PHY 741 Quantum Mechanics
12-12:50 AM MWF Olin 103

Plan for Lecture 27:

Chap. 17 in Shankar: Magnetic field effects – atoms, charged particles

1. **Perturbation theory -- Zeeman and Paschen-Back effects**
2. **Effects of a magnetic field on free charged particles**

	Fri, 10/13/2017		*Fall break -- No class*		
19	Mon, 10/16/2017		Discuss exam questions and topics for presentations	Topic	10/18/2017
20	Wed, 10/18/2017	Chap. 14	Intrinsic spin	#11	10/20/2017
21	Fri, 10/20/2017	Chap. 15	Addition of Angular Momentum	#12	10/23/2017
22	Mon, 10/23/2017	Chap. 15	Multi-electron atoms	#13	10/25/2017
23	Wed, 10/25/2017	Chap. 15	Multi-electron atoms	#14	10/30/2017
24	Fri, 10/27/2017		Effects of nuclear motion		
25	Mon, 10/30/2017	Chap. 17	Time-independent perturbation theory	#15	11/3/2017
26	Wed, 11/01/2017	Chap. 17	Time-independent perturbation theory		
27	Fri, 11/03/2017		Effects of a static magnetic field		
28	Mon, 11/06/2017				
29	Wed, 11/08/2017				
30	Fri, 11/10/2017				
31	Mon, 11/13/2017				
32	Wed, 11/15/2017				
33	Fri, 11/17/2017				
34	Mon, 11/20/2017				
	Wed, 11/22/2017		*Thanksgiving Holiday -- No class*		
	Fri, 11/24/2017		*Thanksgiving Holiday -- No class*		

Degenerate perturbation theory example for effects of a constant magnetic field B on an atom

Vector potential $\mathbf{A}=\frac{1}{2}\mathbf{r}\times\mathbf{B}$

$$H=\frac{\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2}{2m}+V(r)+g\mu_B\mathbf{B}\cdot\mathbf{S}/\hbar \qquad \mu_B=\frac{e\hbar}{2mc}$$

$$H^0=\frac{\mathbf{p}^2}{2m}+V(r) \qquad |g|=2.00231930436182$$

Keeping only terms to linear order in $\mathbf{B}$:

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

Detail:

$$\frac{1}{2}\mathbf{p}\cdot\mathbf{r}\times\mathbf{B}+\frac{1}{2}\mathbf{r}\times\mathbf{B}\cdot\mathbf{p}=\mathbf{L}\cdot\mathbf{B}$$

Degenerate perturbation theory example for effects of a constant magnetic field B on an atom – including the effects of spin-orbit interaction

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

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

Keeping only terms to linear order in $\mathbf{B}$:

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

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

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

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

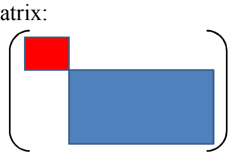
$$H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$$

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

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

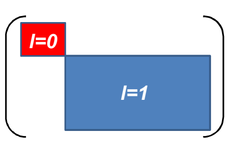
$\Rightarrow 8\times 8$ perturbation matrix:

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



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

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



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

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

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

mm_s \ $m'm_s'$	$1\frac{1}{2}$	$1-\frac{1}{2}$	$0\frac{1}{2}$	$0-\frac{1}{2}$	$-1\frac{1}{2}$	$-1-\frac{1}{2}$
$1\frac{1}{2}$	X					
$1-\frac{1}{2}$		X	X			
$0\frac{1}{2}$		X	X			
$0-\frac{1}{2}$				X	X	
$-1\frac{1}{2}$				X	X	
$-1-\frac{1}{2}$						X

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

$$J_\pm|jm\rangle = \hbar\sqrt{j^2 - m^2 + j \mp m}\,|j(m\pm1)\rangle$$

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

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

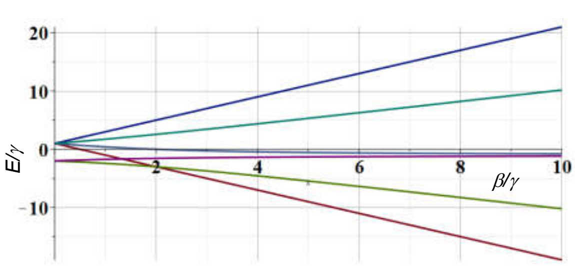
$\beta \equiv \mu_B \mathrm{B}_0$

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

mm_s \ $m'm_s'$	$1\frac{1}{2}$	$1-\frac{1}{2}$	$0\frac{1}{2}$	$0-\frac{1}{2}$	$-1\frac{1}{2}$	$-1-\frac{1}{2}$
$1\frac{1}{2}$	$\gamma+\beta(1+g/2)$	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	$\gamma-\beta(1+g/2)$

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

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



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:

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

For a constant and uniform magnetic field $B_0\hat{\mathbf{z}}$ can choose $\mathbf{A}(\mathbf{r}) = -B_0 y\hat{\mathbf{x}}$

$$H = \frac{1}{2m}\left(p_x + \frac{qB_0 y}{c}\right)^2 + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

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Constants of the motion: p_x, p_z

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

Energy eigenstates:

$$H\Psi = E\Psi$$

$$H = \frac{1}{2m}\left(p_x + \frac{qB_0 y}{c}\right)^2 + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

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

where $\omega_c \equiv \frac{qB_0}{mc}$ $\quad y_0 = -\frac{cp_x}{qB_0}$

$$-\frac{\hbar^2}{2m}\frac{d^2\chi(y)}{dy^2}+\frac{1}{2}m\omega_c^2(y-y_0)^2\chi(y)$$

$$=\left(E-\frac{p_z^2}{2m}\right)\chi(y)$$

Energy eigenvalues:

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

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Eigenfunctions

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

$$\text{where } \alpha\equiv\sqrt{\frac{\hbar c}{qB_0}}=\sqrt{\frac{\hbar}{m\omega_c}} \quad y_0=-\frac{cp_x}{qB_0}$$

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:

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

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

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

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

Eigenvalues in cylindrical coordinates

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

Equivalent to Cartesian gauge;   full solution includes intrinsic spin

Comment on current density operator in presence of magnetic field

$$\mathbf{j} = \frac{ie\hbar}{2m_e}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right) - \frac{e^2}{m_e c}\mathbf{A}\Psi^*\Psi$$