r^2}{2x}-\frac{\omega\rho^2}{2}\left(\operatorname{cth} x-\frac{1}{x}\right)\right]\frac{dx}{x^{1/2}}. \tag{3.5}$$

We consider now Φ_0 and $\Phi_{\pm1}$ on a bounding sphere of radius r_0. The term $(1/2)\omega\rho^2(\coth x-1/x)$ in the argument of the experimental does not exceed $(1/2)\omega r_0^2$. The quantity ωr_0^2 is the square of the ratio of the well radius to the magnetic length $\omega^{-1/2}$ and is assumed to be small (otherwise the fixed boundary condition cannot be used). We therefore neglect this term. Next, to separate the singular part in the wave function, we add and subtract the quantity $1/x$ under the integral sign in (3.4) and $1/x^2$ in (3.5). The singular part is expressed in terms of the spherical Hankel function $h_1^{(1)}(i\alpha r_0)$, in which we take into account three terms of the series expansion. In the remaining regular part we retain the terms that do not depend on r_0 and the terms proportional to r_0, and discard all others. Substituting the approximate expressions obtained in this manner for Φ_0 and $\Phi_{\pm1}$ in (3.1), we obtain equations[1)] for the determination of α:

$$\alpha_0^2/2-\alpha_0^3 r_0/3=\alpha^2/2-\alpha^3 r_0/3-\omega-(A_0-\omega\alpha)r_0, \quad m=0, \tag{3.6}$$

$$\alpha_0^2/2-\alpha_0^3 r_0/3=\alpha^2/2-\alpha^3 r_0/3-2\omega-(A_1-2\omega\alpha)r_0, \quad m=\pm1, \tag{3.7}$$

$$A_0=\frac{\omega^{3/2}}{(2\pi)^{1/2}}\int_0^\infty\left(\operatorname{cth}x-\frac{1}{x}\right)\exp\left(-\frac{\alpha^2x}{2\omega}\right)\frac{dx}{x^{3/2}}$$
$$=-\alpha\omega-\frac{\alpha^3}{3}-4\omega^{3/2}\zeta\left(\frac{1}{2},1+\frac{\alpha^2}{4\omega}\right),\qquad(3.8)$$
$$A_1=\frac{\omega^{3/2}}{(2\pi)^{1/2}}\int_0^\infty\left(1+2\operatorname{cth}x-\frac{2}{x}+\operatorname{cth}^2x-\frac{1}{x^2}\right)\exp\left(-\frac{\alpha^2x}{2\omega}\right)\frac{dx}{x^{3/2}}.$$

We consider two limiting cases.

1. *Weak fields*, $\omega\ll\alpha_0^2/2$. In this case α is close to α_0. In the integrals A_0 and A_1 the main contribution is made by the region of small x, and the values of the integrals can be estimated by replacing the pre-exponential factor by the first term of the expansion in powers of x. We obtain

$$A_0=\frac{1}{3}\frac{\omega^2}{\alpha},\quad A_1=\frac{5}{3}\frac{\omega^2}{\alpha}.$$

The equations (3.6) are solved by successive approximations. In the first-order approximation we neglect all the quantities proportional to r_0, and retain only the terms independent of r_0. In the second approximation we find the correction proportional to r_0, in which we retain the terms not higher than ω^2. We obtain

$$\frac{\alpha^2}{2}=\frac{\alpha_0^2}{2}+\omega-\frac{\omega^2r_0}{6\alpha_0},\quad m=0,$$
$$\frac{\alpha^2}{2}=\frac{\alpha_0^2}{2}+2\omega-\frac{\omega^2r_0}{3\alpha_0},\quad m=\pm1.\qquad(3.9)$$

Changing from the quantity $-\alpha^2/2$ to the energy ε (with allowance for the position of the boundary of the continuous spectrum), we obtain

$$\varepsilon=\varepsilon_0+\omega^2r_0/6\alpha_0,\quad m=0,$$
$$\varepsilon=\varepsilon_0+\omega^2r_0/3\alpha_0\pm\omega,\quad m=\pm1.\qquad(3.10)$$

The term $\pm\omega$ is the paramagnetic energy shift. The terms proportional to ω^2 are the diamagnetic energy shift and agree (in first order in r_0) with the result of the perturbation-theory calculation.

2. *Strong fields*, $\omega\gg\alpha_0^2/2$. In this case the terms $(1/3)\alpha^3r_0$ and $\omega\alpha r_0$ are small corrections and can be neglected. Equations (3.6) take the form

$$\alpha^2/2=\omega+A_0r_0,\quad m=0,$$
$$\alpha^2/2=2\omega+A_1r_0,\quad m=\pm1.\qquad(3.11)$$

To estimate the integral A_0 we can take the limit as $\alpha^2/\omega\to0$ in the argument of the exponential. We obtain

$$A_0=\frac{\omega^{3/2}}{(2\pi)^{1/2}}\int_0^\infty\left(\operatorname{cth}x-\frac{1}{x}\right)\frac{dx}{x^{3/2}}=\frac{1}{\pi}\zeta\left(\frac{3}{2}\right)\omega^{3/2}\approx0.2647\omega^{3/2}.\qquad(3.12)$$

As for the integral A_1, the limit as $\alpha^2/\omega\to0$ cannot be taken, since the integral then diverges. Replacing by way of estimate the pre-exponential factor by its limiting value as $x\to\infty$ and calculating the integral, we have

$$A_1=8\omega^2/\alpha.\qquad(3.13)$$

Finally, we consider the possibility of appearance of a level in the case when there is no level in the absence of a field, that is, $\alpha_0^2/2<0$. We designate $-\alpha_0^2/2$ by E_0. If a level can appear under the influence of the field, then one must expect this level to be close to the boundary of the continuous spectrum, i.e., $\alpha_2/2\ll\omega$. To determine α under these conditions, we have the relations

$$\alpha^2/2=\omega-E_0+\pi^{-1}\zeta(3/2)\,\omega^{3/2}r_0,\quad m=0,\qquad(3.14)$$
$$\alpha^2/2=2\omega-E_0+8\omega^2r_0/\alpha,\quad m=\pm1.\qquad(3.15)$$

As seen from (3.14), the appearance of a level at a given E_0 and $m=0$ is possible only starting with a certain threshold value of the field, determined by the relation

$$\omega+\pi^{-1}\zeta(3/2)\,\omega^{3/2}r_0=E_0.\qquad(3.16)$$

On the contrary, at $m=\pm1$, as seen from (3.15), a level can appear at any arbitrarily small but finite value of ω.

Neglecting in (3.15) ω and $\omega^2/2$ compared with E_0, we obtain an estimate for α:

$$\alpha=8\omega^2r_0/E_0.\qquad(3.17)$$

Accordingly, the binding energy W of the level, which appears under the influence of the field, is equal to

$$W=32\omega^4r_0^2/E_0^2.\qquad(3.18)$$

4. EFFECT OF ELECTRIC FIELD ON A LOOSELY BOUND PARTICLE IN THE p-STATE

In the presence of an electric field of intensity $\mathscr{E}$, the energy becomes complex. The imaginary part, as is well known, characterizes the probability of penetrating through the potential barrier. Of greatest physical interest is the case when the ratio of the imaginary and real parts of the energy is small. This case is realized when the dimension of the potential barrier along the field, which is of the order of $\alpha_0^2/\mathscr{E}$, greatly exceeds the characteristic dimension α_0^{-1} (the "radius" of the wave function, i.e., when $\mathscr{E}/\alpha_0^3\ll1$. In this case $\mathscr{E}r_0/\alpha_0^2$ will be all the smaller. Under these conditions, the term $(1/3)\alpha^3r_0$ in the boundary condition (2.8) is a small correction which we shall disregard.

The problem consists of finding a suitable singular solution of the Schrödinger equation Φ_m in an electric field $\mathscr{E}$ directed along the z axis and satisfying the boundary condition at $r=r_0$

$$\int\Phi_mY_{1m}^*d\Omega=\frac{1}{r_0^2}-\frac{\alpha_0^2}{2}.$$

Just is in the case of magnetic field, Φ_m is expressed in terms of derivatives of the Green's function G, which is equal to[6]

$$G=\left(\frac{i}{2\pi}\right)^{3/2}\int_0^\infty\exp i\left[\frac{r^2}{2t}-\frac{1}{2}(\alpha^2-\mathscr{E}z)t-\frac{\mathscr{E}^2t^3}{24}\right]\frac{dt}{t^{3/2}}.\qquad(4.1)$$

The derivative $(\partial G/\partial\rho)e^{\pm i\varphi}$ satisfies in obvious fashion the Schrödinger equation. We therefore put ($m=1,\pi$-state)

$$\Phi_\pm=(3\pi/2)^{1/2}e^{\pm i\varphi}\partial G/\partial\rho.\qquad(4.2)$$

We consider now Φ on a bounding sphere of radius r_0. Assuming that $\mathscr{E}r_0\ll\alpha^2$, we neglect the term $\mathscr{E}_z$ in the argument of the integrand. Then

$$\Phi_{\pm1}=-\left(\frac{i}{2\pi}\right)^{1/2}r_0\int_0^\infty\exp i\left(\frac{r_0^2}{2t}-\frac{\alpha^2}{2}t-\frac{\mathscr{E}^2t^3}{24}\right)\frac{dt}{t^{5/2}}Y_{1,\pm1}.\qquad(4.3)$$

The method of calculating the integral in the right-hand side of (4.3) is indicated in Appendix III. We write out here the final result:

$$\Phi_{\pm 1}=\left[\frac{1}{r_0^2}-\frac{\alpha^2}{2}+\frac{\mathscr{E}^2 r_0}{24\alpha_0^3}+i\frac{\mathscr{E}^2 r_0}{8\alpha_0^3}\exp\left(-\frac{2\alpha_0^3}{3\mathscr{E}}\right)\right] Y_{1,\pm 1}. \qquad (4.4)$$

We have left out of (4.4) a corrections of higher order of r_0. Substituting (4.4) in the boundary condition, we obtain

$$\frac{\alpha^2}{2}=\frac{\alpha_0^2}{2}+\frac{\mathscr{E}^2 r_0}{24\alpha_0^3}+i\frac{\mathscr{E}^2 r_0}{8\alpha_0^3}\exp\left(-\frac{2\alpha_0^3}{3\mathscr{E}}\right). \qquad (4.5)$$

The real part of the energy shift Δ is equal to

$$\Delta_\pi=-\mathscr{E}^2 r_0/24\alpha_0^3 \qquad (4.6)$$

and coincides with the value obtained by perturbation theory (neglecting the corrections of higher order in r_0). The imaginary part of the shift is half the level width Γ_π. As follows from (4.5),

$$\Gamma_\pi=\frac{\mathscr{E}^2 r_0}{4\alpha_0^3}\exp\left(-\frac{2\alpha_0^3}{3\mathscr{E}}\right). \qquad (4.7)$$

We turn now to the case $m=0$ (σ-state). It is easy to verify that the expression $\partial G/\partial z+2\mathscr{E}\partial G/\partial\alpha^2$ satisfies the Schrödinger equation for a particle in a homogeneous electric field. Starting from this, we put

$$\Phi_0=(3\pi)^{1/2}\left[\frac{\partial G}{\partial z}+2\mathscr{E}\frac{\partial G}{\partial\alpha^2}\right]. \qquad (4.8)$$

Substituting here (4.1), we obtain

$$\Phi_0=-\frac{(3i)^{1/2}}{2^{3/2}\pi}\left[r_0\cos\theta\int_0^\infty \exp i\left(\frac{r_0^2}{2t}-\frac{\alpha^2}{2}t+\frac{\mathscr{E}r_0\cos\theta}{2}t-\frac{\mathscr{E}^2t^3}{24}\right)\frac{dt}{t^{5/2}}\right.$$
$$\left.-\frac{\mathscr{E}}{2}\int_0^\infty \exp i\left(\frac{r_0^2}{2t}-\frac{\alpha^2}{2}t+\frac{\mathscr{E}r_0\cos\theta}{2}t-\frac{\mathscr{E}^2t^3}{24}\right)\frac{dt}{t^{1/2}}\right]. \qquad (4.9)$$

In the argument of the exponential in the first integral of the right-hand side of (4.9) we neglect, just as in (4.3), the quantity $\mathscr{E}r_0\cos\theta$. As for the second integral, we retain two terms of the series expansion of $\exp(i\mathscr{E}r_0 t\cos\theta/2)$ in powers of t, i.e., we replace this exponential by $1+(1/2)i\mathscr{E}r_0 t\cos\theta$. We obtain

$$\Phi_0=-\left(\frac{i}{2\pi}\right)^{1/2}\left[Y_{1,0}r_0\int_0^\infty\left(\frac{1}{t^{5/2}}-i\frac{\mathscr{E}}{4}t^{1/2}\right)\exp i\left(\frac{r_0^2}{2t}-\frac{\alpha^2}{2}t-\frac{\mathscr{E}^2t^3}{24}\right)dt\right.$$
$$\left.-\frac{\sqrt{3}}{2}\mathscr{E}Y_{0,0}\int_0^\infty \exp i\left(\frac{r_0^2}{2t}-\frac{\alpha^2}{2}t-\frac{\mathscr{E}^2t^3}{24}\right)\frac{dt}{t^{1/2}}\right]. \qquad (4.10)$$

The term containing Y_{00} makes no contribution whatever to the boundary condition, by virtue of the orthogonality of the spherical functions.

The integrals in (4.10) are calculated by the method indicated in Appendix III. The expression for $\alpha^2/2$, which follows from the boundary condition, is of the form

$$\frac{\alpha^2}{2}=\frac{\alpha_0^2}{2}+\frac{7}{24}\frac{\mathscr{E}^2 r_0}{\alpha_0^3}+i\left(\frac{\mathscr{E}}{4}+\frac{\mathscr{E}^2}{8\alpha_0^3}\right)r_0\exp\left(-\frac{2\alpha_0^3}{3\mathscr{E}}\right). \qquad (4.11)$$

The real part of the energy shift is

$$\Delta_\sigma=-\frac{7}{24}\frac{\mathscr{E}^2 r_0}{\alpha_0^3}, \qquad (4.12)$$

which also agrees with the perturbation-theory result (accurate to higher powers of r_0) for the polarizability. For the width we obtain

$$\Gamma_\sigma=(\mathscr{E}/2+\mathscr{E}^2/4\alpha_0^3)r_0\exp(-2\alpha_0^3/3\mathscr{E}). \qquad (4.13)$$

The term $\mathscr{E}^2/4\alpha_0^3$ in the parentheses is a small correction to the principal term.

In conclusion we examine the dependence of the real part of the energy shift $\Delta=-\beta_1\mathscr{E}^2/2$ on α_0 and r_0 at different l. We confine ourselves to the case of a maximum value of the projection of the angular momentum $m=l$, for which the calculation reduces to the determination of the l-th derivative of the Green's function

$$\lambda_l=\rho^l(\partial/\partial\rho^2)^l G$$

(in the same approximation as before).

With the aid of the boundary condition (2.8) we find that the polarizability β_l is proportional to the quantity $r_0^{l-1}(\partial\lambda_l/\partial\mathscr{E}^2)_{\mathscr{E}=0}$. Leaving out all the numerical coefficients, we have

$$\beta_l\sim\alpha^{l-5/2}r_0^{l+3/2}H^{(1)}_{l-5/2}(i\alpha r_0).$$

Since $\alpha r_0\ll 1$, we can replace $H^{(1)}_{l-5/2}$ by the first term of the series expansion.

At $l=1$ and 2, the first term is proportional to $(\alpha r_0)^{l-5/2}$, so that

$$\beta_l\sim\alpha^{2l-5}r_0^{2l-1}. \qquad (4.14)$$

At $l=1$ we obtain the already-known result. At $l=2$

$$\beta_l\sim\alpha^{-1}r_0^3.$$

At $l\geqslant 3$, however, the first term of the expansion of $H^{(1)}_{l-5/2}(i\alpha r_0)$ is proportional to $(\alpha r_0)^{5/2-l}$. In this case

$$\beta_l\sim r_0^4 \qquad (4.15)$$

and is independent of α.

5. COMPARISON WITH THE RESULTS OF OTHER CALCULATIONS

Dalidchik and Slonim[6] have considered an electron in the field of several zero-radius potentials in the presence of an external homogeneous electric field. They simulated the p-state by an odd wave function in the field of two centers separated by a distance R under the condition $\alpha R\ll 1$. However, the question of how the distance R is connected with the radius r_0 in the potential well for which the two-center model is constructed, remained open in their paper. Comparing the formulas (4.6) and (4.12) for the energy shift with the results of the calculation of the shift in Ref. 6, we arrive at the conclusion that $R=2r_0$. In Ref. 6 is calculated also the level width. The final expressions (30) and (31) of that reference contain errors in the numerical coefficients. If Γ is recalculated using the general Eq. (29) of Ref. 6, but with $R=2r_0$, full agreement is obtained with our expressions (4.7) and (4.13).

We note also Refs. 7 and 8, in which the approximation of several zero-radius wells in an external field and perturbation theory were also considered.

An expression for the width was derived also by Smirnov and Chibisov[9] for a more general case, by another method that made it possible to obtain only the first term of the pre-exponential series. A comparison with our results has revealed errors in Ref. 9. One error is that the expression for $\sin\theta$ in terms of the parabolic coordinates $\xi=r+z$ and $\eta=r-z$ at small angles is taken in the form $(2\eta/\xi)^{1/2}$, whereas the correct expression is $2(\eta/\xi)^{1/2}$. The second error is that in place of $(l-m)!(l+m)!$ the final expression contains $(l+m)!/(l-m)!$ (which changes the result very greatly at $m \neq 0$).

Retaining the notation of Ref. 9, we present the correct expression for the electron-detachment probability per unit time:

$$W = B^2 \frac{2l+1}{2\gamma^m} \frac{m!(l-m)!}{(l+m)!} 2^{(2Z/\gamma)-1} \left(\frac{\gamma^2}{F}\right)^{(2Z/\gamma)-m-1} \exp\left(-\frac{2\gamma^3}{F}\right). \quad (5.1)$$

In the notation of the present paper, $\gamma = \alpha_0$, $F = \mathscr{E}$, $W = \Gamma$, and m means $|m|$. In addition, we must put $Z = 0$, inasmuch as in our case there is no Coulomb field. If we use the expression (2.4) for B_1 at $l = 1$, then the results of calculation by means of (5.1) agree with (4.7) and (4.13) (without the second term in the parentheses).

The indicated corrections allow us to resolve the contradiction in Ref. 10, where, when the coefficients B were determined by comparing the theory with experiment for the σ and π states of He^-, a difference by a factor of 1.5 was obtained. After making the corrections and including in B the additional factor $2^{1/2}$, the two coefficients agree within the limits of experimental error.

6. REGION OF APPLICABILITY OF THE APPROXIMATION

We discuss now the region of applicability of the approximation considered here. Actually in both considered problems (magnetic and electric fields) there are three independent parameters with the dimension of length: 1) the effective radius r_0; 2) the "wave-function radius" α^{-1}; 3) the characteristic scale R of the external field. For the magnetic field this is the magnetic length $R = \omega^{-1/2}$, for the electric field this is the width of the potential barrier $R = \alpha^2/2\mathscr{E}$. The theory is valid if $\alpha r_0 \ll 1$ and $r_0/R \ll 1$, and we take into account below only the lowest terms in the expansion in these parameters. At the same time, αR can be either larger than unity (weak fields) or less than unity (strong fields), as well as of the order of unity, although in real cases we are dealing usually with weak fields (even at a negative-ion binding energy 0.01 eV we have $\alpha^{-1} = 2 \cdot 10^{-7}$ cm, $\alpha R = 1$ at $\mathscr{E} = 5 \cdot 10^4$ V/cm or $\mathscr{H} = 2 \cdot 10^{-6}$ G $= 200$ T). In addition, at $\alpha R \sim 1$ the level width Γ in an electric field becomes large, and it is practically impossible to observe the corresponding state. We therefore assume $(\alpha R)^{-1} \ll 1$ in Eqs. (3.10) and (4.13) and expand the sought quantities in powers of this parameter, taking into account the necessary number of terms, this being an additional and generally speaking not obligatory approximation.

The second assumption with which the relation between the effective radius and the asymptotic normalization factor is connected is that the potential well and the external region are separated by a centrifugal potential barrier. If in addition there is a comparable potential barrier of a different type (non-centrifugal) at the edge of the well, then this relation is violated. A similar violation results, for example, from a Feshbach-like state of a strongly bound system (detachment of electron as a result of a two-electron transition in the presence of a weak dynamic coupling between the electrons in a negative ion). In all these cases, introduction of an effective radius is also possible but calls for a more detailed examination of the problem.

Finally, we have used throughout implicitly the assumption that an interaction takes place only with states with a given angular momentum, i.e., there is no "accidental" degeneracy at low energies of states with different l, while for the considered potential other bound and quasistationary states lie substantially farther from the origin on the complex energy plane, on both the physical and unphysical sheets, with the same relation preserved also in the presence of external fields. This assumption is perfectly natural for negative ions and, to a lesser degree, for scattering of slow neutrons by nuclei (as a result of the complicated structure of the low-energy scattering for many nuclei). It should be noted that the specific symmetry of the atomic potential[11] can lead to an almost simultaneous appearance of weakly bound states with different l when the nuclear charge Z is increased, but a more accurate allowance for the polarization and other interactions makes the splitting of these states sufficiently large, so that apparently this interaction can be disregarded for most real negative ions in really attainable fields.

It must be emphasized that although the results depend little on the shape of the potential well (except for the restrictions noted above), in contrast to the s-state they depend substantially on the spherical-symmetry assumption and, correspondingly, on the $(2L+1)$-fold degeneracy of the levels in the absence of an external field. Nonspherical small-radius potential wells and the parametrization with the aid of boundary conditions call for a more detailed analysis. This is precisely why simulation of spherically potential well with the aid of a system of zero-radius potential[6] must be carried out with caution.

7. CONCLUSION

The results of the present paper, jointly with Ref. 3, demonstrate clearly that it is natural to use a two-parameter approximation, similar to the two-parameter approximation for s-states (Ref. 5, § 133), for the description of weakly bound states with an arbitrary angular momentum in a short-range force field. One of these parameters (α_0^2) is connected with the energy of the bound state $(\alpha_0^2 > 0)$ of with the position of the quasistationary state–resonance in the scattering $(\alpha_0^2 < 0)$. The force parameter, on the other hand, characterizes the effective radius of the forces and is correspondingly connected with the relative contribution made to the normalization integral by the regions of space inside and outside the potential well. By the same token, it can be expressed in terms of the normalization coefficient of the wave function of the bound state outside the well. The effective radius is convenient as a second parameter in view of its clarity, of the connection with the analogous parameter for the s-states, and of its suitability for use for both bound and quasistationary states.

The behavior of a weakly bound p-state in a magnetic field can be explained qualitatively by starting from simple physical considerations. Indeed, when the magnetic field is turned on, the problem becomes quasi-one-dimensional[2] since the magnetic field prevents the particle from moving away in directions perpendicular to the field. For the $p\sigma$ states there is, in addition, a nodal surface at $z=0$, and we obtain a quasi-one-dimensional problem on a semi-infinite interval. The bound state is formed in this case only after the potential well reaches a certain depth, as is in fact observed. For the $p\pi$ states, the plane $z=0$ is not a node, the wave function is symmetrical with respect to the replacement of z by $-z$, and then there is a bound state in the one-dimensional problem in any potential well. In this case, however, the wave function vanishes on the z axis, the influence of the potential well is weaker than for the $s\sigma$ state considered in Ref. 2, and the binding energy is proportional not to the second power of the field (as for the $s\sigma$ case) but to the fourth power. Such states can be apparently observed in semiconductors with low effective electron or hole masses in superstrong magnetic fields at low temperatures, but this is a much more complicated task than the observation of analogous $s\sigma$ states.

For the p state in an electric field, the most interesting is the lifetime and the width of the level Γ, inasmuch as in really attainable fields we can destroy the weakly bound negative ions at a binding energy less than 0.1 eV (Ref. 10) and when an accelerators magnetic field (a Lorentz force equivalent to the electric field) is used this can be done at energies up to ~1 eV, Since Γ depends very strongly on the binding energy E_0, these measurements make it possible to determine E_0 quite reliably and the effective radius somewhat less reliably (field spectroscopy of weakly bound states[10]). In (4.7) and (4.13) the argument of the exponential is trivial and is equal to the phase integral for a trivial and is equal to the phase integral for a triangular potential barrier. However, the pre-exponential factor is not trivial, is proportional in our approximation to the effective radius, and contains an additional power of the small parameter $\mathscr{E}/\alpha_0^3$ for the π state, so that to reach the same accuracy in the calculation of Γ_σ it is necessary to retain two terms in the pre-exponential factor.

The quantity $\bar{\Gamma}=(1/3)\Gamma_\sigma+(2/3)\Gamma_\pi$ averaged over the σ and π states is meaningful when the time of stay of the ion in the field is short compared with the half-lives, so that the decay exponential can be expanded in a series and only the terms linear in Γ retained. Under real conditions allowance for Γ_π and for the second term in Γ_σ can change $\bar{\Gamma}$ by up to 15–20%.

Quantities such as the polarizability, diamagnetism, and others, which are not connected with tunnel transitions, do not depend on the binding energy at all at sufficiently large l in this simplest approximation. The centrifugal potential clamps the particle in this case to the edge of the potential well, so that we obtain the rigid-rotator model, and the below-barrier part of the wave function both inside and outside the well becomes negligible. This transition can take place at different l for different values; for the polarizability, as we have already found, it takes place at $l=3$.

Inasmuch as for all the negative ions the electron-affinity energy is much less than the polarization potential (the energy of the detachment of the next electron), the single-electron approximation used here and earlier[1,2] is quite satisfactory; the collective effects are important only inside the atom, where the behavior of the wave function has little influence on the phenomena considered here.

In some cases the effective radius may not enter in the final formulas. This is precisely the situation in the calculation of the spectrum of electrons emitted in slow collisions between negative ions and atoms, when this process is regarded as "pushing out" of a bound state with a specified l into the continuous spectrum from a small-radius nonstationary potential well.

We note finally that most monatomic negative ions have a weakly bound electron precisely in the p-state, so that the case $l=1$ considered here is particularly important from the point of view of possible applications.

APPENDIX I

We determine the coefficient a_l in (2.3) at $\alpha=0$ for a rectangular well. Inside the well, the radial wave function is of the form

$$R_l(r)=bj_l(\varkappa r),\quad \varkappa=(2V_0)^{1/2}, \tag{I.1}$$

where V_0 is the depth of the potential well. Outside the wall, at $\alpha=0$ we have from (2.3)

$$R_l=a(2l-1)!!r^{-l-1}. \tag{I.2}$$

From the normalization condition

$$\int_0^\infty R^2r^2dr=1$$

it follows that

$$b^2\int_0^{r_0} j_l^2(\varkappa r)r^2dr+a_l^2[(2l-1)!!]^2(2l-1)^{-1}r_0^{1-2l}=1. \tag{I.3}$$

Using the relation

$$\int_0^{r_0} j_l^2(\varkappa r)r^2dr=\frac{r_0^3}{3}[j_l^2(\varkappa r_0)-j_{l-1}(\varkappa r_0)j_{l+1}(\varkappa r_0)], \tag{I.4}$$

taking into account the condition for the appearance of a level with angular momentum l

$$j_{l-1}(\varkappa r_0)=0 \tag{I.5}$$

and the continuity of R_l at $r=r_0$, we obtain

$$a_l=\left(2\frac{2l-1}{2l+1}\right)^{1/2}\frac{r_0^{l-1/2}}{(2l-1)!!}. \tag{I.6}$$

We derive also Eq. (2.4) for B_l, by considering the residue of the scattering amplitude at the pole. According to Ref. 3, the scattering amplitude in the effective-radius approximation is of the form

$$f=-\frac{r_0^{2l-1}k^{2l}}{k^2+\alpha^2}\cdot 2\left(\frac{2l-1}{2l+1}\right)[(2l-1)!!]^2=-\frac{Ck^{2l}}{k^2+\alpha^2}.$$

Its residue at the pole $k^2=-\alpha^2$ is $(-1)^{l+1}\alpha^{2l}C$. On the other hand, from general scattering theory it follows that this residue should be equal, apart from the factor $(-1)^{l+1}$, to the square of the coefficient B_l in the asymptotic expression for the radial wave function $B_l r^{-1}\exp(-\alpha r)$. From this we get expression (2.4).

APPENDIX II

The Green's function for an electron in a magnetic field can be represented in the form of the series

$$G=-\sum_n R_n(\rho)R_n(0)\frac{\exp(-\alpha_n|z|)}{2\alpha_n},$$
$$\alpha_n=\left[2\omega\left(n+\frac{1}{2}\right)-\varepsilon\right]^{1/2}, \qquad (\text{II}.1)$$

where R_n is the normalized radial wave function of the electron in a magnetic field at zero projection of the angular momentum on the field direction. It is equal to[5]

$$R_n=(2\omega)^{1/2}\exp(-\omega\rho^2/2)F(-n,1,\omega\rho^2). \qquad (\text{II}.2)$$

Here F is a confluent hypergeometric function.

To prove that $(\partial G/\partial\rho-\omega\rho G)e^{\pm i\varphi}$ satisfies the Schrödinger equation in a magnetic field at an angular-momentum projection ± 1, it suffices to show that $dR_n/d\rho-\omega\rho R_n$ is the radial wave function for the case of an angular-momentum projection ± 1. Differentiating R_n with respect to ρ, we obtain

$$\frac{dR_n}{d\rho}=(2\omega)^{1/2}\exp\left(-\frac{\omega\rho^2}{2}\right)\left[\frac{d}{d\rho}F(-n,1,\omega\rho^2)-\omega\rho F(-n,1,\omega\rho^2)\right]. \qquad (\text{II}.3)$$

Using the known relations

$$\frac{d}{dz}F(\alpha,\beta,z)=\frac{\alpha}{\beta}F(\alpha+1,\beta+1,z),$$
$$F(\alpha,\beta,z)=\frac{\beta-\alpha}{\beta}F(\alpha,\beta+1,z)+\frac{\alpha}{\beta}F(\alpha+1,\beta+1,z),$$

we obtain

$$\frac{dR_n}{d\rho}-\omega\rho R_n=(-2\omega)^{1/2}(n+1)\rho F(-n,2,\omega\rho^2)\exp(-\omega\rho^2/2). \qquad (\text{II}.4)$$

According to Ref. 5, this expression is apart from the normalization, exactly the required radial wave function.

APPENDIX III

To investigate the integrals in (4.3) and (4.10) it is advisable to introduce first of all a new integration variable $\tau=\alpha^2 t/2$. The integrals obtained are of the form

$$J=\int_0^\infty \exp i\left[\frac{(\alpha r_0)^2}{4\tau}-\tau-\frac{1}{3}\left(\frac{\mathscr{E}}{\alpha^3}\right)^2\tau^3\right]\frac{d\tau}{\tau^\lambda},$$

and contain two dimensionless parameters: αr_0 and $\mathscr{E}/\alpha^3$. We apply to this integral the artifice employed in Ref. 6. We deform the integration contour so that it follows the lower imaginary semi-axis of the complex τ plane to the stationary-phase point τ_0, and then a straight line parallel to the real axis to ∞. If $\alpha^3/\mathscr{E}\gg 1$, then the stationary-phase point is located far from the origin and its position is given, accurate to small corrections, by the relation $\tau_0=-i\alpha^3/\mathscr{E}$.

In the integral over the segment $(0,\tau_0)$, we expand $\exp[-(1/3)i(\mathscr{E}/\alpha^3)^2\tau^3]$ in powers of $(\mathscr{E}/\alpha^3)^2$ and confine ourselves to the first two terms. We obtain integrals of the type

$$\int_0^{\tau_0}\frac{d\tau}{\tau^\mu}\exp i\left[\frac{(\alpha r_0)^2}{4\tau}-\tau\right].$$

Since $\alpha r_0\ll 1$, we can replace the upper limit τ_0 by ∞, after which the integral is expressed in terms of a Hankel function of the argument $i\alpha r_0$.

The integral over the section (τ_0,∞) is calculated by the stationary-phase method.

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