PHY 742 Quantum Mechanics II
1-1:50 AM MWF Olin 103

Plan for Lecture 3

Quantum particle interacting with classical electromagnetic fields

Reading: Chapter 9 in Carlson's textbook

a. **Example of charged particle in a magnetostatic field**
b. **Example of a hydrogen atom in a magnetostatic field**

PHY 742 Quantum Mechanics II>

MWF 1-1:50 PM	**OPL 103**	**http://www.wfu.edu/~natalie/s20phy742/**

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Course schedule for Spring 2020

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/13/2020	Chap. 9	Quantum mechanics of electromagnetic forces	#1	01/22/2020
2	Wed: 01/15/2020	Chap. 9	Quantum mechanics of particle in electrostatic field	#2	01/24/2020
3	Fri: 01/17/2020	Chap. 9	Quantum mechanics of particle in magnetostatic field	#3	01/27/2020
	Mon: 01/20/2020	No class	Martin Luther King Holiday		
4	Wed: 01/22/2020				
5	Fri: 01/24/2020				
6	Mon: 01/27/2020				
7	Wed: 01/29/2020				
8	Fri: 01/31/2020				

For electrostatic and/or magnetostatic fields, the time dependence of the fields becomes trivial, and we expect stationary state solutions to the Schrödinger equation

Hamiltonian: $H(\mathbf{r})=\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r}) + qU(\mathbf{r})$

Time-dependent Schrödinger Eq: $i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = H(\mathbf{r})\Psi(\mathbf{r},t)$

Stationary state solution at energy E: $\Psi(\mathbf{r},t) = \psi(\mathbf{r})e^{iEt/\hbar}$

Time-independent Schrödinger Eq: $E\psi(\mathbf{r}) = H(\mathbf{r})\psi(\mathbf{r})$

Consideration of effects of a static magnetic field on quantum states of a charged free particle. First consider the spatial degrees of freedom (ignoring intrinsic spin).

Assume particle has charge q and mass m; $V(\mathbf{r})=0$ and $U(\mathbf{r})=0$

$$H=\frac{1}{2m}\left(-i\nabla-q\mathbf{A}(\mathbf{r})\right)^2$$

For a constant and uniform magnetic field $B_0\hat{\mathbf{z}}$

can choose $\mathbf{A}(\mathbf{r})=-B_0 y\hat{\mathbf{x}}$

$$H=\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}+qB_0 y\right)^2+\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$$

$$H = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} + qB_0 y\right)^2 + \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

Constants of the motion: p_x, p_z

$$\Psi(x,y,z) = e^{i(p_x x + p_z z)/\hbar}\psi(y)$$

Energy eigenstates:

$$H\Psi = E\Psi$$

$$H = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} + qB_0 y\right)^2 + \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$H\Psi = e^{i(p_x x + p_z z)/\hbar}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \left(\frac{1}{2}m\omega_c^2(y-y_0)^2 + \frac{p_z^2}{2m}\right)\psi(y)\right) = E\Psi$$

Differential equation for $\psi(y)$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \frac{1}{2}m\omega_c^2(y-y_0)^2\psi(y) = \left(E - \frac{p_z^2}{2m}\right)\psi(y)$$

where $\omega_c \equiv \frac{qB_0}{m}$ $\qquad y_0 = -\frac{p_x}{qB_0}$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2}+\frac{1}{2}m\omega_c^2(y-y_0)^2\psi(y)=\left(E-\frac{p_z^2}{2m}\right)\psi(y)$$

where $\omega_c \equiv \frac{qB_0}{m}$

Energy eigenvalues:

$$E=E_n(p_z)=\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{p_z^2}{2m}$$

Energy eigenvalues:

$$E_n(p_z) = \hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{p_z^2}{2m} \qquad \text{where} \quad \omega_c \equiv \frac{qB_0}{m}$$

Eigenfunctions

Hermite polynomial

$$\psi_n(y) = \mathcal{N} e^{-(y-y_0)^2/\left(2\alpha^2\right)} H_n((y-y_0)/\alpha)$$

$$\text{where } \alpha \equiv \sqrt{\frac{\hbar}{qB_0}} = \sqrt{\frac{\hbar}{m\omega_c}} \qquad y_0 = -\frac{p_x}{qB_0}$$

Notion of density of states

$$\text{DOS}(\epsilon) = \sum_{\text{states}} \delta(E - \epsilon)$$

For discrete spectrum: $\text{DOS}(\epsilon) = \sum_{n} \delta(E_n - \epsilon)$

For continuum spectrum such as 3-dimensional free-particle:

$$\text{DOS}(\epsilon) = \sum_{p_x, p_y, p_z} \delta\left(\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} - \epsilon\right)$$

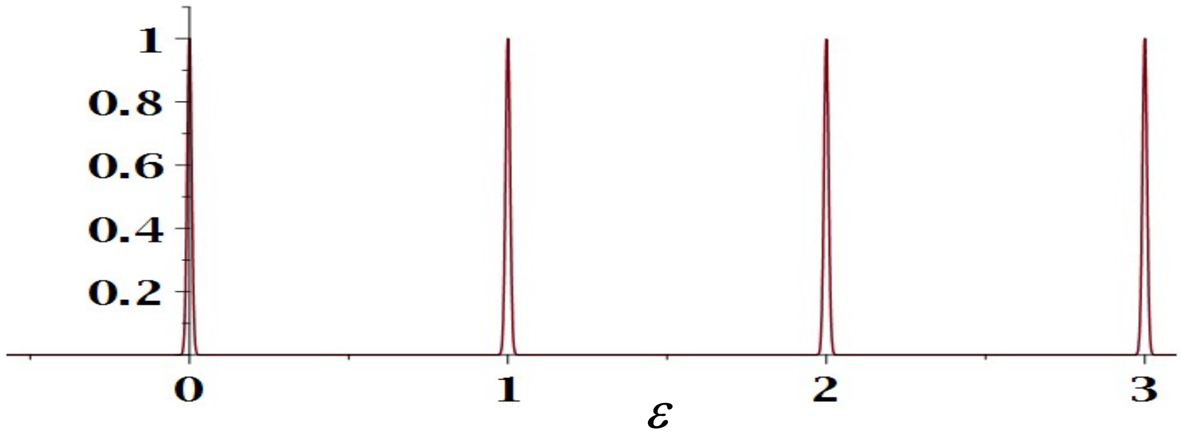
$$= C \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} dp_z \delta\left(\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} - \epsilon\right)$$

For isotropic case:

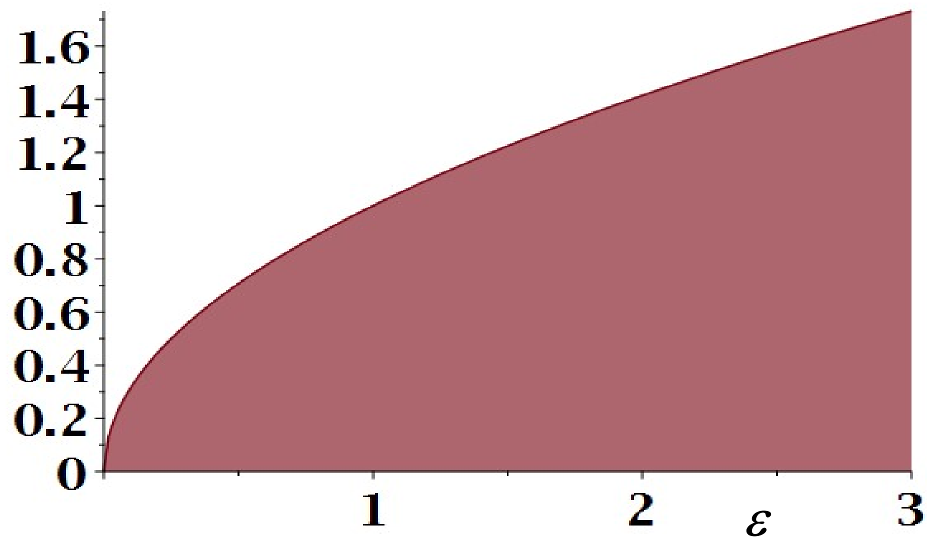
$$\text{DOS}(\epsilon) = C 4\pi \int_0^{\infty} p^2 dp \delta\left(\frac{p^2}{2m} - \epsilon\right) = C 4\pi (2m)^{3/2} \sqrt{\epsilon}$$

DOS plots –

Discrete spectrum



Continuous spectrum for a free particle in three dimensions

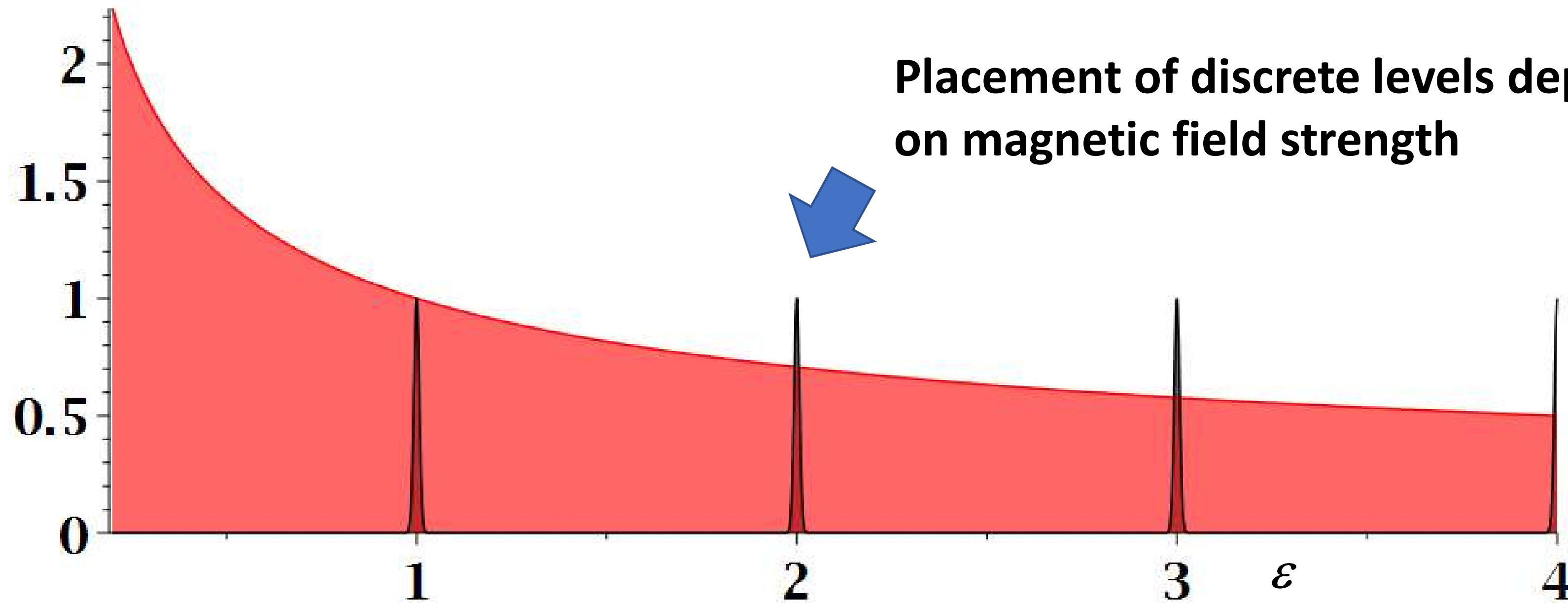


DOS plot for magnetostatic acting on charged particle

Energy eigenvalues:

$$E_n(p_z) = \hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{p_z^2}{2m} \qquad \text{where} \quad \omega_c \equiv \frac{qB_0}{m}$$

Note that this is an approximate model of an ideal metal in a magnetic field which results in oscillatory resistivity for example.



Placement of discrete levels depends on magnetic field strength

Treating the same problem with a different Gauge:

$$\mathbf{A}(x,y,z) = -\frac{1}{2}\left(y\hat{\mathbf{x}} - x\hat{\mathbf{y}}\right)B_0$$

In cylindrical coordinates:

$$\mathbf{A}(\rho,\phi,z) = \frac{1}{2}\rho\ \hat{\phi}B_0$$

$$\left\{-\frac{\hbar^2}{2m_e}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) - \frac{i\hbar\omega_c}{2}\frac{\partial}{\partial\phi} + \frac{1}{8}m_e\omega_c^2\rho^2\right\}\Psi(\rho,\phi,z)$$

$$= \left(E - \frac{p_z^2}{2m_e}\right)\Psi(\rho,\phi,z)$$

Here m_e is electron mass rather than integer azimuthal eigenvalue m.

$$\Psi(\rho,\phi,z) = R(\rho)e^{im\phi}e^{ip_z z/\hbar}$$

Eigenvalues in cylindrical coordinates

$$E_{\nu m}(p_z) = \hbar\omega_c\left(\nu + \frac{1}{2} + \frac{1}{2}\left(m + |m|\right)\right) + \frac{p_z^2}{2m_e}$$

Note that (with a non-trivial proof) it can be shown that this spectrum is equivalent to Cartesian gauge; full solution includes intrinsic spin

Full solution including eigenfunctions are worked out in Landau and Lifshitz. It is shown that the eigenstates are related to harmonic oscillator eigenstates.

Effects of magnetostatic fields on particles' intrinsic magnetic moment.

If a particle has an intrinsic magnetic moment $\mathbf{m}$, its interaction potential with a magnetostatic field is $-\mathbf{m}\cdot\mathbf{B}$. For an electron, $\mathbf{m}=-g\mu_B\mathbf{S}/\hbar$ where $\mathbf{S}$ the spin angular momentum operator of the electron with eigenvalues $\pm\frac{1}{2}\hbar$, $\mu_B=\dfrac{e\hbar}{2m_e}$, and $|g|=2.00231930436256$. This adds an interaction to the Hamiltonian $\Delta H_{spin}=g\mu_B\mathbf{B}\cdot\mathbf{S}/\hbar$. This formalism is appropriate for all particles with intrinsic spin, each with its own gyromagnetic ratio. For example, there is also an interaction of the magnetic field with a proton, with a smaller factor by 10^{-3}.

Interaction of magnetostatic field B with a hydrogen atom (including contribution of intrinsic electron spin, omitting contribution of intrinsic proton spin).

Isolated H atom: $$H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$$

H atom in magnetic field $\mathbf{B}$ and vector potential $\mathbf{A} = -\frac{1}{2}\mathbf{r}\times\mathbf{B}$

$$H = \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + V(r) + g\mu_B \mathbf{S}\cdot\mathbf{B}/\hbar = H^0 + H^1 + H^2$$

Terms of linear order in $\mathbf{A}$:

$$\frac{e}{2m}(\mathbf{p}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{p}) = -\frac{e}{4m}\big(\mathbf{p}\cdot(\mathbf{r}\times\mathbf{B}) + (\mathbf{r}\times\mathbf{B})\cdot\mathbf{p}\big) = \frac{e}{2m}(\mathbf{r}\times\mathbf{p})\cdot\mathbf{B} = \frac{e}{2m}\mathbf{L}\cdot\mathbf{B}$$

$$H^1 = \mu_B(\mathbf{L}+g\mathbf{S})\cdot\mathbf{B}/\hbar$$

$$\mu_B = \frac{e\hbar}{2m} \qquad |g| = 2.00231930436256$$

Analysis of magnetostatic effects on atomic structure using perturbation theory, also including the effects of spin-orbit interation

$$H = \frac{(\mathbf{p} + e\mathbf{A})^2}{2m} + V(r) + G(r)\mathbf{S}\cdot\mathbf{L} + g\mu_B\mathbf{B}\cdot\mathbf{S}/\hbar$$

$$H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$$

Keeping terms of linear order in $\mathbf{B}$ and spin-orbit interation :

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B\left(\mathbf{L} + g\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

$$= \frac{G(r)}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) + \mu_B\left(\mathbf{J} + (g-1)\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

Perturbation theory treatment of uniform and constant magnetic fields on atomic states -- continued

$$H = H^0 + H^1$$

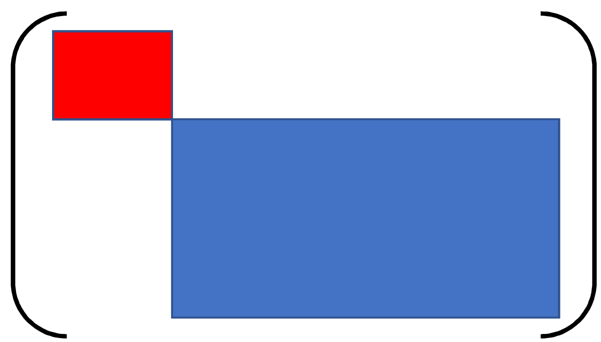
$$H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B\left(\mathbf{L} + g\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

For the effects on a H atom in the $n = 2$ states:

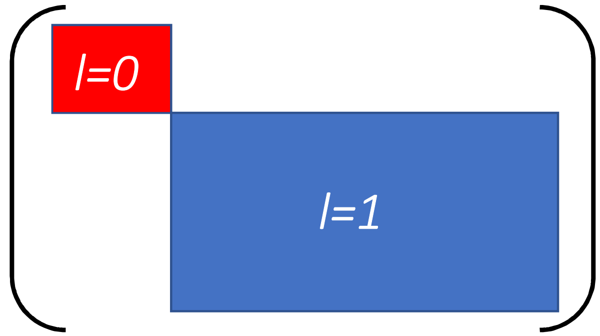
$\Rightarrow 8\times 8$ perturbation matrix:

$$\left\langle 2lmm_s \middle| H^1 \middle| 2lm'm_s' \right\rangle =$$



$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B\left(\mathbf{L} + g\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

$$\langle 2lmm_s | H^1 | 2lm'm_s' \rangle =$$



$$\begin{array}{c} \\ \langle 200m_s | H^1 | 200m_s' \rangle = \end{array} \begin{array}{c} \\ m_s = \tfrac{1}{2} \\ m_s = -\tfrac{1}{2} \end{array} \begin{array}{cc} m_s' = \tfrac{1}{2} & -\tfrac{1}{2} \\ \multicolumn{2}{c}{\begin{pmatrix} \frac{g\mu_B B}{2} & 0 \\ 0 & -\frac{g\mu_B B}{2} \end{pmatrix}} \end{array}$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B\left(\mathbf{L} + g\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

$$\langle 21mm_s|H^1|21m'm_s'\rangle = \begin{array}{r} m'm_s' = \\ mm_s = 1\tfrac{1}{2} \\ 1-\tfrac{1}{2} \\ 0\tfrac{1}{2} \\ 0-\tfrac{1}{2} \\ -1\tfrac{1}{2} \\ -1-\tfrac{1}{2} \end{array} \begin{array}{c} \begin{array}{cccccc} 1\tfrac{1}{2} & 1-\tfrac{1}{2} & 0\tfrac{1}{2} & 0-\tfrac{1}{2} & -1\tfrac{1}{2} & -1-\tfrac{1}{2} \end{array} \\ \begin{pmatrix} X & & & & & \\ & X & X & & & \\ & X & X & & & \\ & & & X & X & \\ & & & X & X & \\ & & & & & X \end{pmatrix} \end{array}$$

$$\mathbf{S}\cdot\mathbf{L} = \tfrac{1}{2}\left(S_-L_+ + S_+L_-\right) + S_zL_z$$

$$J_\pm\left|jm\right\rangle = \hbar\sqrt{j^2 - m^2 + j \mp m}\left|j\left(m \pm 1\right)\right\rangle$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B\left(\mathbf{L} + g\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

$$\text{Let } \gamma \equiv \frac{\langle 21|G(r)|21\rangle}{2\hbar^2}$$

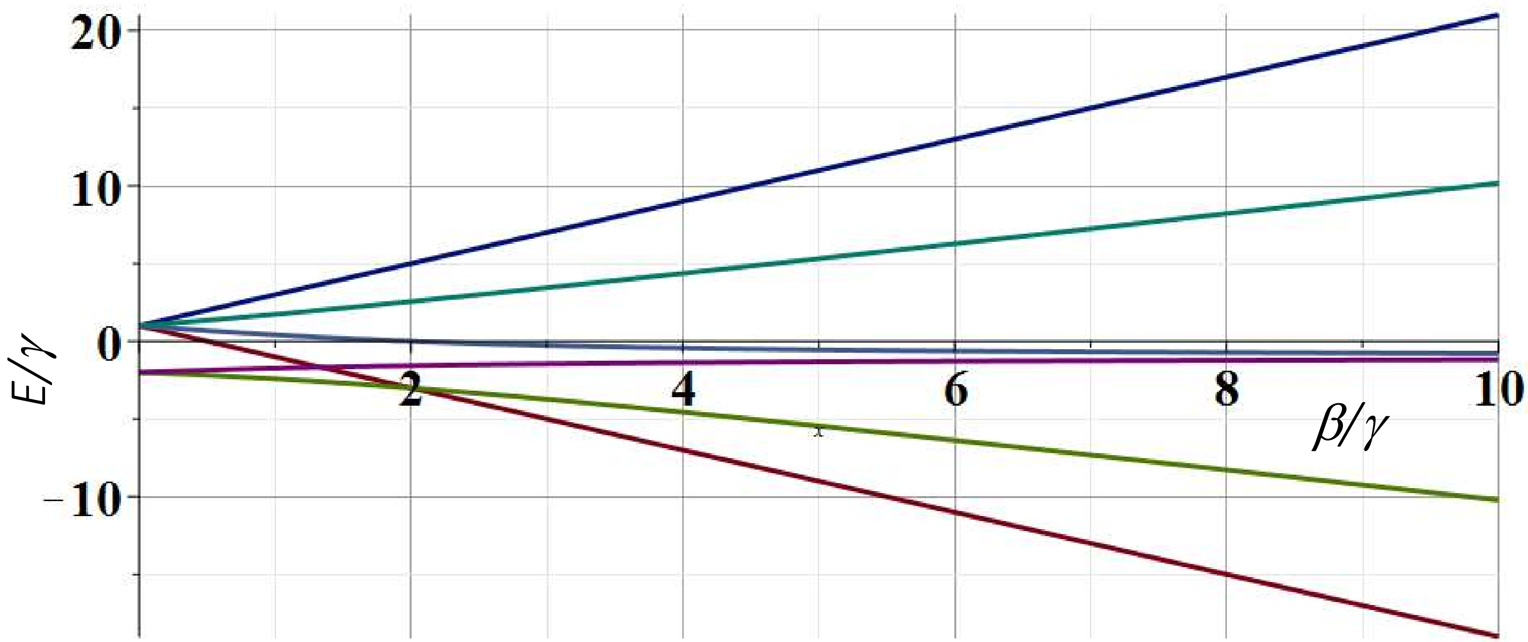
$$\beta \equiv \mu_B \mathrm{B}_0$$

$$\langle 21mm_s|H^1|21m'm_s'\rangle =$$

$$
\begin{array}{c|cccccc}
 & m'm_s' = 1\,\frac{1}{2} & 1-\frac{1}{2} & 0\,\frac{1}{2} & 0-\frac{1}{2} & -1\,\frac{1}{2} & -1-\frac{1}{2} \\
\hline
mm_s = 1\frac{1}{2} & \gamma+\beta(1+g/2) & 0 & 0 & 0 & 0 & 0 \\
1-\frac{1}{2} & 0 & -\gamma+\beta(1-g/2) & \sqrt{2}\gamma & 0 & 0 & 0 \\
0\frac{1}{2} & 0 & \sqrt{2}\gamma & \beta g/2 & 0 & 0 & 0 \\
0-\frac{1}{2} & 0 & 0 & 0 & -\beta g/2 & \sqrt{2}\gamma & 0 \\
-1\frac{1}{2} & 0 & 0 & 0 & \sqrt{2}\gamma & -\gamma-\beta(1-g/2) & 0 \\
-1-\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & \gamma-\beta(1+g/2)
\end{array}
$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B\left(\mathbf{L} + g\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

Evaluated for degenerate states $\left|nlmm_s\right\rangle = \left|21mm_s\right\rangle$



Zeeman effect

Paschen-Backb effect