Modification of Coulomb law and energy levels of hydrogen atom in superstrong magnetic field

M.I.Vysotsky

ITEP, Moscow

Baikal School of Physics of Elementary Particles and AstroPhysics, July 3 -10, 2011

Recently solved QM + QED (almost) textbook problem.

A.E.Shabad, V.V.Usov (2007,2008) - numerically;
M.I.Vysotsky, JETP Lett. **92** (2010)15; B.Machet, M.I.Vysotsky, PR D **83** (2011)025022 - analytically;

For this talk:

strong magnetic field: $B > m_e^2 e^3$
(Gauss units; $e^2 = \alpha = 1/137$)

superstrong magnetic field: $B > m_e^2/e^3$
$a_H = 1/\sqrt{eB}$ - Landau radius, magnetic length

uncertainty relation

Electron moving in a transverse to magnetic field plane;
Lorentz force:
$evB = mv^2/r, \;\; eBp = p^2/r, \;\; r/p = 1/(eB)$

Classically: in a given B radius diminishes when momentum diminishes.

Quantum Mechanics: $\Delta r \Delta p > 1$, $\quad r > 1/\sqrt{eB}$
$a_H = 1/\sqrt{eB}$ - ground state radius in a transverse plane, along B - free motion

Atom; Lorentz force: $e^2/r^2 = mv^2/r, \;\; e^2 m = p^2 r$
$r > 1/(me^2), \;\; a_B = 1/(me^2)$ - Bohr radius.

plan

- $a_B, a_H,\ a_H << a_B \Longrightarrow B >> e^3 m_e^2$
  electrons on Landau levels feel weak Coulomb potential moving along axis z;
  Loudon, Elliott 1960, numerical solution of Schrodinger equation; (Wang, Hsue 1995)
  LL QM (after 1974), GKK(1992):
  $E_0 = -(me^4/2) \times \ln^2(B/(m^2 e^3))$. Ground level goes to $-\infty$ when B goes to ∞

  NO

- $D = 2$ QED - Schwinger model with massive electrons, radiative "corrections" to Coulomb potential in $d = 1$;
  $\Pi_{\mu\nu}$, interpolating formula, analytical formula for $\Phi(z)$,
  $g > m$ - photon "mass" $m_\gamma \sim g$, screening at ALL z when $g > m$

- $D=4$ QED; photon “mass” $m_\gamma^2 = e^3 B$ at superstrong magnetic fields $B > m_e^2/e^3 = 137 \times 4.4 \times 10^{13}$ gauss; analytical formula for $\Phi(z)$
- Electron in magnetic field - general consideration; LLL - nonrelativistic at all B
- The shallow-well approximation
- The Karnakov-Popov equation for atomic energies
- Equation for the energies of even states with account of screening
- Magnetic fields in laboratory and in stars; excitons
- References
- Conclusions

hydrogen atom in strong B

$$d = 3 : (p^2/(2m) - e^2/r)\chi(r) = E\chi(r)$$

$$R(r) = \chi(r)/r, r \geq 0, \chi(0) = 0$$

$$(\chi(0) \neq 0 \;\; \triangle 1/r = \delta(r))$$

$$d = 1 : (p^2/(2m) - e^2/|z|)\Psi(z) = E\Psi(z)$$

$$-\infty < z < \infty, \;\; \Psi(0) \neq 0$$

variational method for ground state energy:

$$\Psi(z) \sim exp(-|z|/b);$$

$$< V > \sim -\ln(1/\epsilon)$$

The fall on the center in $d = 1$ occurs for Coulomb potential, while in $d = 3$ it occurs when $V < -1/(8mr^2)$.
$d = 1 \Longrightarrow d = 3$ at $z < a_H \equiv 1/\sqrt{eB}$

$$U(z) = -e^2/\sqrt{z^2 + a_H^2}$$

$$\ln(1/\epsilon) \Longrightarrow 2\ln(a_B/a_H) = \ln(B/(m^2e^3))$$

($a_B = 1/(me^2)$ - Bohr radius). LL, GKK:

$$E_0 = -2m\left(\int_{a_H}^{a_B} U(z)dz\right)^2$$

$$E_0 = -(me^4/2) \times \ln^2(B/(m^2e^3))$$

BUT: Elliott, Loudon - numerical solution of d=1 Schrodinger equation - very bad accuracy of ln^2 formula, though qualitatively correct.
First excited level: $\Psi_1(0) = 0, E_1 \Longrightarrow -me^4/2 \ (B \Longrightarrow \infty)$;

degeneracy of odd and even levels; the only nondegenerate level - $E_0 \Longrightarrow -\infty$. One-dimensional Coulomb problem - Loudon (1959).

Rad. “corrections” : NO, NO

$D = 2$ QED: screening of Φ

$$\Phi(\bar{k}) \equiv A_0(\bar{k}) = \frac{4\pi g}{\bar{k}^2} \; ; \quad \mathbf{\Phi} \equiv \mathbf{A}_0 = D_{00} + D_{00}\Pi_{00}D_{00} + ...$$

$$L = -1/4F^2_{\mu\nu} \Longrightarrow [A_\mu] = 0; [g] = m.$$

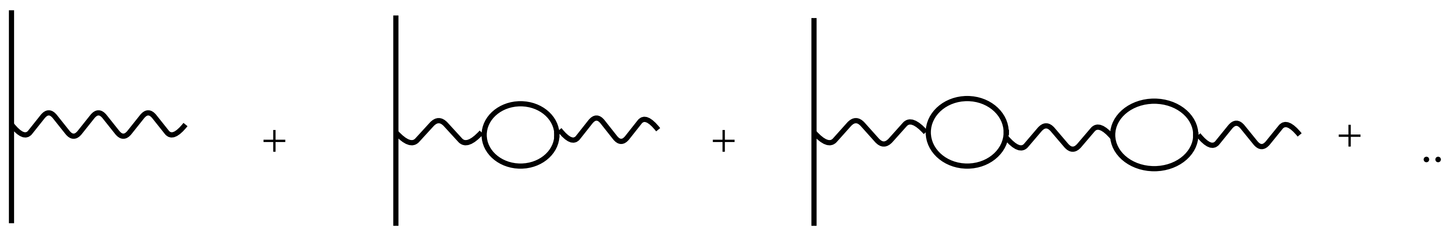


Fig 1. *Modification of the Coulomb potential due to the dressing of the photon propagator.*

Summing the series we get:

$$\mathbf{\Phi}(k) = -\frac{4\pi g}{k^2 + \Pi(k^2)} \, , \quad \Pi_{\mu\nu} \equiv \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right) \Pi(k^2)$$

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

$t \equiv -k^2/4m^2$, $[g] =$mass. (dim. reg: $D = 4-\epsilon, \epsilon = 2$)
Why in $D = 2$ Π is finite?
Taking $k = (0, k_{\|})$, $k^2 = -k_{\|}^2$ for the Coulomb potential in the coordinate representation we get:

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

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

Rad. corr. to Coulomb potential

Uehling-Serber correction to Coulomb potential.

Who knows?

QED in $D = 4$, no magnetic field
Berestetskii, Lifshitz, Pitaevskii, 4 volume of LL Theor.Phys.

e^2 correction; $exp(-2mr), r >> 1/m$ - very small correction;

logarithmic enhancement of potential (charge growth) for $r << 1/m$ (YM - opposite sign, asymptotic freedom)

back to D=2

Asymptotics of $P(t)$ are:

$$P(t) = \begin{cases} \frac{2}{3}t & , \quad t \ll 1 \\ 1 & , \quad t \gg 1 \quad . \end{cases}$$

Let us take as an interpolating formula for $P(t)$ the following expression:

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

The accuracy of this approximation is not worse than 10% for the whole interval of t variation, $0 < t < \infty$.

$$\mathbf{\Phi} = 4\pi g \int_{-\infty}^{\infty} \frac{e^{ik_\| z} dk_\| / 2\pi}{k_\|^2 + 4g^2 (k_\|^2/2m^2)/(3 + k_\|^2/2m^2)} =$$

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

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

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.

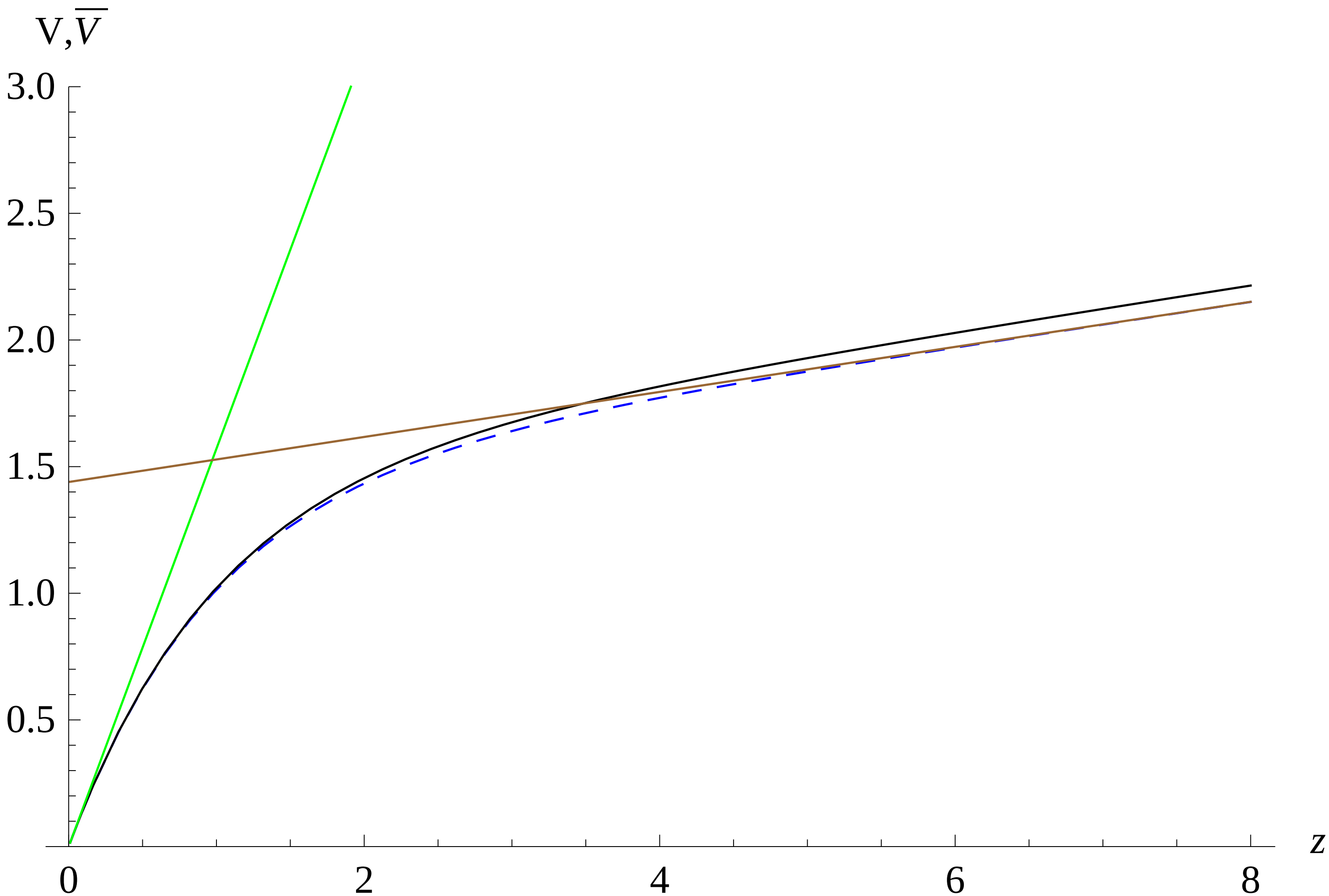
In case of light fermions ($m \ll g$):

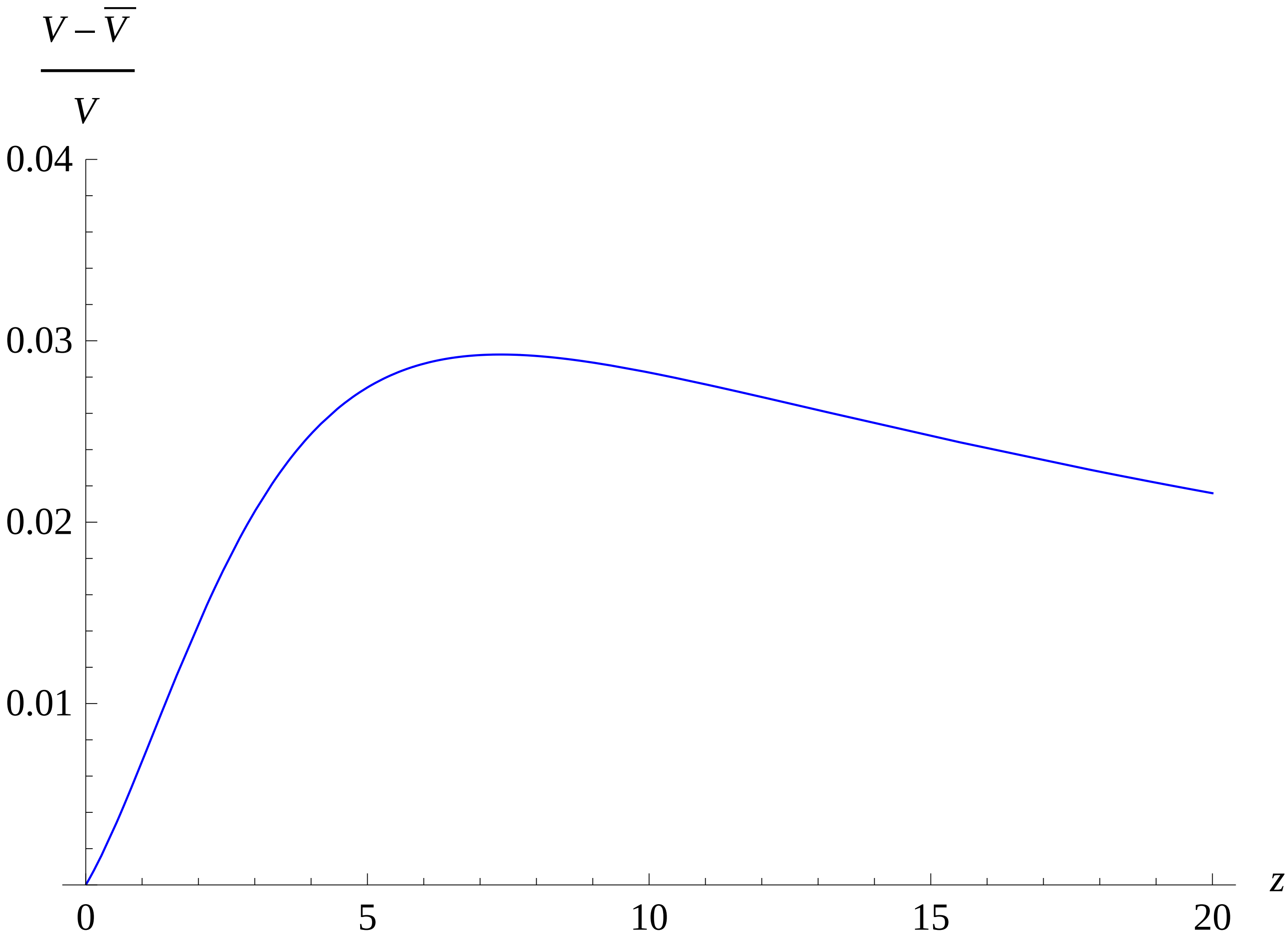
$$\Phi(z)\Big|_{m \ll g} = \begin{cases} \pi e^{-2g|z|} & , \quad z \ll \frac{1}{g}\ln\left(\frac{g}{m}\right) \\ -2\pi g\left(\frac{3m^2}{2g^2}\right)|z| & , \quad z \gg \frac{1}{g}\ln\left(\frac{g}{m}\right) \end{cases} .$$

$m = 0$- Schwinger model; photon get mass. The first gauge invariant theory with massive vector boson (electroweak theory: W, Z).

Light fermions - continuous transition from $m > g$ to $m = 0$.

Next two figures correspond to $g = 0.5, \;\; m = 0.1$:


V,$\overline{V}$
3.0
2.5
2.0
1.5
1.0
0.5
0
2
4
6
8
z



$\frac{V-\overline{V}}{V}$
0.04
0.03
0.02
0.01
0
5
10
15
20
z

$D = 4$ QED

In order to find potential of pointlike charge we need P in strong B. One starts from electron propagator G in strong B. Solutions of Dirac equation in homogenious 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 $B >> m^2/e$ and $k_\|^2 << eB$ in sum over levels LLL ($n = 0$) dominates. In coordinate representation transverse part of LLL wave function is: $\Psi \sim exp((-x^2 - y^2)eB)$ which in momentum representation gives $\Psi \sim exp((-k_x^2 - k_y^2)/eB)$ (gauge in which $\vec{A} = 1/2[\vec{B}\vec{r}]$ is used).
Substituting electron Green functions into polarization operator we get:

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

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

$$= e^3 B * exp(-\frac{k_\perp^2}{2eB}) * \Pi_{\mu\nu}^{(2)}(k_\parallel \equiv k_z);$$

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

$$\mathbf{\Phi}(z) =$$

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

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

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

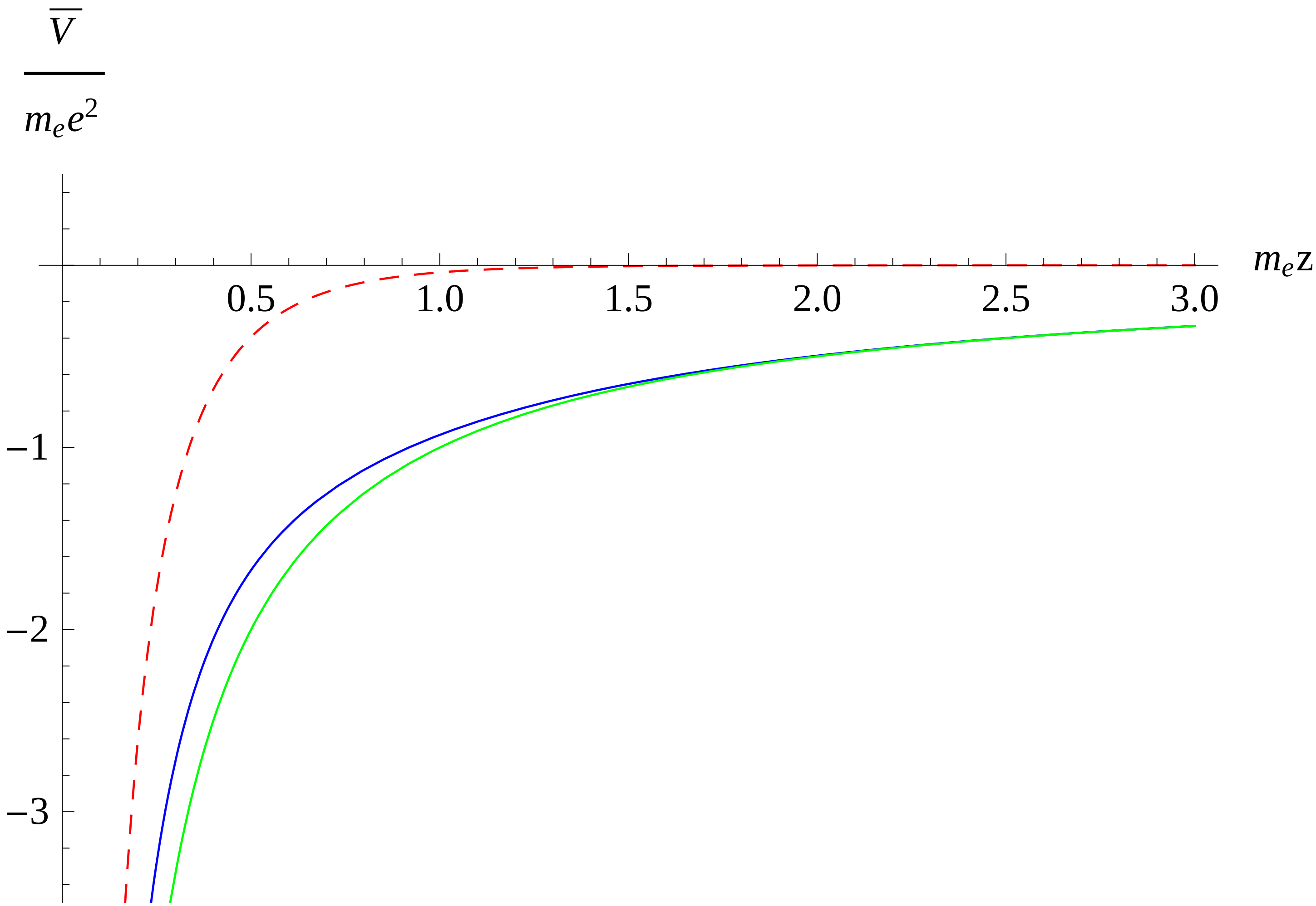
$$\mathbf{\Phi}(z)\Bigg|_{e^3 B \ll m_e^2} = \frac{e}{|z|}\left[1 + O\left(\frac{e^3 B}{m_e^2}\right)\right]$$

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

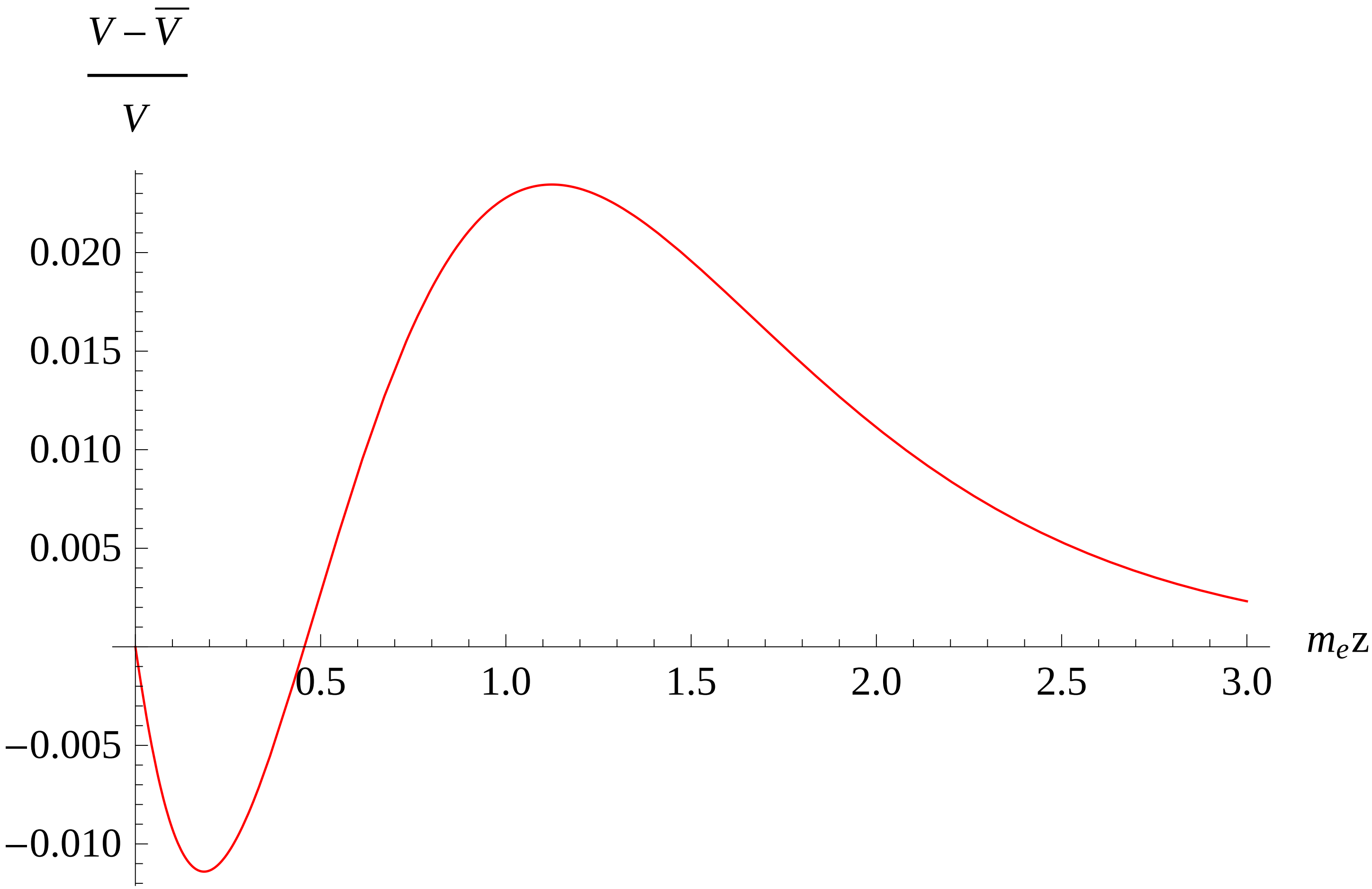
In the opposite case of superstrong magnetic fields $B \gg 3\pi m_e^2/e^3$ we get:

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

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



Modified Coulomb potential at $B = 10^{17}$G (blue) and its long distance (green) and short distance (red) asympotics.



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

electron in magnetic field

spectrum of Dirac eq:

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

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

spectrum of Schrödinger eq. in cylindrical coordinates $(\bar{\rho}, z)$ in the gauge, where $\bar{A} = \frac{1}{2}[\bar{B}\bar{r}]$:

LL QM

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

LLL: $n_\rho = 0,\ \sigma_z = -1,\ m = 0, -1, -2, ...$

$$R_{0m}(\bar{\rho}) = \left[\pi (2a_H^2)^{1+|m|} (|m|!) \right]^{-1/2} \rho^{|m|} e^{(im\varphi - \rho^2/(4a_H^2))} \quad ,$$

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:

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

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

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

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

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

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

$$U_{eff}(z)\Bigg|_{z \gg a_H} = -\frac{e^2}{|z|}$$

and is regular at $z = 0$:

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

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

The shallow-well approximation

$$E^{sw} = -2m_e \left[\int_{a_H}^{a_B} U(z)dz \right]^2 = -(m_e e^4/2) ln^2(B/(m_e^2 e^3))$$

Used to calculate the ground state energy of hydrogen in strong B in LL QM (after 1974 editions); GKK; Shabad, Usov.

Derivation:

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

Neglecting E_0 in comparison with U and integrating we get:

$$\chi'(a) = 2\mu \int_0^a U(x)\chi(x)dx \quad ,$$

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

$$|E_0| = 2\mu \left[\int_0^a U(x)dx \right]^2 \quad .$$

For

$$\mu|U|a^2 \ll 1$$

(condition for the potential to form a shallow well) we get that, indeed, $|E_0| \ll |U|$ and that the variation of χ 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.

Karnakov - Popov equation

It provides a several percent accuracy for the energies of EVEN states for $H > 10^3$ ($H \equiv B/(m_e^2 e^3)$.
Main idea: to integrate Sh eq with effective potential from $x = 0$ till $x = z$, where $a_H << z << a_B$ and to equate obtained expression for $\chi'(z)/\chi(z)$ to the logarithmic derivative of Whittaker function - the solution of Sh eq with Coulomb potential, which exponentially decreases at $z >> a_B$:

$$2\ln\left(\frac{z}{a_H}\right) + \ln 2 - \psi(1+|m|) + O(a_H/z) =$$

$$2\ln\left(\frac{z}{a_B}\right) + \lambda + 2\ln\lambda + 2\psi\left(1 - \frac{1}{\lambda}\right) + 4\gamma + 2\ln 2 + O(z/a_B)$$

$$E = -(m_e e^4/2)\lambda^2$$

The energies of the ODD states are:

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

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

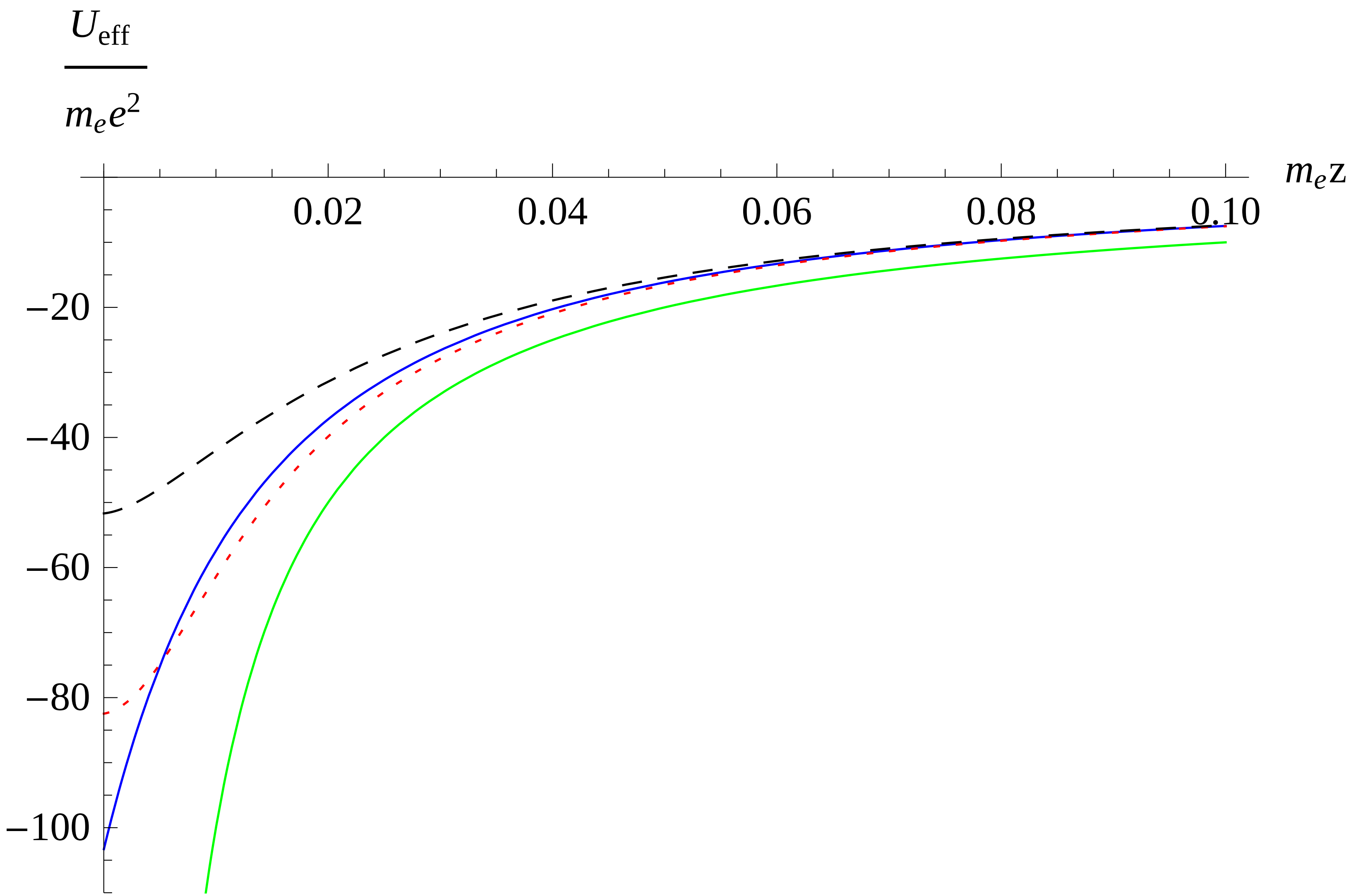
Energies of even states; screening

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

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

$$U_{simpl}(z) = -e^2 \frac{1}{\sqrt{a_H^2 + z^2}} \left[1 - e^{-\sqrt{6m_e^2}\, z} + e^{-\sqrt{(2/\pi)e^3 B + 6m_e^2}\, z}\right]$$

Eff potential - figures



Effective potentials at $B = 10^{17}$*G*

Modified KP equation

The original KP equation for LLL splitting by Coulomb potential:

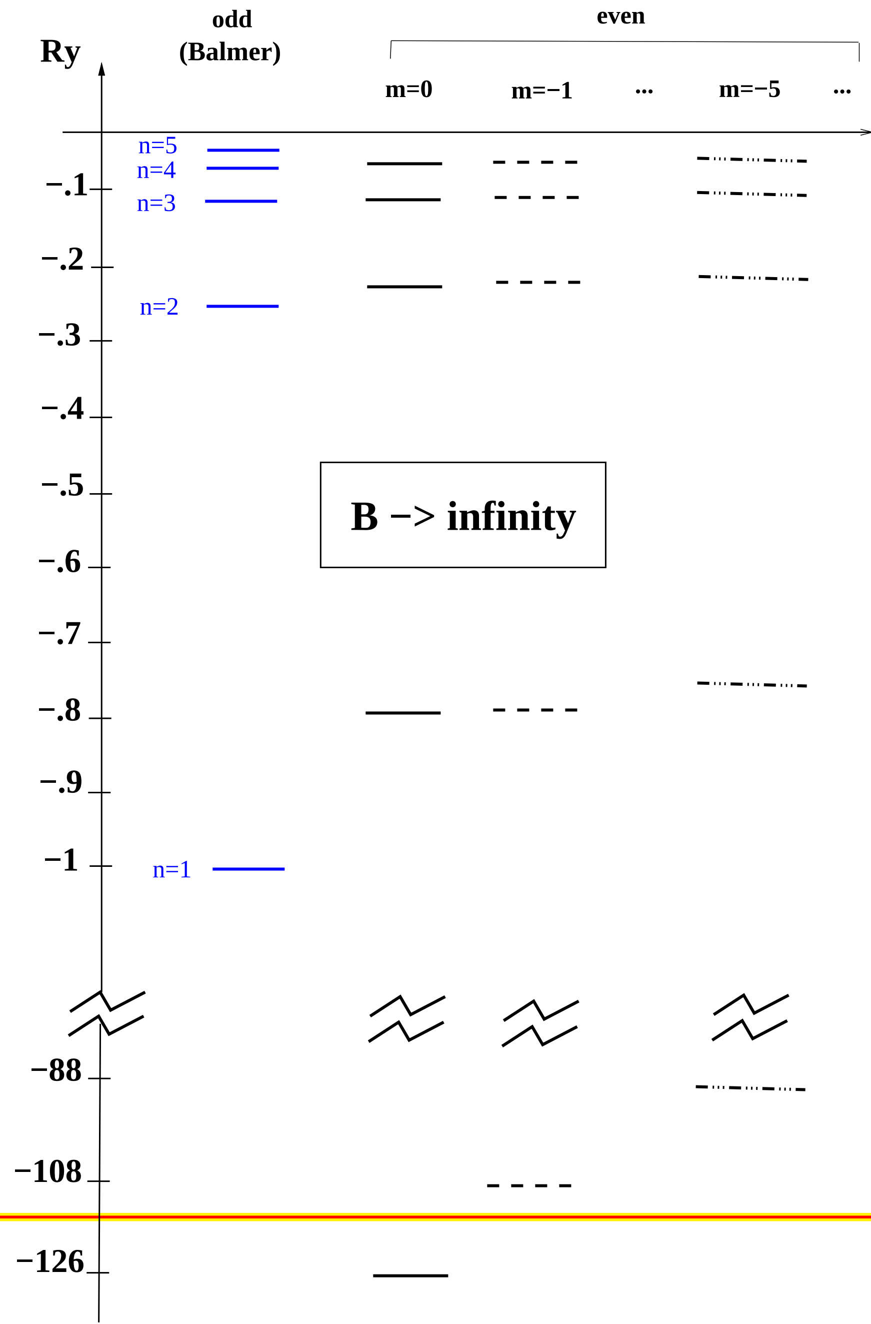
$$\ln(H) = \lambda + 2\ln\lambda + 2\psi\left(1 - \frac{1}{\lambda}\right) + \ln 2 + 4\gamma + \psi(1 + |m|) \quad .$$

$\psi(x)$ - 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:

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

$E = -(m_e e^4/2)\lambda^2$

spectrum


odd
(Balmer)
even
Ry
m=0
m=−1
...
m=−5
...
n=5
n=4
−.1
n=3
−.2
n=2
−.3
−.4
−.5
B −> infinity
−.6
−.7
−.8
−.9
−1
n=1
−88
−108
−126

B values

$B > m_e^2 e^3 = 2.4 * 10^9$Gauss - strong B,
$B > m_e^2/e^3 = 6 * 10^{15}$Gauss - superstrong B.

$B_{cr} = m_e^2/e = 4.4 * 10^{13}$Gauss - critical B

B in laboratories:
$10^6 - 10^7$Gauss - magnetic cumulation, A.D.Saharov, 1952,
$H * r^2 =$const

Pulsars: $B \sim 10^{13}$Gauss;   Magnetars: $B \sim 10^{15}$Gauss

Elliott, Loudon: excitons in semiconductors,
$m^* \ll m_e, \ \ e^* << e \ \ B > 2000$ Gauss - strong B

superstrong B - graphene: $m << m_e, \ \ \alpha \sim 1$???

References

Shabad, Usov (2007,2008): $D = 4$ screening of Coulomb potential, freezing of the energy of ground state for $B >> m^2/e^3$ - numerical calculations;
Batalin, Shabad (1971): Π at $B > B_{cr}$ calculation;
Skobelev(1975), Loskutov, Skobelev(1976): linear in B term and $D = 4 \Longrightarrow D = 2$ correspondence in photon polarization operator for $B > m^2/e$;
Loskutov, Skobelev(1983); Kuznetsov, Mikheev, Osipov (2002): in $B >> m^2/e^3$ photon “mass” emerge;
Loudon(1959), Elliott, Loudon(1960) - atomic energies in strong $B > m^2e^3$ - numerical calculations;
Karnakov, Popov(2003) - analytical formulas for atomic energies in strong $B > m^2e^3$;
Vysotsky; Machet, Vysotsky(2010) - analytical formulas for Coulomb potential screening and LLL spectrum.

Conclusions

- analytical expression for charged particle electric potential in $d = 1$ is given; for $m < g$ screening take place at all distances
- analytical expression for charged particle electric potential at superstrong B at $d = 3$ is found: $\Phi(z, \rho = 0)$; screening take place at distances $|z| < 1/m_e$
- an algebraic formula for the energy levels of a hydrogen atom originating from the lowest Landau level in superstrong B has been obtained
- NOT THE END: Dirac equation for LLL in Coulomb field; power in B corrections to E_0