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# MODIFICATION OF THE COULOMB LAW AND ENERGY LEVELS OF HYDROGEN ATOM IN SUPERSTRONG MAGNETIC FIELD

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The screening of the Coulomb potential by superstrong magnetic field is studied. Its influence on the spectrum of a hydrogen atom is determined.

Изучается экранировка кулоновского потенциала сверхсильным магнитным полем и ее влияние на спектр атома водорода.

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I will discuss recently solved Quantum Mechanical – Quantum Electrodynamical problem in this lecture. It was solved numerically in papers [1, 2], and then analytical solution was found in papers [3, 4].

We will use Gauss units convenient in atomic physics: $e^2 = \alpha = 1/137$. We will call magnetic fields $B > m_e^2 e^3$ strong, while $B > m_e^2/e^3$ will be called superstrong. An important quantity in the problem under consideration is Landau radius $a_H = 1/\sqrt{eB}$ called magnetic length in condensed matter physics.

Let us consider hydrogen atom in external homogeneous magnetic field $B$. At strong $B$, Bohr radius $a_B$ is larger than $a_H$, so there are two time scales in the problem: fast motion in the plane perpendicular to magnetic field and slow motion along the magnetic field. That is why adiabatic approximation is applicable: averaging over fast motion, we get one-dimensional motion of electron along the magnetic field in effective potential

$$U(z) \approx \frac{-e^2}{\sqrt{z^2 + a_H^2}}. \tag{1}$$

The energy of a ground state can be estimated as

$$E_0 = -2m \left( \int_{a_H}^{a_B} U(z)\, dz \right)^2 \sim -me^4 \ln^2(B/m^2 e^3), \tag{2}$$

and it goes to minus infinity when $B$ goes to infinity.

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We will see that radiative corrections qualitatively change this result: ground-state energy goes to finite value when $B$ goes to infinity. This happens due to screening of the Coulomb potential.

Since at strong $B$ reduction of the number of space dimensions occurs and motion takes place in one space and one time dimensions, it is natural to begin systematic analysis from QED in $D = 2$. At tree level the Coulomb potential is

$$\Phi(k) \equiv A_0(\bar{k}) = \frac{4\pi g}{\bar{k}^2}, \tag{3}$$

while, taking into account loop insertions into photon propagator, we get

$$\Phi(k) \equiv \mathbf{A}_0 = D_{00} + D_{00}\Pi_{00}D_{00} + \ldots = -\frac{4\pi g}{k^2 + \Pi(k^2)}, \tag{4}$$

where the photon polarization operator equals

$$\Pi_{\mu\nu} \equiv \left( g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right) \Pi(k^2), \tag{5}$$

$$\Pi(k^2) = 4g^2 \left[ \frac{1}{\sqrt{t(1+t)}} \ln\left(\sqrt{1+t} + \sqrt{t}\right) - 1 \right] \equiv -4g^2 P(t), \tag{6}$$

$t \equiv -k^2/4m^2$, and the dimension of charge $g$ equals mass in $D = 2$.

Taking $k = (0, k_\parallel)$, $k^2 = -k_\parallel^2$ for the Coulomb potential in the coordinate representation, we get

$$\mathbf{\Phi}(z) = 4\pi g \int\limits_{-\infty}^{\infty} \frac{\mathrm{e}^{ik_\parallel z}\, dk_\parallel/2\pi}{k_\parallel^2 + 4g^2 P(k_\parallel^2/4m^2)}, \tag{7}$$

and the potential energy for the charges $+g$ and $-g$ is finally: $V(z) = -g\mathbf{\Phi}(z)$.

In order to perform integration in (7), we need a simplified expression for $P(t)$. Taking into account that asymptotics of $P(t)$ are

$$P(t) = \begin{cases} (2/3)t, & t \ll 1, \\ 1, & t \gg 1, \end{cases} \tag{8}$$

let us take as an interpolating formula the following expression:

$$\overline{P}(t) = \frac{2t}{3 + 2t}. \tag{9}$$

The accuracy of this approximation is better than 10%.

Substituting (9) into (7), we get

$$\mathbf{\Phi} = 4\pi g \int\limits_{-\infty}^{\infty} \frac{\mathrm{e}^{ik_\parallel z}\, dk_\parallel/2\pi}{k_\parallel^2 + 4g^2(k_\parallel^2/2m^2)/(3 + k_\parallel^2/2m^2)} =$$

$$= \frac{4\pi g}{1 + 2g^2/3m^2} \int\limits_{-\infty}^{\infty} \left[\frac{1}{k_\parallel^2} + \frac{2g^2/3m^2}{k_\parallel^2 + 6m^2 + 4g^2}\right] \mathrm{e}^{ik_\parallel z} \frac{dk_\parallel}{2\pi} =$$

$$= \frac{4\pi g}{1 + 2g^2/3m^2} \left[-\frac{1}{2}|z| + \frac{g^2/3m^2}{\sqrt{6m^2 + 4g^2}} \exp\left(-\sqrt{6m^2 + 4g^2}|z|\right)\right]. \quad (10)$$

In the case of heavy fermions ($m \gg g$) the potential is given by the tree level expression; the corrections are suppressed as $g^2/m^2$.

In the case of light fermions ($m \ll g$),

$$\mathbf{\Phi}(z)\Big|_{m \ll g} = \begin{cases} \pi\, \mathrm{e}^{-2g|z|}, & z \ll \dfrac{1}{g} \ln\left(\dfrac{g}{m}\right), \\ -2\pi g \left(\dfrac{3m^2}{2g^2}\right) |z|, & z \gg \dfrac{1}{g} \ln\left(\dfrac{g}{m}\right). \end{cases} \quad (11)$$

For $m = 0$ we have Schwinger model — the first gauge invariant theory with a massive vector boson. Light fermions make a continuous transition from $m > g$ to $m = 0$ case. The next two figures correspond to $g = 0.5$, $m = 0.1$. The expression for $\bar{V}$ contains $\bar{P}$.

To find the modification of the Coulomb potential in $D = 4$, we need an expression for $\Pi$ in strong $B$.

One starts from electron propagator $G$ in strong $B$. Solutions of the Dirac equation in homogeneous constant in time $B$ are known, so one can write spectral representation of electron Green function. Denominators contain $k^2 - m^2 - 2neB$, and for $B \gg m^2/e$ and $k_\parallel^2 \ll eB$ in sum over levels the lowest Landau level (LLL, $n = 0$) dominates. In coordinate

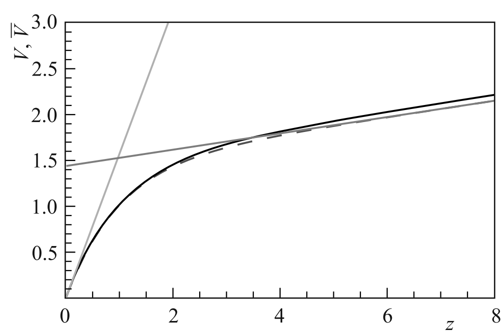


Fig. 1. Potential energy of the charges $+g$ and $-g$ in $D = 2$. The solid curve corresponds to $P$; the dashed curve corresponds to $\bar{P}$

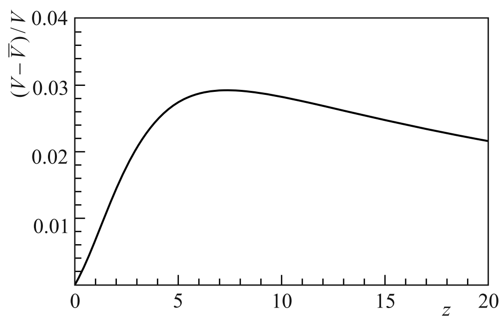


Fig. 2. Relative difference of potential energies calculated with the exact and interpolating formulae for the polarization operator for $g = 0.5$, $m = 0.1$

representation the transverse part of the LLL wave function is $\Psi \sim \exp\left((-x^2-y^2)eB\right)$, which in momentum representation gives $\Psi \sim \exp\left((-k_x^2-k_y^2)/eB\right)$ (gauge in which $\mathbf{A} = 1/2[\mathbf{B}\times\mathbf{r}]$ is used).

Substituting electron Green functions into the polarization operator, we get

$$\Pi_{\mu\nu} \sim e^2 eB \int \frac{dq_x\, dq_y}{eB} \exp\left(-\frac{q_x^2+q_y^2}{eB}\right) \times$$

$$\times \exp\left(-\frac{(q+k)_x^2+(q+k)_y^2}{eB}\right) dq_0\, dq_z \gamma_\mu \frac{1}{\hat{q}_{0,z}-m}\gamma_\nu \frac{1}{\hat{q}_{0,z}+\hat{k}_{0,z}-m} =$$

$$= e^3 B \exp\left(-\frac{k_\perp^2}{2eB}\right)\Pi_{\mu\nu}^{(2)}(k_\parallel \equiv k_z), \quad (12)$$

$$\mathbf{\Phi} = \frac{4\pi e}{(k_\parallel^2+k_\perp^2)\left(1-\frac{\alpha}{3\pi}\ln\left(\frac{eB}{m^2}\right)\right)+\frac{2e^3B}{\pi}\exp\left(-\frac{k_\perp^2}{2eB}\right)P\left(\frac{k_\parallel^2}{4m^2}\right)}, \quad (13)$$

$$\mathbf{\Phi}(z) = 4\pi e \int \frac{\mathrm{e}^{ik_\parallel z} dk_\parallel d^2k_\perp/(2\pi)^3}{k_\parallel^2+k_\perp^2+\frac{2e^3B}{\pi}\exp\left(\frac{-k_\perp^2}{2eB}\right)\frac{k_\parallel^2/2m_e^2}{3+k_\parallel^2/2m_e^2}}, \quad (14)$$

$$\mathbf{\Phi}(z) = \frac{e}{|z|}\left[1-\mathrm{e}^{-\sqrt{6m_e^2}|z|}+\exp\left(-\sqrt{\frac{2}{\pi}e^3B+6m_e^2}|z|\right)\right]. \quad (15)$$

For magnetic fields $B \ll 3\pi m^2/e^3$ the potential is the Coulomb up to small power suppressed terms:

$$\mathbf{\Phi}(z)\Big|_{e^3B \ll m_e^2} = \frac{e}{|z|}\left[1+O\left(\frac{e^3B}{m_e^2}\right)\right] \quad (16)$$

in full accordance with the $D=2$ case, where $g^2$ plays the role of $e^3B$.

In the opposite case of superstrong magnetic fields $B \gg 3\pi m_e^2/e^3$, we get

$$\mathbf{\Phi}(z) = \begin{cases} \frac{e}{|z|}\exp\left(-\sqrt{\frac{2}{\pi}e^3B}|z|\right), & \frac{1}{\sqrt{(2/\pi)e^3B}}\ln\left(\sqrt{\frac{e^3B}{3\pi m_e^2}}\right) > |z| > \frac{1}{\sqrt{eB}}, \\ \frac{e}{|z|}\left(1-\exp\left(-\sqrt{6m_e^2}|z|\right)\right), & \frac{1}{m} > |z| > \frac{1}{\sqrt{(2/\pi)e^3B}}\ln\left(\sqrt{\frac{e^3B}{3\pi m_e^2}}\right), \\ \frac{e}{|z|}, \quad |z| > \frac{1}{m}, \end{cases} \quad (17)$$

$$V(z) = -e\mathbf{\Phi}(z). \quad (18)$$

The spectrum of the Dirac equation in magnetic field constant in space and time is well known:

$$\varepsilon_n^2 = m_e^2 + p_z^2 + (2n+1+\sigma_z)eB, \quad (19)$$

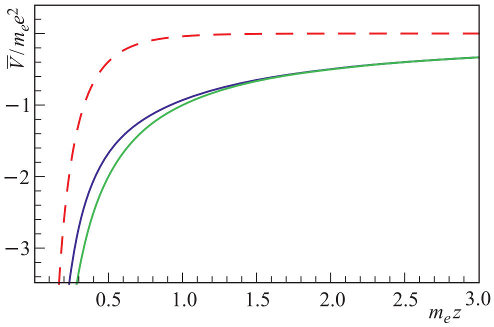


Fig. 3 (color online). The modified Coulomb potential at $B = 10^{17}$ G (blue) and its long distance (green) and short distance (red) asympotics

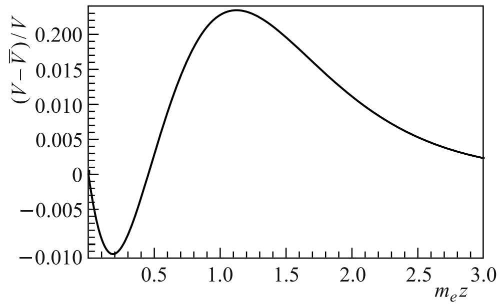


Fig. 4. Relative accuracy of analytical formula for the modified Coulomb potential at $B = 10^{17}$ G

$n = 0, 1, 2, 3, \ldots$; $\sigma_z = \pm 1$. For $B > B_{\rm cr} = m_e^2/e$ the electrons are relativistic with only one exception: electrons from lowest Landau level ($n = 0$, $\sigma_z = -1$) can be nonrelativistic.

In what follows, we will study the spectrum of electrons from LLL in the Coulomb field of the proton modified by the superstrong $B$.

The spectrum of Schrödinger equation in cylindrical coordinates $(\bar{\rho}, z)$ in the gauge where $\bar{A} = (1/2)\,[\bar{B}\bar{r}]$ is

$$E_{p_z n_\rho m \sigma_z} = \left(n_\rho + \frac{|m| + m + 1 + \sigma_z}{2}\right)\frac{eB}{m_e} + \frac{p_z^2}{2m_e}; \tag{20}$$

LLL corresponds to $n_\rho = 0$, $\sigma_z = -1$, $m = 0, -1, -2, \ldots$

A wave function factorizes on those describing free motion along a magnetic field with momentum $p_z$ and those describing motion in the plane perpendicular to magnetic field:

$$R_{0m}(\bar{\rho}) = \left[\pi(2a_H^2)^{1+|m|}(|m|!)\right]^{-1/2} \rho^{|m|} \exp\left(\frac{im\varphi - \rho^2}{4a_H^2}\right). \tag{21}$$

Now we should take into account electric potential of atomic nuclei situated at $\bar{\rho} = z = 0$. For $a_H \ll a_B$ adiabatic approximation is applicable and the wave function in the following form should be looked for:

$$\Psi_{n0m-1} = R_{0m}(\bar{\rho})\chi_n(z), \tag{22}$$

where $\chi_n(z)$ is the solution of the Schrödinger equation for electron motion along a magnetic field:

$$\left[-\frac{1}{2m}\frac{d^2}{dz^2} + U_{\rm eff}(z)\right]\chi_n(z) = E_n\chi_n(z). \tag{23}$$

Without screening the effective potential is given by the following formula:

$$U_{\rm eff}(z) = -e^2 \int \frac{|R_{0m}(\rho)|^2}{\sqrt{\rho^2 + z^2}} d^2\rho, \tag{24}$$

For $|z| \gg a_H$ the effective potential equals the Coulomb potential:

$$U_{\rm eff}(z)|_{z \gg a_H} = -\frac{e^2}{|z|}, \tag{25}$$

and the effective potential is regular at $z = 0$:

$$U_{\rm eff}(0) \sim -\frac{e^2}{|a_H|}. \tag{26}$$

Since $U_{\rm eff}(z) = U_{\rm eff}(-z)$, the wave functions are odd or even under reflection $z \to -z$; the ground states (for $m = 0, -1, -2, \ldots$) are described by even wave functions.

To calculate the ground state of hydrogen atom, in the textbook «Quantum Mechanics» by L. D. Landau and E. M. Lifshitz the shallow-well approximation is used:

$$E^{\rm sw} = -2m_e \left[ \int\limits_{a_H}^{a_B} U(z)\, dz \right]^2 = -\left(\frac{m_e e^4}{2}\right) \ln^2 \left(\frac{B}{m_{e^2} e^3}\right). \tag{27}$$

Let us derive this formula. The starting point is one-dimensional Schrödinger equation:

$$-\frac{1}{2\mu}\frac{d^2}{dz^2}\chi(z) + U(z)\,\chi(z) = E_0\chi(z). \tag{28}$$

Neglecting $E_0$ in comparison with $U$ and integrating, we get

$$\chi'(a) = 2\mu \int\limits_0^a U(x)\chi(x)\, dx, \tag{29}$$

where we assume $U(x) = U(-x)$, that is why $\chi$ is even.

The next assumptions are: 1) the finite range of the potential energy: $U(x) \neq 0$ for $a > x > -a$; 2) $\chi$ undergoes very small variations inside the well. Since outside the well $\chi(x) \sim {\rm e}^{-\sqrt{2\mu|E_0|}\,x}$, we readily obtain

$$|E_0| = 2\mu \left[ \int\limits_0^a U(x)\, dx \right]^2. \tag{30}$$

For

$$\mu|U|a^2 \ll 1 \tag{31}$$

(condition for the potential to form a shallow well) we get that, indeed, $|E_0| \ll |U|$ and that the variation of $\chi$ inside the well is small, $\Delta\chi/\chi \sim \mu|U|a^2 \ll 1$. Concerning the one-dimensional Coulomb potential, it satisfies this condition only for $a \ll 1/(m_e e^2) \equiv a_B$.

This explains why the accuracy of $\log^2$ formula is very poor.

A much more accurate equation for atomic energies in strong magnetic field was derived by B. M. Karnakov and V. S. Popov [5]. It provides a several percent accuracy for the energies of EVEN states for $H > 10^3$ ($H \equiv B/(m_e^2 e^3)$).

The main idea is to integrate the Schrödinger equation with effective potential from $x = 0$ till $x = z$, where $a_H \ll z \ll a_B$ and to equate the obtained expression for $\chi'(z)/\chi(z)$ to the logarithmic derivative of Whittaker function — the solution of Schrödinger equation with the Coulomb potential, which exponentially decreases at $z \gg a_B$:

$$2\ln\left(\frac{z}{a_H}\right) + \ln 2 - \psi(1+|m|) + O\left(\frac{a_H}{z}\right) = \\ = 2\ln\left(\frac{z}{a_B}\right) + \lambda + 2\ln\lambda + 2\psi\left(1-\frac{1}{\lambda}\right) + 4\gamma + 2\ln 2 + O\left(\frac{z}{a_B}\right), \quad (32)$$

$$E = -\left(\frac{m_e e^4}{2}\right)\lambda^2. \quad (33)$$

The energies of the ODD states are

$$E_{\text{odd}} = -\frac{m_e e^4}{2n^2} + O\left(\frac{m_e^2 e^3}{B}\right), \quad n = 1, 2, \ldots \quad (34)$$

So, for superstrong magnetic fields $B \sim m_e^2/e^3$ the deviations of odd states energies from the Balmer series are negligible.

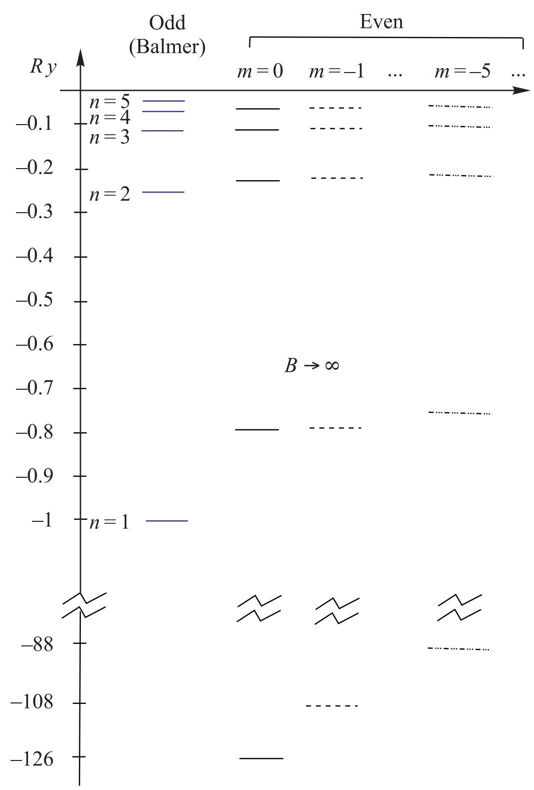


Fig. 5. Spectrum of hydrogen levels in the limit of infinite magnetic field. Energies are given in Rydberg units, $Ry \equiv 13.6$ eV

When screening is taken into account, an expression for effective potential transforms into

$$\tilde{U}_{\text{eff}}(z) = -e^2 \int \frac{|R_{0m}(\boldsymbol{\rho})|^2}{\sqrt{\rho^2 + z^2}} d^2\rho \left[1 - \mathrm{e}^{-\sqrt{6m_e^2}\,z} + \exp\left(-\sqrt{\frac{2}{\pi}\,e^3 B + 6m_e^2}\,z\right)\right]. \tag{35}$$

The original KP equation for LLL splitting by the Coulomb potential is

$$\ln(H) = \lambda + 2\ln\lambda + 2\psi\left(1 - \frac{1}{\lambda}\right) + \ln 2 + 4\gamma + \psi(1 + |m|), \tag{36}$$

where $\psi(x)$ is the logarithmic derivative of the gamma function; it has simple poles at $x = 0, -1, -2, \ldots$

The modified KP equation, which takes screening into account, looks like

$$\ln\left(\frac{H}{1 + \dfrac{e^6}{3\pi}H}\right) = \lambda + 2\ln\lambda + 2\psi\left(1 - \frac{1}{\lambda}\right) + \ln 2 + 4\gamma + \psi(1 + |m|), \tag{37}$$

$E = -(m_e e^4/2)\lambda^2$. In particular, for a ground state $\lambda = -11.2$, $E_0 = -1.7$ keV.

In conclusion,

1) analytical expression for charged particle electric potential in $d = 1$ is given; for $m < g$ screening takes place at all distances;

2) analytical expression for charged particle electric potential $\Phi(z, \rho = 0)$ at superstrong $B$ at $d = 3$ is found; screening takes place at distances $|z| < 1/m_e$;

3) an algebraic formula for the energy levels of a hydrogen atom originating from the lowest Landau level in superstrong $B$ has been obtained.

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