

PARTICLE OF LOW BINDING ENERGY IN A MAGNETIC FIELD

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An exact solution is given to the problem of finding the bound state of a charged particle in a zero-range force field in a uniform magnetic field. It is shown that if no bound state exists in the potential well in the absence of the magnetic field, turning on the field always leads to the appearance of such bound states. The possibility of detecting this effect in semiconductors is discussed.

1. INTRODUCTION

IN an earlier paper^[1] we considered a particle in a potential well of small radius (a negative ion) placed in a strong electric field. Here we treat the same system, but now placed in a uniform magnetic field.

First we consider, qualitatively the case of a shallow potential well, where in the absence of the field there is no bound state. If we switch on a magnetic field, the motion of the particle transverse to the field will be hindered, and consequently the problem becomes similar to the one-dimensional problem. We know that for the one-dimensional problem there is a bound state in any well. We may therefore assume (and will prove later) that for an arbitrarily shallow three-dimensional well, when we switch on an arbitrarily weak field a bound state always appears. In first approximation the binding energy is proportional to the square of the field, so that the phenomenon is reminiscent of diamagnetism, but acts in the opposite direction, so that we might call it antidiagnetism.

The magnetic field thus appears to exert a stabilizing influence on the particle. Real magnetic fields are too weak for such an effect to be observable with free atoms or electrons. But in semiconductors at liquid helium temperatures and for low values of the effective mass of electrons or holes, we shall see that the binding energy may be comparable to kT , so that the bound states that are formed may be observed experimentally.

In addition to an antidiagnetism downward shift of the energy, proportional to the square of the field, there is also an upward shift, linear in the field, of the limit of the continuous spectrum, the shift being $\Delta E = \hbar\omega_L$ ($\omega_L = eh/2mc$ is the

Larmor frequency). This is related to the fact that, unlike a classical particle, a quantum particle with zero spin and sufficiently low energy cannot penetrate into a region of strong magnetic field, moving along a force line; the quantity ΔE is a sort of potential barrier, related to the presence of an ambiguity of the coordinate and momentum transverse to the field, and equal to the zero point energy of a two-dimensional oscillator of frequency ω_L . The term ΔE increases the total energy and is analogous to a paramagnetic shift, but it also acts in the opposite direction (antiparamagnetism) and causes the system to be repelled from a region of strong magnetic field. But if the particle has a spin and is oriented along the field then, for example, for an electron, because of the anomalous gyromagnetic ratio, the antiparamagnetic and paramagnetic terms compensate completely, and there remains only the quadratic antidiagnetism term, which will lead to an attraction of the system into the field.

If the potential well is sufficiently deep, so that there is a bound state in the absence of the magnetic field, there is the usual diamagnetic effect, which increases the total energy by an amount proportional to the square of the field and leads to expulsion of the system from the field. The linear shift of the edge of the continuous spectrum also appears, but it has no effect on the total energy, and only has the consequence that, despite the upward diamagnetic energy shift, the binding energy of the particle increases with field, so that the magnetic field exerts a stabilizing influence on the particle in both the cases considered.

2. THE WAVE FUNCTION

Consider a charged particle of mass m and charge e , in the field of a potential well of small

radius and a uniform magnetic field \mathcal{H} , where we assume that the projection of the angular momentum along the field direction is zero. We shall not consider the spin of the particle.

Assuming that the main part of the wave function is outside the potential well, we use the familiar approximation (cf., for example, [1]), in which the actual potential well is replaced by a well of zero radius that has the same scattering length a . Then the wave function ψ at small r can be written as

$$\psi = (4\pi)^{-1}(r^{-1} - a^{-1}) + O(r) \quad (1)$$

and has a $1/r$ singularity when $r \rightarrow 0$. The normalization factor $(4\pi)^{-1}$ simplifies the later formulas. If $a > 0$, then in the absence of the magnetic field there is a bound state of energy $E = -\hbar^2/2ma^2$ and wave function $\psi = (4\pi r)^{-1}e^{-r/a}$. But if $a < 0$, then without the field there is no bound state.

We introduce the notation

$$\varepsilon = 2mE/\hbar^2, \quad \lambda = e\mathcal{H}/2\hbar c.$$

Then, considering the singularity for $r \rightarrow 0$, we obtain the equation for the wave function in the cylindrical polar coordinates ρ, z :

$$\frac{\partial^2 \psi}{\partial z^2} + \frac{\partial^2 \psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} + (\varepsilon - \lambda^2 \rho^2) \psi = -\delta(\mathbf{r}). \quad (2)$$

Thus ψ is the Green's function for a particle in a uniform magnetic field. Formula (1) enables us to express the energy of the bound state in terms of the parameters a and λ .

The time-dependent Green's function for a particle in a uniform magnetic field has been treated by several authors; [2,3] the required function ψ can be obtained from it by a simple integration. We shall construct the ψ function directly, using the formula

$$\psi(\rho, z) = \sum_n \varphi_n(\rho) \varphi_n(0) g_n(z). \quad (3)$$

Here φ_n is the regular normalized solution of the equation

$$\frac{d^2 \varphi_n}{d\rho^2} + \frac{1}{\rho} \frac{d\varphi_n}{d\rho} + (\beta_n - \lambda^2 \rho^2) \varphi_n = 0, \quad (4)$$

i.e., eigenfunctions of the two-dimensional isotropic oscillator, having cylindrical symmetry:

$$\varphi_n = (\lambda/\pi)^{1/2} e^{-\lambda \rho^2/2} L_n(\lambda \rho^2), \quad (5)$$

where the L_n are Laguerre polynomials. The eigenvalues β_n are

$$\beta_n = 4\lambda(n + 1/2). \quad (6)$$

The functions g_n are one-dimensional Green's functions satisfying the equations

$$\frac{d^2 g_n}{dz^2} - \alpha_n^2 g_n = -\delta(z), \quad \alpha_n^2 = \beta_n - \varepsilon, \quad (7)$$

and vanishing for $|z| \rightarrow \infty$ (since we are considering only bound states).

The functions g_n have the form

$$g_n = \frac{1}{2\alpha_n} e^{-\alpha_n |z|}, \quad (8)$$

and consequently the required wave function can be represented as a sum:

$$\psi(\rho, z) = \frac{\lambda}{2\pi} \sum_n e^{-\lambda \rho^2/2} L_n(\lambda \rho^2) \frac{1}{\alpha_n} e^{-\alpha_n |z|}. \quad (9)$$

For what follows we need only consider the behavior of ψ for $\rho = 0$ on the z axis. We have

$$\psi = \frac{\lambda}{2\pi} \sum_{n=0}^{\infty} e^{-\alpha_n |z|/\alpha_n}; \quad (10)$$

$$\alpha_n = (\lambda(4n + \xi))^{1/2}, \quad \xi = 2 - \varepsilon/\lambda. \quad (11)$$

In this case the series can be summed, using the formula

$$\int_0^{\infty} \exp\left(-bt^2 - \frac{c}{t^2}\right) dt = \frac{1}{2} \sqrt{\frac{\pi}{b}} \exp(-2\sqrt{bc}) \quad (12)$$

and setting $c = \lambda z^2$, $b = n + \xi/4$. Then, interchanging the order of summation and integration and summing the geometrical progression under the integral, we get

$$\psi(0, z) = \frac{\lambda^{1/2}}{2\pi^{3/2}} \int_0^{\infty} \frac{\exp(-\xi t^2/4 - \lambda z^2/t^2)}{1 - e^{-t^2}} dt. \quad (13)$$

When $z \rightarrow 0$ the integral diverges at its lower limit. Separating off the divergent part, we have

$$\begin{aligned} \psi(0, z) &= \frac{1}{4\pi|z|} \exp(-\sqrt{\lambda\xi}|z|) \\ &+ \frac{\lambda^{1/2}}{2\pi^{3/2}} \int_0^{\infty} \left(\frac{1}{2} \coth \frac{t^2}{2} + \frac{1}{2} - \frac{1}{t^2} \right) \\ &\times \exp\left(-\frac{\xi t^2}{4} - \frac{\lambda z^2}{t^2}\right) dt. \end{aligned} \quad (14)$$

For large z the factor multiplying the exponential in the integrand can be replaced by unity, and consequently

$$\psi(0, z) \sim \frac{1}{4\pi} \sqrt{\frac{\lambda}{\xi}} \exp(-\sqrt{\lambda\xi}|z|) [1 + O(|z|^{-1})], \quad (15)$$

i.e., at infinity the behavior of ψ is determined by the first term of the sum (10) and is the same as

in the one-dimensional case. It follows that the edge of the continuous spectrum is reached for $\xi = 0$, which coincides with the condition $E = h\omega_L$.

3. ENERGY OF THE BOUND STATE

We now use condition (1) and go to the limit $r \rightarrow 0$ along the z axis. Then, after taking out the divergent part $(4\pi|z|)^{-1}$, the remaining part of the function ψ must be equal to $-(4\pi a)^{-1}$. We get an equation for determining the energy:

$$\frac{1}{a\sqrt{\lambda}} = \sqrt{\xi} - \frac{2}{\sqrt{\pi}} \int_0^{\infty} \left(\frac{1}{2} \coth \frac{t^2}{2} + \frac{1}{2} - \frac{1}{t^2} \right) \exp\left(-\frac{\xi t^2}{4}\right) dt. \quad (16)$$

The right side can be expressed in terms of the generalized Riemann ζ -function (cf. the Appendix):

$$1/a\sqrt{\lambda} = -\zeta(1/2, \xi/4) = F(\xi) \quad (17)$$

and can be represented to high accuracy by the expression¹⁾

$$F(\xi) \approx (\xi + 4)^{1/2} - 2\xi^{-1/2} - (\xi + 4)^{-1/2} - 1/3(\xi + 4)^{-3/2}. \quad (18)$$

Finally, when $\xi \ll 1$ and $\xi \gg 1$ we get

$$1/a\sqrt{\lambda} = -2\xi^{-1/2} - \zeta(1/2) + O(\xi), \quad \xi \ll 1; \quad (19)$$

$$1/a\sqrt{\lambda} = \xi^{1/2} - \xi^{-1/2} - 1/3\xi^{-3/2} + O(\xi^{-7/2}), \quad \xi \gg 1, \quad (20)$$

where $\zeta(s)$ is the usual Riemann ζ -function.

As we see from these expressions, the case $\xi \gg 1$ occurs when $a > 0$, where there is a bound state in the well even in the absence of the magnetic field. The case $\xi \ll 1$ occurs for $a < 0$, when there are no bound states in the absence of the field. In both cases the right side of the equation is a large number and consequently $a\sqrt{\lambda} \ll 1$, i.e., the radius of the first Larmor orbit is much greater than the dimensions of the electron cloud in the absence of the field. We shall regard such a field as weak, whereas a field for which the opposite criterion $a\sqrt{\lambda} \gg 1$ is satisfied will be considered strong.

Now let us consider the different limiting cases.

1. $a > 0$, weak field. Using formula (20), we

get

$$\varepsilon a^2 = -1 + 1/3\lambda^2 a^4 + O(\lambda^4 a^8), \quad (21)$$

or, changing to the usual units,

$$E = E_0 + \frac{e^2 \mathcal{H}^2 a^2}{24mc^2}. \quad (22)$$

Using the equation

$$\langle r^2 \rangle = 1/2a^2, \quad (23)$$

which comes from the expression for the wave function in the absence of the field,

$$\psi = (4\pi r)^{-1} e^{-r/a}, \quad (24)$$

we get

$$E - E_0 = \frac{e^2 \mathcal{H}^2}{12mc^2} \langle r^2 \rangle \quad (25)$$

the familiar result for the diamagnetic energy shift.

Arguments similar to those in [1] for the electric field permit the conclusion that for a given binding energy E_0 , in the absence of potential barriers, the diamagnetic susceptibility

$$\kappa = \frac{e^2 E_0}{6c^2} = \left(\frac{\partial^2 E}{\partial \mathcal{H}^2} \right)_{\mathcal{H}=0} \quad (26)$$

for our case will be minimal relative to all other potential wells with zero range of the forces. For example, for the long range Coulomb field, $\langle r^2 \rangle$ and consequently also the diamagnetic susceptibility is six times greater. It is interesting that in this same case the polarizability in an electric field changes by a factor of 18, [1] so that the diamagnetic susceptibility is less sensitive to the shape of the potential well than the electric polarizability.

2. $a < 0$, weak field. Using (19), we get

$$2\lambda - \varepsilon = \frac{4\lambda^2 a^2}{[1 + a\lambda^{1/2} \zeta(1/2)]^2} + O(\lambda^{7/2} a^7). \quad (27)$$

From our earlier remarks, the value $\varepsilon = 2\lambda$ is the edge of the continuous spectrum, so that the difference $2\lambda - \varepsilon$ gives us the binding energy E_0 . In ordinary units this quantity is equal to

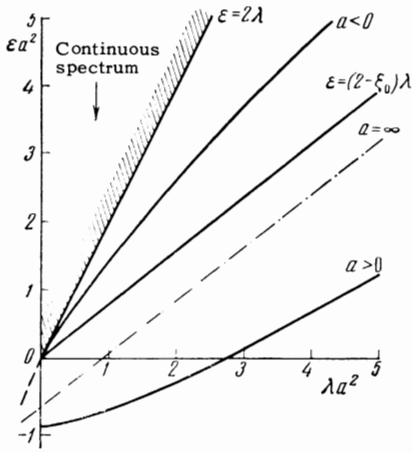
$$E_0 = \frac{e^2 \mathcal{H}^2 a^2}{2mc^2} \left[1 + 1.46|a| \left(\frac{e\mathcal{H}}{2hc} \right)^{1/2} \right]^{-2}. \quad (28)$$

As we remarked in the Introduction this downward energy shift from the edge of the continuous spectrum may be called antdiamagnetism. The first term of (28), which is quadratic in the field, coincides with the result of Bychkov [4] who treated the scattering of electrons by a force center in a mag-

¹⁾If we replace the sum (10) by an integral, after separating off the first term, we easily get the cruder approximate expression

$$F(\xi) \approx (2 + \xi)^{1/2} - 2\xi^{-1/2},$$

which gives fair results for cases 2 and 3 (where the numerical constants in formulas (28) and (29) are changed by only a few percent). We thank O. B. Firsov for pointing this out. But in case 1 this formula is not applicable (it gives no diamagnetic shift).



netic field. But the second term is significant—even when $\lambda a^2 = 0.01$, the correction is 30%.

3. $|a| = \infty$, arbitrary field. This is the limiting case where in zero field there is no bound state, but such a state appears for an arbitrarily small increase in the well depth. In this case the left side of (17) is zero and we must find the value of ξ_0 for which the right side vanishes. Using the approximate formula (18) we easily find $\xi_0 = 1.21$. Thus in this limiting case the binding energy E_0 increases linearly with the field:

$$2\lambda - \varepsilon = \xi_0 \lambda; \quad E_0 = 0.30 e h \mathcal{H} / mc. \quad (29)$$

4. a arbitrary, strong field. In this case we must expand the function $F(\xi)$ in series in the neighborhood of the point ξ_0 :

$$F(\xi) = F'(\xi_0)(\xi - \xi_0) + \frac{1}{2} F''(\xi_0)(\xi - \xi_0)^2 + \dots \quad (30)$$

Using the approximate formula (18) we easily find

$$F'(\xi_0) = 1.02, \quad F''(\xi_0) = -0.95.$$

For the total energy of the bound state in the magnetic field we then get the formula

$$\begin{aligned} \varepsilon a^2 &= (2 - \xi_0) \lambda a^2 - \frac{a \sqrt{\lambda}}{F'(\xi_0)} + \frac{F''(\xi_0)}{2[F'(\xi_0)]^3} + O\left(\frac{1}{a \sqrt{\lambda}}\right) \\ &= 0.79 \lambda a^2 - 0.98 a \sqrt{\lambda} - 0.45 + O[(\lambda a^2)^{-1/2}]. \end{aligned} \quad (31)$$

The figure shows the dependence of the energy εa^2 on the field λa^2 in dimensionless units for the different cases. In addition it shows the edge of the continuous spectrum and the line $\varepsilon = (2 - \xi_0) \lambda$, corresponding to the case of $|a| \rightarrow \infty$, which determines the slopes of the other two curves when $\lambda \rightarrow \infty$. The curves for $a > 0$ and $a < 0$ are the two branches of a curve which is similar to a parabola; the extension of the curve $a < 0$ into the nonphysical region of negative λa^2 is shown as a dashed line. Within the accuracy of the computa-

tion the two branches are symmetric around the axis shown in the figure as a dot-dash line.

4. DISCUSSION

The present approximate treatment is applicable if the following two conditions are satisfied.

A. The dimensions of the electron cloud should be much greater than the radius r_0 of the potential well. It follows that if $a > 0$, for a bound state in the absence of the field the inequality $a \gg r_0$ must be satisfied. This condition does not contain the magnetic field \mathcal{H} and is a general condition for all cases in which one uses the zero range approximation. If $a < 0$ it is not necessary to require that $|a| \gg r_0$. In this case the wave function of the bound state will fall off very slowly in reasonably strong fields. If $E_0(\mathcal{H})$ is the binding energy, our condition can be written as

$$(2mE_0(\mathcal{H}))^{1/2} r_0 / h \ll 1,$$

or, replacing $E_0(\mathcal{H})$ by the first term in (28), we get

$$e \mathcal{H} a r_0 / hc \ll 1.$$

This condition is practically always satisfied: for example, if $a = 10^{-7}$ cm, $r_0 = 10^{-8}$ cm, we get $\mathcal{H} \ll 10^8$ Oe. A bound state near the edge of the continuous spectrum will always appear in a magnetic field if the scattering length a is negative, even if the well is deep and contains other bound states with large binding energies.

B. The radius of the first Larmor orbit should be much greater than the size of the well r_0 , i.e.,

$$r_0 \sqrt{\lambda} \ll 1. \quad (e \mathcal{H} / 2hc)^{1/2} r_0 \ll 1.$$

This condition is surely satisfied for actual fields and not too large r_0 . Even assuming $r_0 = 10^{-7}$ cm, we get $\mathcal{H} \ll 10^7$ Oe.

Let us estimate the energy of the bound state in a semiconductor under favorable conditions. Setting $m_{\text{eff}} = 0.01 m_e$, $a = 10^{-7}$ cm, $\mathcal{H} = 10^5$ Oe, we get $E = 10^{-3}$ eV. Thus at a temperature of a few degrees Kelvin these levels may have an effect on the concentration of electrons or holes in the conduction band of the semiconductor, resulting, for example, in a decrease in the electrical conductivity along the magnetic field.

For an anisotropic uniaxial crystal with the magnetic field along the axis, so that there are two effective masses m_{\parallel} and m_{\perp} , all the arguments of Secs. 2 and 3 remain valid except for changes in some of the factors; in the final expressions for the energy we must replace m by m_{\perp} and multiply the whole expression by $(m_{\parallel} / m_{\perp})^{1/2}$.

In conclusion we thank A. G. Zhilich and A. V. Tulub for valuable discussions of the problems treated in this paper.

APPENDIX

The generalized Riemann ζ -function^[5] can be represented as an integral:

$$\zeta(s, q) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{x^{s-1} e^{-qx}}{1 - e^{-x}} dx = \sum_{n=0}^\infty \frac{1}{(n+q)^s};$$

Re $s > 1$; Re $q > 0$. (1)

In order to extend this definition to the required region $0 < \text{Re } s < 1$, we take out the factor $(1 - e^{-x})^{-1}$ which is divergent at the lower limit. We get

$$\zeta(s, q) = -\frac{q^{1-s}}{1-s} + \frac{1}{\Gamma(s)} \int_0^\infty \left(\frac{1}{1 - e^{-x}} - \frac{1}{x} \right) x^{s-1} e^{-qx} dx. \quad (2)$$

We have thus separated out the pole of the ζ -function at $s = 1$, and the formula is applicable over the entire right halfplane of the variable s . Setting $x = t^2$, $s = 1/2$, $q = \xi/4$, we get precisely the integral in formula (16) and arrive at formula (17).

Expanding the expression in parentheses in the integrand and calculating the integrals term by term, we get an asymptotic expansion for large q :

$$\zeta(s, q) = \frac{1}{2q^s} + \sum_{n=0}^\infty \frac{\Gamma(2n + s - 1)}{\Gamma(2n + 1)\Gamma(s)} B_{2n} q^{1-s-2n}$$

$$= -\frac{q^{1-s}}{1-s} + \frac{1}{2q^s} + \frac{s}{12q^{s+1}} - \frac{s(s+1)(s+2)}{720q^{s+3}}$$

$$+ O\left(\frac{1}{q^{s+5}}\right), \quad (3)$$

where B_{2n} are the Bernoulli numbers. If we substitute the first three terms of the series in (17), we get formula (20). The error is given by the fourth term, which for $s = 1/2$, $q = 1$ ($\xi = 4$) is equal to 0.0026.

We then use the recursion relation

$$\zeta(s, q) = 1/q^s + \zeta(s, q + 1), \quad (4)$$

which follows from the definition (1). Substituting the first three terms of the asymptotic expansion on the right side, we get an approximate expression for the ζ -function in the interval $0 < q < \infty$,

which leads to formula (18).

Finally, expanding the right side of (4) in series for small q and using the formula $\zeta(s, 1) = \zeta(s)$, we get

$$\zeta(s, q) = \frac{1}{q^s} + \sum_{n=0}^\infty (-1)^n \frac{\Gamma(s+n)\zeta(s+n)}{\Gamma(s)\Gamma(n+1)} q^n. \quad (5)$$

Only two terms of this expansion are used in formulas (19), (27), and (28).

Another important development is the asymptotic expansion in inverse powers of $q - 1/2$, which can be gotten by using the formula

$$\zeta(s, q) = \frac{1}{2\Gamma(s)} \int_0^\infty e^{-(q-1/2)x} x^{s-1} \text{cosech } \frac{x}{2} dx, \quad \text{Re } s > 1. \quad (6)$$

Expanding the cosecant in series and evaluating the integrals, we get the expansion

$$\zeta(s, q) = \sum_{k=0}^\infty \frac{\Gamma(s+2k-1)}{\Gamma(s)} \times (2^{1-2k} - 1) B_{2k} \left(q - \frac{1}{2} \right)^{1-2k-s}, \quad (7)$$

which is easily shown to be valid also in the region $0 < \text{Re } s < 1$. Thus the function $(q - 1/2)^{s-1} \zeta(s, q)$ is expanded in an asymptotic series involving only even powers of $(q - 1/2)^{-1}$. In our case, $q - 1/2 = -\epsilon/4\lambda$, and using formula (7) and Eq. (17) we find that for $a > 0$ and small λ , the function $\epsilon(\lambda)$ is expanded in a series containing only even powers of λ , a fact that is not directly evident from (17). We should, however, remark that this is an asymptotic series and diverges for arbitrarily small λ , which is related to the unboundedness of the perturbation operator.

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