Quantum Mechanics - 1: HW 7 Solutions

Leo Radzihovsky
Paul Martens

November 28, 2007

1 Problem 1

3D Spherical square-well potential. Suppose

$$V(r) = \begin{cases} -V_0 & r < d \\ 0 & r > d \end{cases} \tag{1}$$

1.1 a: Boundstates

For these states $E < 0$. Define:

$$R_{n\ell}(r) = \frac{U_{n\ell}(r)}{r} \tag{2}$$

The radial equation for U

$$-\frac{\hbar^2}{2m}\frac{d^2U_{n\ell}(r)}{dr^2} + \left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)U_{n\ell} = E_{n\ell}U_{n\ell} \tag{3}$$

1.1.1 i: spectrum for general ℓ

Solve for internal and external separately then match boundary conditions. $0 < r < d \Rightarrow V(r) = -V_0 \Rightarrow$ free schr. solutions with $E \to E + V_0$

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(\kappa^2 - \frac{\ell(\ell+1)}{r^2}\right)R = 0 \tag{4}$$

where

$$\kappa \equiv \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}} \tag{5}$$

we require a regular solution at $r = 0$; therefore

$$R_{n\ell}(r) = Aj_\ell(\kappa r) \tag{6}$$

for the external solution

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(-\alpha^2 - \frac{\ell(\ell+1)}{r^2}\right)R = 0 \tag{7}$$

where

$$\alpha \equiv \sqrt{\frac{2m\left|E\right|}{\hbar^2}} \tag{8}$$

outer solution is

$$R\left(r\right) = Bj_\ell\left(\imath\alpha r\right) + Cn_\ell\left(\imath\alpha r\right) \tag{9}$$

we need a decaying solution, which is a spherical Hankel function of the first kind. $h_\ell^{(1)} \equiv j_\ell + \imath n_\ell$. Matching boundary conditions leads to a discrete spectrum.

$$\kappa\frac{j_\ell'\left(\kappa d\right)}{j_\ell\left(\kappa d\right)} = \imath\alpha\frac{h_\ell^{(1)\prime}\left(\imath\alpha d\right)}{h_\ell\left(\imath\alpha d\right)} \tag{10}$$

1.1.2 ii: $\ell = 0$ case

$$\begin{cases} U'' + \kappa^2 U = 0 & 0 < r \leq d \\ U'' - \alpha^2 U = 0 & d < r \end{cases} \tag{11}$$

Solution is

$$U\left(r\right) = \begin{cases} A\sin\kappa r & 0 < r \leq d \\ Be^{-\alpha r} & d < r \end{cases} \tag{12}$$

BC

$$\frac{B}{A} = e^{\alpha d}\sin\kappa d \tag{13}$$

The wavefunction is

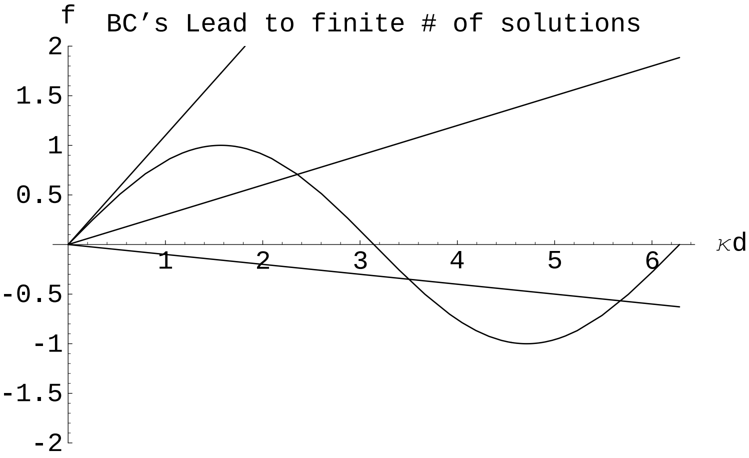
$$\Psi_{E0}\left(r\right) = \begin{cases} \frac{A}{r}\sin\kappa r & 0 < r \leq d \\ \frac{B}{r}e^{-\alpha r} & d < r \end{cases} \tag{14}$$

spectrum is found through the relation

$$\kappa\frac{\cos\kappa d}{\sin\kappa d} = -\alpha = -\sqrt{\frac{2m}{\hbar^2}V_0 - \kappa^2} \tag{15}$$

$$\kappa^2 = \underbrace{\left(\kappa^2 + \alpha^2\right)}_{\frac{2m}{\hbar^2}V_0}\sin^2\kappa d \tag{16}$$

$$\sin\kappa d = \pm\sqrt{\frac{\hbar^2}{2md^2V_0}}\kappa d \tag{17}$$



1.1.3 iii: n-th boundstate requirement

The relation above has the form $\delta x = \sin x$. So we get the n-th bound state when

$$\delta\left(2n-1\right)\frac{\pi}{2}=1 \tag{18}$$

or

$$V_{0C}^{(n)}=\frac{\pi^2\hbar^2}{8md^2}\left(2n-1\right)^2 \tag{19}$$

The first bound state appears

$$V_{0C}^{(1)}=\frac{\pi^2\hbar^2}{8md^2} \tag{20}$$

Note that this is somewhat different then the one dimensional case where there is always an even bound solution for an attractive potential. Our boundstate here corresponds to the first odd boundstate in the one dimensional case. This is a result of the $U\left(0\right)=0$ condition, which in effect requires that all solutions are odd.

1.1.4 iv: Deep well approximation

consider the limit $\alpha \to \infty$ for low energy states. In this limit $R_{outer} \to 0$. We now have the simple BC.

$$j_\ell\left(\kappa d\right)=0 \tag{21}$$

Bessel zeroes can be looked up in a table. I list some here

$n =$	1	2	3
$\ell = 0$	3.14	6.28	9.42
$\ell = 1$	4.49	7.73	10.9
$\ell = 2$	5.76	9.10	12.3
$\ell = 3$	6.99	10.4	
$\ell = 4$	8.20		
$\ell = 5$	9.35		

(22)

In atomic language. The lowest states are:
1s, 1p, 1d, 2s, 1f, 2p, 1g, 2d, 1h, 3s

1.2 b: continuum states

1.2.1 i

$$k^2 = \frac{2mE}{\hbar^2} \tag{23}$$

$$\kappa^2 = \frac{2m}{\hbar^2}\left(E + V_0\right) \tag{24}$$

$$R_\ell\left(r\right) = \begin{cases} Bj_\ell\left(kr\right) + Cn_\ell\left(kr\right) & d < r \\ Aj_\ell\left(\kappa r\right) & 0 < r \leq d \end{cases} \tag{25}$$

matching boundary conditions

$$j_\ell\left(\kappa d\right) = \frac{B}{A} j_\ell\left(kd\right) + \frac{C}{A} n_\ell\left(kd\right) \tag{26}$$

$$\kappa j_\ell'\left(\kappa d\right) = \frac{B}{A} k j_\ell'\left(kd\right) + \frac{C}{A} k n_\ell'\left(kd\right) \tag{27}$$

$$\kappa \frac{j_\ell'\left(\kappa d\right)}{j_\ell\left(\kappa d\right)} = k \frac{j_\ell'\left(kd\right) + \frac{C}{B} n_\ell'\left(kd\right)}{j_\ell\left(kd\right) + \frac{C}{B} n_\ell\left(kd\right)} \tag{28}$$

from the above expression $\frac{C}{B}$ can be calculated.

1.2.2 ii

$$R_\ell\left(r\right) \underbrace{\approx}_{r\to\infty} B\left[\frac{1}{kr}\sin\left(kr - \frac{\pi}{2}\ell\right) - \frac{C}{B}\frac{1}{kr}\cos\left(kr - \frac{\pi}{2}\ell\right)\right] \tag{29}$$

$$\underbrace{\approx}_{r\to\infty} \frac{1}{kr}\sin\left(kr - \frac{\pi}{2}\ell + \delta_\ell\right) \tag{30}$$

$$\underbrace{\approx}_{r\to\infty} \frac{1}{kr}\left[\sin\left(kr - \frac{\pi}{2}\ell\right)\cos\delta_\ell + \cos\left(kr - \frac{\pi}{2}\ell\right)\sin\delta_\ell\right] \tag{31}$$

therefore

$$\frac{C}{B} = -\tan\delta_\ell\left(k\right) \tag{32}$$

1.2.3 iii

For $\ell = 0$

$$R_0\left(r\right) = \begin{cases} \frac{1}{r}\left(B\sin kr - C\cos kr\right) & r > d \\ \frac{A}{r}\sin kr & 0 \leq r \leq d \end{cases} \tag{33}$$

¿From Continuity BC's

$$A\sin\kappa d = B\sin kd - C\cos kd \tag{34}$$

$$A\kappa\cos\kappa d = Bk\cos kd + Ck\sin kd \tag{35}$$

$$\kappa\cot\kappa d = k\frac{B\cos kd + C\sin kd}{B\sin kd - C\cos kd} \tag{36}$$

$$\frac{\kappa}{k}\cot\kappa d = \frac{\cot kd - \frac{C}{B}}{1 - \frac{C}{B}\cot kd} \tag{37}$$

$$\frac{\kappa}{k}\cot\kappa d - \cot kd = \frac{C}{B}\left(\frac{\kappa}{k}\cot\kappa d\cot kd - 1\right) \tag{38}$$

$$\frac{C}{B} = \frac{\frac{\kappa}{k}\cot\kappa d - \cot kd}{\frac{\kappa}{k}\cot\kappa d\cot kd - 1} \tag{39}$$

$$\frac{C}{B} = -\tan\delta_0\left(k\right) = \frac{\tan kd - \frac{k}{\kappa}\tan\kappa d}{1 - \frac{k}{\kappa}\tan kd\tan\kappa d} \tag{40}$$

define

$$\kappa_0 \equiv \sqrt{emV_0}\hbar^2 \tag{41}$$

$$x \equiv kd \tag{42}$$

$$x_0 \equiv \kappa_0 d \tag{43}$$

in terms of these new parameters

$$\kappa = \kappa_0\sqrt{1 + \left(\frac{k}{\kappa_0}\right)^2}\cot\delta_0 \qquad = \frac{\frac{x\tan x\tan\left[x_0\sqrt{1+\left(\frac{x}{x_0}\right)^2}\right]}{x_0\sqrt{1+\left(\frac{x}{x_0}\right)^2}} - 1}{x\left(1 + \frac{1}{3}x^2 - \frac{1}{x_0}\frac{\tan\left[x_0\sqrt{1-\left(\frac{x}{x_0}\right)^2}\right]}{\sqrt{1+\left(\frac{x}{x_0}\right)^2}}\right)} \tag{44}$$

one can expand this in terms of k

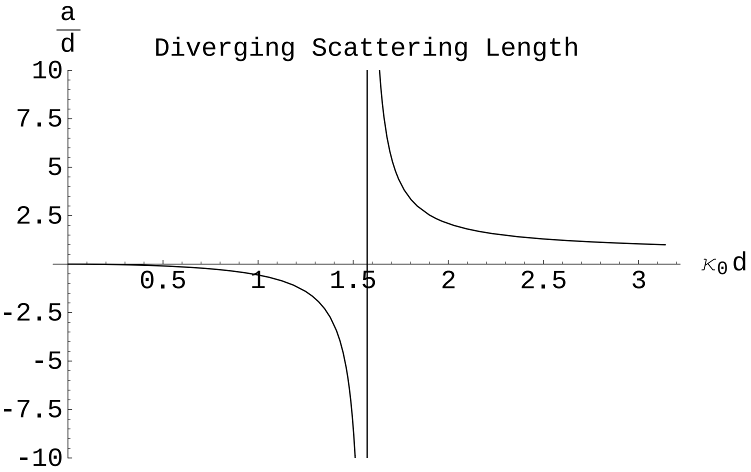
$$k\cot\delta_0 \approx -\frac{1}{a} + \frac{1}{2}r_0k^2 \tag{45}$$

$$a \equiv \left(1 - \frac{\tan \kappa_0 d}{\kappa_0 d}\right) d \tag{46}$$

$$r_0 \equiv \frac{2d\left(\frac{1}{\kappa_0 d}\tan \kappa_0 d + \frac{1/3 - \frac{1}{2\kappa_0^2 d^2} + \frac{\tan \kappa_0 d}{2(\kappa_0 d)^{3/2}} - \frac{\tan^2 \kappa_0 d}{2\kappa_0^2 d^2}}{1 - \frac{\tan \kappa_0 d}{\kappa_0 d}}\right)}{1 - \frac{\tan \kappa_0 d}{\kappa_0 d}} \tag{47}$$

$$a = d\left(1 - \frac{tan \kappa_0 d}{\kappa_0 d}\right) \tag{48}$$

$$r_0 = 2d\left[\frac{\frac{1}{\kappa_0 d}\tan \kappa_0 d}{1 - \tan \kappa_0 d} + \frac{\frac{1}{3} - \frac{1}{2\kappa_0^2 d^2} + \frac{\tan \kappa_0 d}{2(\kappa_0 d)^{3/2}} - \frac{\tan^2 \kappa_0 d}{2\kappa_0^2 d^2}}{\left(1 - \frac{\tan \kappa_0 d}{\kappa_0 d}\right)^2}\right] \tag{49}$$



Note that:

(1): scattering length a diverges (changing sign from negative to positive) at $\kappa_0 d = \frac{\pi}{2}$, which implies

$$\frac{2mV_0^* d^2}{\hbar^2} = \frac{\pi^2}{4} \Rightarrow V_0^* = \frac{\pi^2 \hbar^2}{8md^2} = V_{0C} \tag{50}$$

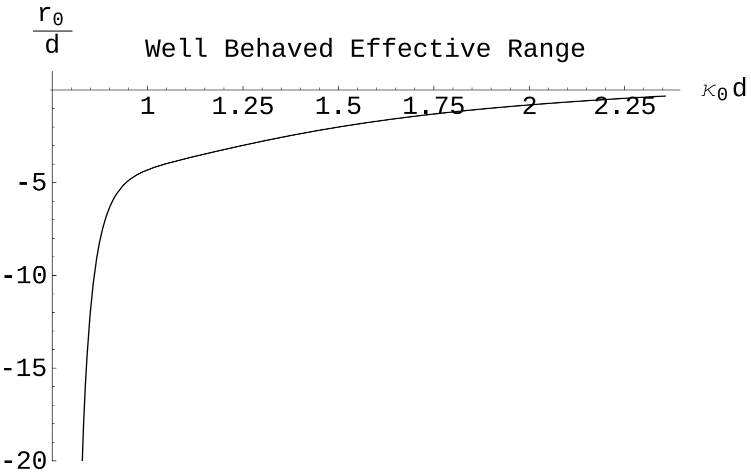
ie. $a \to \infty$ when $V_0 \to V_{0C}^-$ as a bound state comes in

(2): r_0 is smooth and finite near V_{0C}.

1.2.4 iv

for $V_0 \to \infty$, $\kappa_0 d \to \infty$.

$$a = d\left(1 - \frac{\tan \kappa_0 d}{\kappa_0 d}\right) \to d \tag{51}$$



1.2.5 v

$$\kappa \frac{j_\ell'(\kappa d)}{j_\ell(\kappa d)} = k \frac{j_{ell}'(kd) + \frac{C}{B} n_\ell'(kd)}{j_\ell(kd) + \frac{C}{B} n_\ell(kd)} \tag{52}$$

$$\kappa \frac{j_\ell'(\kappa d)}{j_\ell(\kappa d)} j_\ell(kd) + \kappa \frac{j_\ell'(\kappa d)}{j_\ell(\kappa d)} n_\ell(kd) \frac{C}{B} = k \left(j_\ell'(kd) + \frac{C}{B} n_\ell'(kd) \right) \tag{53}$$

$$\Rightarrow \frac{C}{B} \left(\kappa \frac{j_\ell(\kappa d)}{j_\ell(\kappa d)} n_\ell(kd) - k n_\ell'(kd) \right) = k j_\ell'(kd) - \kappa \frac{j_\ell'(\kappa d)}{j_\ell(\kappa d)} j_\ell(kd) \tag{54}$$

in the limit $kd \to \infty$

$$n_\ell(kd) \to -\frac{(kd)^\ell}{(2\ell+1)!!} \tag{55}$$

$$j_\ell(kd) \to \frac{(kd)^\ell}{(2\ell+1)!!} \tag{56}$$

$$\Rightarrow \frac{C}{B} \left(-\kappa_0 \frac{j_\ell(\kappa_0 d)}{j_\ell(\kappa_0 d)} \frac{(kd)^{-(\ell+1)}}{(2\ell+1)!!} - \frac{k(\ell+1)(kd)^{-(\ell+2)}}{(2\ell+1)!!} \right) \tag{57}$$

$$\approx \frac{\ell}{(2\ell+1)!!} k (kd)^{\ell-1} - \kappa_0 \frac{j_\ell'(\kappa_0 d)}{j_\ell(\kappa d)} \frac{(kd)^\ell}{(2\ell+1)!!} \tag{58}$$

solving the above expression for $\frac{C}{B}$.

$$\frac{C}{B} = -(kd)^{2\ell+1} \frac{\frac{\ell}{d} - \kappa_0 \frac{j_\ell'(\kappa_0 d)}{j_\ell(\kappa_0 d)}}{\frac{\ell+1}{d} + \kappa_0 \frac{j_\ell'(\kappa_0 d)}{j_\ell(\kappa_0 d)}} \tag{59}$$

so

$$\delta_\ell(k) \underbrace{\approx}_{kd\to 0} (kd)^{2\ell+1} \frac{\ell - \kappa_0 d \frac{j'_\ell(\kappa_0 d)}{j_\ell(\kappa_0 d)}}{\ell + 1 + \kappa_0 d \frac{j'_\ell(\kappa_0 d)}{j_\ell(\kappa_0 d)}} \tag{60}$$

$$\delta_\ell(k) \sim O\left(k^{2\ell+1}\right) \tag{61}$$

2 Problem 2: Hydrogen Atom

2.1 a

suppose

$$\Psi(r) = Ae^{-\frac{r}{r_0}} \tag{62}$$

$A = \sqrt{\frac{1}{\pi r_0^3}}$ can be found via normalization

The Probability to be in a state $\Psi_{m\ell m}$ is

$$P_{n\ell m} = \left|\langle \Psi_{n\ell m}|\Psi\rangle\right|^2 \tag{63}$$

$$= \left| \int_0^\infty dr r^2 R_{n\ell}(r)\Psi(r) \underbrace{\int_{-1}^{-1} d(\cos\theta) \int_0^{2\pi} d\phi Y_\ell^{m*}(\theta,\phi)}_{\sqrt{4\pi}\delta_{\ell,0}\delta_{m,0}} \right|^2 \tag{64}$$

$$P_{100} = \frac{(4\pi)^2}{\pi r_0^3} \left| \int_0^\infty dr r^2 \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} e^{-\frac{r}{r_0}} \right|^2 \tag{65}$$

$$= \left(\frac{16}{r_0^3 a_0^3}\right) \left| \int_0^\infty dr r^2 e^{-\left(\frac{1}{a_0}+\frac{1}{r_0}\right)r} \right|^2 \tag{66}$$

$$P_{100} = 64 \frac{a_0^3 r_0^3}{(a_0+r_0)^6} \tag{67}$$

$$P_{100}(\alpha) = 64 \frac{\alpha^3}{(\alpha+1)^6} \tag{68}$$

in which the $\alpha = \frac{r_0}{a_0}$.

$$P_{100}(\alpha = 1) = 1 \tag{69}$$

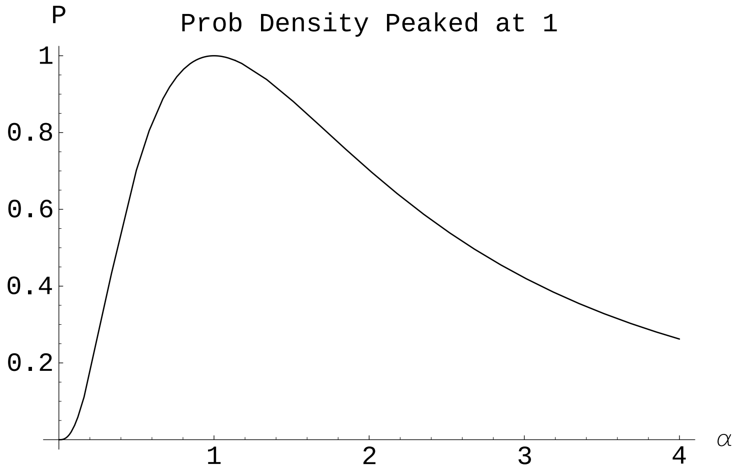
2.2 b

Ψ is separable

$$\Psi_{n\ell m} = R_{n\ell}(r) Y_\ell^m(\theta,\phi) \tag{70}$$

under parity $\vec{r} \to -\vec{r}$. In spherical coordinates $\theta \to \pi - \theta$, $\phi \to \phi + \pi$, and $r \to r$.

$$P\Psi_{n\ell m} = R_{n\ell}(r) Y_\ell^m(\pi - \theta, \phi + \pi) \tag{71}$$



Recall

$$Y_\ell^m = N_{\ell m} e^{\imath m\theta} \frac{1}{(\sin\theta)^m} \frac{d^{\ell-m}}{d(\cos\theta)^{\ell-m}} (\sin\theta)^{2\ell} \tag{72}$$

$$Y_\ell^m(\pi-\theta,\phi+\pi) = N_{\ell m} e^{\imath m\theta} e^{\imath m\pi} \frac{1}{(-\sin\theta)^m} \frac{d^{\ell-m}}{d(-\cos\theta)^{\ell-m}} (-\sin\theta)^{2\ell} \tag{73}$$

$$= (-1)^m (-1)^{\ell-m} Y_\ell^m \tag{74}$$

$$P\Psi_{n\ell m} = (-1)^\ell \Psi_{n\ell m} \tag{75}$$

3 Problem 3: Angular Momentum

3.1 a:$\vec{\sigma}$

Recall

$$J_\pm |j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\, |j, m\pm 1\rangle \tag{76}$$

$$J_z |j,m\rangle = \hbar m |j,m\rangle \tag{77}$$

and that

$$J_\pm = J_x \pm \imath J_y \tag{78}$$

$$J_x = \frac{1}{2}(J_+ + J_-) \tag{79}$$

$$J_y = \frac{1}{2\imath}(J_+ - J_-) \tag{80}$$

consider a spin-$\frac{1}{2}$ particle. ($j = \frac{1}{2}$ and $m \in \left\{-\frac{1}{2}, \frac{1}{2}\right\}$). Then

$$\begin{aligned} \langle jm \left| J_x \right| jm' \rangle &\equiv J^x_{mm'} && (81) \\ &= \frac{\hbar}{2}\left(\sqrt{\frac{3}{4}+\frac{1}{4}}\delta_{m,m-1} + \sqrt{\frac{3}{4}+\frac{1}{4}}\delta_{m,m+1}\right) && (82) \\ \langle jm \left| J_x \right| jm' \rangle &\equiv \frac{\hbar}{2}\sigma_x && (83) \end{aligned}$$

likewise

$$J^y_{m,m'} = \frac{\hbar}{2\imath}\left(\delta_{m,m-1} - \delta_{m,m+1}\right) \equiv \frac{\hbar}{2}\sigma_y \quad (84)$$

$$J^z_{m,m'} = \hbar m \delta_{m,m'} \equiv \frac{\hbar}{2}\sigma_z \quad (85)$$

Therefore

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix} \qquad (86)$$
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

3.2 b

$$\begin{aligned} \left[\sigma_i, \sigma_j\right] &= 2\imath\epsilon_{ijk}\sigma_k && (87) \\ \left\{\sigma_i, \sigma_j\right\} &= 2\delta_{ij} && (88) \end{aligned}$$

3.2.1 i

$$\begin{aligned} 2\sigma_i\sigma_j &= \left[\sigma_i, \sigma_j\right] + \left\{\sigma_i, \sigma_j\right\} && (89) \\ &= 2\delta_{ij} + 2\imath\epsilon_{ijk}\sigma_k && (90) \\ Tr\left[\sigma_i\sigma_j\right] &= 2\delta_{ij} && (91) \end{aligned}$$

3.2.2 ii

$$\begin{aligned} \left(\vec{a}\cdot\vec{\sigma}\right)\left(\vec{b}\cdot\vec{\sigma}\right) &= a_i b_j \sigma_i \sigma_j && (92) \\ &= a_i b_j \left(\delta_{ij} + \imath\epsilon_{ijk}\sigma_k\right) && (93) \\ \left(\vec{a}\cdot\vec{\sigma}\right)\left(\vec{b}\cdot\vec{\sigma}\right) &= \vec{a}\cdot\vec{b} + \imath\left(\vec{a}\times\vec{b}\right)\cdot\vec{\sigma} && (94) \end{aligned}$$

3.3 c

$$\begin{aligned} \hat{n}\cdot\vec{\sigma} &= n_x\sigma_x + n_y\sigma_y + n_z\sigma_z && (95) \\ \hat{n}\cdot\vec{\sigma} &= \begin{pmatrix} \cos\theta & \sin\theta e^{-\imath\phi} \\ \sin\theta e^{\imath\phi} & -\cos\theta \end{pmatrix} && (96) \end{aligned}$$

3.3.1 i: eigen values and vectors

$$\begin{vmatrix} \cos\theta - \lambda & \sin\theta e^{-\imath\phi} \\ \sin\theta e^{\imath\phi} & -\left(\cos\theta + \lambda\right) \end{vmatrix} = 0 \tag{97}$$

$$\Rightarrow \lambda = \pm 1 \tag{98}$$

Finding eigen vectors

$$\left(\cos\theta - 1\right)\alpha_+ + \sin\theta e^{-\imath\phi}\beta_+ = 0 \tag{99}$$

$$\left(-2\sin^2\frac{\theta}{2}\right)\alpha_+ + 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-\imath\phi}\beta_+ = 0 \tag{100}$$

$$\Rightarrow \Psi_+^{\hat{n}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{\imath\phi}\sin\frac{\theta}{2} \end{pmatrix} \tag{101}$$

$$\left(\cos\theta + 1\right)\alpha_- + \sin\theta e^{-\phi}\beta_- = 0 \tag{102}$$

$$\left(2\cos^2\frac{\theta}{2}\right)\alpha_- + 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-\imath\phi}\beta_- = 0 \tag{103}$$

$$\Rightarrow \Psi_-^{\hat{n}} = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{\imath\phi}\cos\frac{\theta}{2} \end{pmatrix} \tag{104}$$

3.3.2 ii: rotating

$$e^{-\imath\frac{\theta}{2}\hat{\theta}\cdot\vec{\sigma}} = \cos\frac{\theta}{2} - \imath\hat{\theta}\cdot\vec{\sigma}\sin\frac{\theta}{2} \tag{105}$$

$$= \begin{pmatrix} \cos\frac{\theta}{2} - \imath\hat{\theta}_z\sin\frac{\theta}{2} & \left(-\imath\hat{\theta}_x - \hat{\theta}_y\right)\sin\frac{\theta}{2} \\ \left(-\imath\hat{\theta}_x + \hat{\theta}_y\right)\sin\frac{\theta}{2} & \cos\frac{\theta}{2} + \imath\hat{\theta}_z\sin\frac{\theta}{2} \end{pmatrix} \tag{106}$$

$$\hat{\theta} = \frac{\hat{z}\times\hat{n}}{\left|\hat{z}\times\hat{n}\right|} = \frac{1}{\sqrt{n_x^2 + n_y^2}}\left(-n_y\hat{x} + n_y\hat{y}\right) \tag{107}$$

where $\hat{n} \equiv \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta$.

$$\hat{\theta} = -\sin\phi\hat{x} + \cos\phi\hat{y} \tag{108}$$

so

$$e^{-\imath\frac{\theta}{2}\hat{\theta}\cdot\vec{\sigma}} = \begin{pmatrix} \cos\frac{\theta}{2} & -e^{-\imath\phi}\sin\frac{\theta}{2} \\ e^{\imath\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \tag{109}$$

Eigenvectors through rotation

$$\Psi_+^{\hat{n}} = e^{-\imath\frac{\theta}{2}\hat{\theta}\cdot\vec{\sigma}}\Psi_+^{\hat{z}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{\imath\theta}\sin\frac{\theta}{2} \end{pmatrix} \tag{110}$$

$$\Psi_-^{\hat{n}} = e^{-\imath \frac{\theta}{2} \hat{\theta} \cdot \vec{\sigma}} = \begin{pmatrix} -\sin\frac{\theta}{2} e^{-\imath\phi} \\ \cos\frac{\theta}{2} \end{pmatrix} \tag{111}$$

In operator language

$$\left(\hat{n} \cdot \vec{\sigma}\right) U_{\hat{n}} U_{\hat{n}}^{\dagger} \Psi_{\pm}^{\hat{n}} = \lambda_{\pm} \Psi_{\pm}^{\hat{n}} \tag{112}$$

$$\underbrace{U_{\hat{n}}^{\dagger} \left(\hat{n} \cdot \vec{\sigma}\right) U_{\hat{n}}}_{\sigma_z} \left(U_{\hat{n}}^{\dagger} \Psi_{\pm}^{\hat{n}}\right) = \lambda_{\pm} \left(U_{\hat{n}}^{\dagger} \Psi_{\pm}^{\hat{n}}\right) \tag{113}$$

$$\sigma_z \left(U_{\hat{n}}^{\dagger} \Psi_{\pm}^{\hat{n}}\right) = \pm \left(U_{\hat{n}}^{\dagger} \Psi_{\pm}^{\hat{n}}\right) \tag{114}$$

eigenvectors

$$\Psi_+^{\hat{n}} = U_{\hat{n}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{115}$$

$$\Psi_-^{\hat{n}} = U_{\hat{n}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{116}$$

3.4 d: Eigenvalues and vectors of $S_x + S_z$ for $S = \frac{\hbar}{2}$

suppose

$$O = S_x + S_z = \frac{\hbar}{2} \left(\sigma_x + \sigma_z\right) = \frac{\hbar}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{117}$$

Eigenvalues from the characteristic equation

$$-1 + \lambda^2 - 1 = 0 \Rightarrow \lambda_{\pm} = \pm\sqrt{2} \tag{118}$$

where

$$\hat{n} = \frac{1}{\sqrt{2}} \left(\hat{x} + \hat{z}\right) \tag{119}$$

or $\phi = 0$, $\theta = \frac{\pi}{4}$. We calculate the eigenvectors directly

$$\left(1 - \sqrt{2}\right) \alpha + \beta = 0 \tag{120}$$

$$\Psi_+ = N \begin{pmatrix} -1 \\ 1 - \sqrt{2} \end{pmatrix} \tag{121}$$

$$\Psi_- = N \begin{pmatrix} 1 - \sqrt{2} \\ 1 \end{pmatrix} \tag{122}$$

where $N = \frac{1}{\sqrt{1+1+2-2\sqrt{2}}} = \frac{1}{\sqrt{4-2\sqrt{2}}}$. This agrees with the result we get by rotating the eigenvectors of σ_z.

$$\Psi_+ = \begin{pmatrix} \cos\frac{\pi}{8} \\ \sin\frac{\pi}{8} \end{pmatrix} = \begin{pmatrix} \sqrt{\left(\cos\pi 4 + 1\right)/2} \\ \sqrt{\left(1 - \cos\frac{\pi}{2}\right)/2} \end{pmatrix} \quad = \frac{1}{2} \frac{1}{\sqrt{1 - 1/\sqrt{2}}} \begin{pmatrix} 1 \\ -\left(1 - \sqrt{2}\right) \end{pmatrix} \tag{123}$$

So the probability that we measure the system to be in the up state is

$$P_+ = \cos^2 \frac{\pi}{8} \approx 0.85 \tag{124}$$

3.5 e: spin precession

$$H = -\vec{\mu} \cdot \vec{B} = g \frac{e}{2mc} \vec{S} \cdot \vec{B} \tag{125}$$

3.5.1 i: Heisenberg

The Heisenberg equations of motion

$$\imath\hbar \dot{O}_i = [O_i, H] \tag{126}$$

In this case

$$\begin{aligned} \imath\hbar \partial_t S_i &= [S_i, H] && (127) \\ &= [S_i, S_j] \frac{ge}{2mc} B_j && (128) \\ &= \imath\hbar \epsilon_{ijk} S_k B_j \frac{ge}{2mc} && (129) \\ \partial_t \vec{S} &= \left(\frac{ge}{2mc}\right) \vec{B} \times \vec{S} && (130) \end{aligned}$$

The frequency can be read off the differential equations above

$$\omega_0 = \frac{ge}{2mc} B \tag{131}$$

Note that $\vec{S} \cdot \vec{B}$ does not change with time. (the S_B component is fixed). They is perhaps easier to see if we re-write the above differential equations as two independent harmonic oscillators.

$$\begin{aligned} \partial_t S_x &= -\omega_0 S_y && (132) \\ \partial_t S_y &= \omega_0 S_x && (133) \end{aligned}$$

plugging one into the other

$$\begin{aligned} \partial_t^2 S_x &= -\omega_0^2 S_x && (134) \\ \partial_t^2 S_y &= -\omega_0^2 S_y && (135) \end{aligned}$$

The solution is

$$\begin{pmatrix} S_x(t) \\ S_y(t) \\ S_z(t) \end{pmatrix} = \begin{pmatrix} \cos\omega_0 t & -\sin\omega_0 t & 0 \\ \sin\omega_0 t & \cos\omega_0 t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} S_x(0) \\ S_y(0) \\ S_z(0) \end{pmatrix} \tag{136}$$

3.5.2 ii

suppose $\Psi_+\left(0\right) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Then

$$\Psi_+\left(t\right) = \left(\cos\frac{\omega_0 t}{2} - \imath\hat{B}\cdot\vec{\sigma}\sin\frac{\omega_0 t}{2}\right)\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{137}$$

where $\omega_0 = \frac{g\mu_B B}{\hbar} = \frac{g\mu_b}{\hbar}\sqrt{B_x^2 + B_y^2}$.

$$\Psi_+\left(t\right) = \begin{pmatrix} \cos\frac{\omega_0 t}{2} - \imath\frac{Bz}{B_x^2+B_z^2}\sin\frac{\omega_0 t}{2} \\ -\imath\frac{B_x}{\sqrt{B_x^2+B_z^2}}\sin\frac{\omega_0 t}{2} \end{pmatrix} \tag{138}$$

Therefore

$$P_+\left(t\right) = \cos^2\frac{\omega_0 t}{2} + \frac{B_z^2}{B_x^2 + B_z^2}\sin^2\frac{\omega_0 t}{2} \tag{139}$$

$$P_+\left(t\right) = \frac{1}{2}\left(1 + \frac{B_z^2}{B_x^2 + B_z^2}\right) + \frac{1}{2}\left(\frac{B_x^2}{B_x^2 + B_z^2}\right)\cos\omega_0 t \tag{140}$$

The Probability oscillates with frequency ω_0 and amplitude $A = \frac{1}{2}\frac{B_x^2}{B_x^2+B_z^2}$. We now check the limits of this solution to see if it makes sense

$$P_+\left(t = 0\right) = 1 \tag{141}$$

$$B_x = 0 \Rightarrow P_+ = 1 \tag{142}$$

$$B_z = 0 \Rightarrow P_+ = \frac{1}{2}\left(1 + \cos\omega_0 t\right) \tag{143}$$

This problem is trivial in the $\hat{B}$-basis. Recall

$$\Psi_+^{\hat{B}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{\imath\phi}\sin\frac{\theta}{2} \end{pmatrix} \tag{144}$$

$$\Psi_-^{\hat{B}} = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{\imath\phi}\cos\frac{\theta}{2} \end{pmatrix} \tag{145}$$

There is not a B_y-component so $\phi = 0$. In this basis the time dependence is trivial

$$\Psi_+\left(t\right) = \alpha\Psi_+^{\hat{B}}\left(0\right)e^{-\frac{\imath\omega_0 t}{2}} + \beta\Psi_-^{\hat{B}}\left(0\right)e^{\frac{\imath\omega_0 t}{2}} \tag{146}$$

with $\alpha = \cos\frac{\theta}{2}$ and $\beta = \sin\frac{\theta}{2}$. One can write the above in terms of the magnetic field components with the help of the following trig identities,

$$\cos^2\frac{\theta}{2} = \frac{1}{2}\left(\cos\theta + 1\right) \tag{147}$$

$$\cos\frac{\theta}{2}\sin\frac{\theta}{2} = \frac{1}{2}\sin\theta \tag{148}$$

$$\tag{149}$$

and by using

$$\cos\theta = \frac{B_z}{\sqrt{B_x^2 + B_z^2}} \tag{150}$$

$$\sin\theta = \frac{B_x}{\sqrt{B_x^2 + B_z^2}} \tag{151}$$

$$\Psi_+(t) = \begin{pmatrix} \cos^2\frac{\theta}{2} e^{-\imath\omega_0 t/2} + \sin^2\frac{\theta}{2} e^{\imath\omega_0 t/2} \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(e^{-\imath\omega_0 t/2} - e^{\imath\omega_0 t/2}\right) \end{pmatrix} \tag{152}$$

$$= \begin{pmatrix} \frac{1}{2}(\cos\theta + 1)(-2\imath)\sin\frac{\omega_0 t}{2} + e^{\imath\omega_0 t/2} \\ -\imath\sin\theta\sin\omega_0 t/2 \end{pmatrix} \tag{153}$$

$$\Psi_+(t) = \begin{pmatrix} \cos\frac{\omega_0 t}{2} - \imath\frac{B_z}{\sqrt{B_x^2+B_z^2}}\sin\frac{\omega_0 t}{2} \\ -\imath\frac{B_x}{\sqrt{B_x^2+B_z^2}}\sin\frac{\omega_0 t}{2} \end{pmatrix} \tag{154}$$

3.6 f

The Maximum eigen value of $S_{tot}^2 = \hbar^2 S_{tot}(S_{tot}+1)$.

Where $S_{tot} = \underbrace{\frac{1}{2} + \frac{1}{2} + \cdots + \frac{1}{2}}_{N} = \frac{N}{2}$. In ket form

$$\left|\frac{N}{2}, \frac{N}{2}\right\rangle = \left|\frac{1}{2}\frac{1}{2}\right\rangle\left|\frac{1}{2}\frac{1}{2}\right\rangle\cdots\left|\frac{1}{2}\frac{1}{2}\right\rangle \tag{155}$$

which is symmetric. The lowering operator

$$S_{tot}^- = S_{tot}^{(x)} - \imath S_{tot}^{(y)} \tag{156}$$

$$= \left(S_1^- + S_2^- + S_3^- + \cdots + S_N^-\right) \tag{157}$$

is also symmetric, which means that

$$\left(S_{tot}^-\right)^n \left|\frac{N}{2}\frac{N}{2}\right\rangle = \left|\frac{N}{2}, \frac{N}{2} - n\right\rangle \tag{158}$$

must also be symmetric.

3.7 g

$$H_d = \frac{1}{r^3}\left[\vec{\mu}_1\cdot\vec{\mu}_2 - 3(\vec{\mu}_1\cdot\hat{r})(\vec{\mu}_2\cdot\hat{r})\right] \tag{159}$$

we choose $\hat{z}$ to be in the same direction as $\hat{r}$.

$$H_d = -\frac{\left(g\mu_B^P\right)^2}{\hbar^2 a^3}\left[\vec{S}_1\cdot\vec{S}_2 - 3S_{1z}S_{2z}\right] \tag{160}$$

$$\left(\vec{S}_1+\vec{S}_2\right)^2 = S_1^2+S_2^2+2\vec{S}_1\cdot\vec{S}_2^2 \tag{161}$$

$$S^2=\hbar^2 S\left(S+1\right)=\hbar^2 S_1\left(S_1+1\right)+\hbar^2 S_2\left(S_2+1\right)+2\vec{S}_1\vec{S}_2 \tag{162}$$

$$\left(S_{1z}+S_{2z}\right)^2=S_{1z}^2+S_{2z}^2+2S_{1z}S_{2z}=S_z^2 \tag{163}$$

so

$$H_d=-\frac{\left(g\mu_B^P\right)^2}{a^3}\left[\frac{1}{2}S\left(S+1\right)-\frac{1}{2}S_1\left(S_1+1\right)-\frac{1}{2}S_2\left(S_2+1\right)-\frac{3}{2}\left(S_z^2-S_{1z}^2-S_{2z}^2\right)\right] \tag{164}$$

$$H_d=-\frac{\left(g\mu_B^P\right)^2}{2a^3}\left[S\left(S+1\right)-\frac{3}{2}-3\left(S_z^2-\frac{1}{2}\right)\right] \tag{165}$$

$$H_d\left|S,S_z;S_1,S_2\right\rangle E_{S,S_z}\left|S,S_z;S_1,S_2\right\rangle \tag{166}$$

$$\begin{array}{r} S=0;1 \\ S_z=0;0,\pm1 \end{array}\left\{\Rightarrow E_{S,S_z}=-2\frac{\mu_B^{(P)2}}{a^3}\left(S\left(S+1\right)-s_z^2\right)\right. \tag{167}$$

Energy levels are

$$E_{0,0}=0 \tag{168}$$

$$E_{1,0}=-\frac{4\mu_B^{(P)2}}{a^3} \tag{169}$$

$$E_{1,\pm1}=\frac{2\mu_B^{(P)2}}{a^3} \tag{170}$$

4 Problem 4: 3D charge particle in constant B-field

4.1 a

$$H=\left(\vec{p}-\frac{q\vec{A}}{c}\right)^2/2m \tag{171}$$

$$\vec{A}=\frac{1}{2}\vec{B}\times\vec{r}=\begin{pmatrix}-\frac{By}{2}\\ \frac{Bx}{2}\\ 0\end{pmatrix} \tag{172}$$

we use the the radiation gauge $\vec{\nabla}\cdot A=0$, in which case $\vec{p}\cdot\vec{A}=\vec{A}\cdot\vec{p}$.

$$H=\frac{p^2}{2m}-\frac{q}{2mc}\underbrace{(\vec{B}\times\vec{r})\cdot\vec{p}}_{\vec{r}\times\vec{p}\cdot\vec{B}}+\frac{q^2B^2}{8mc^2}\left(x^2+y^2\right) \tag{173}$$

$$=\frac{P_{perp}^2}{2m}-\frac{q}{2mc}BL_z+\frac{q^2B^2}{8mc^2}r_{perp}^2-\frac{p_z^2}{2m} \tag{174}$$

$$H\left|k_z\right\rangle = \left(\frac{p_{perp}^2}{2m} + \frac{q^2B^2}{8mc^2}r_{perp}^2 - \frac{qB}{2mc}L_z + \frac{\hbar^2k_z^2}{2m}\right)\left|k_z\right\rangle = E\left|k_z\right\rangle \tag{175}$$

This is an effective 2D H.O. with an extra $-\frac{qB}{2mc}L_z$ term.

$$H_{2D}\left|E_2D\right\rangle = E_{2D}\left|E_{2D}\right\rangle \tag{176}$$

$$E_{2D} + \frac{\hbar^2k_z^2}{2m} = E \tag{177}$$

$$H_{2D} = \frac{p_{perp}^2}{2m} + \frac{m\omega_0^2}{2}r_{perp}^2 - \Omega L_z \tag{178}$$

with

$$\omega_0 = \frac{qB}{2mc} \tag{179}$$

$$\Omega = \frac{qB}{2mc} \tag{180}$$

4.2 b

This has energy spectrum

$$E_{n,m} = \hbar\omega_0\left(n+1\right) \tag{181}$$

note that when $4\omega_0 = \Omega = \frac{1}{2}\omega_B$ that the Landau levels are spaced $\hbar\omega_B$ apart. This agrees with our result done in Cartesian coordinates.

4.3 c

Compare $-\frac{qB}{2mc}L_z$ and diamagnetic $\frac{q^2B^2}{8mc^2}r_{perp}^2$ for an e^- in an atom.

$$R = \frac{\frac{q^2B^2}{8mc^2}\left\langle r_{perp}^2\right\rangle}{\frac{qB}{2mc}\left\langle L_Z\right\rangle} = \frac{qBa_0^2}{4\hbar c} \tag{182}$$

become comparable for $R \approx 1$.

$$B_* = \frac{\hbar c}{ea_0^2} \tag{183}$$

$$R = \frac{e^2}{4\hbar c}\frac{B}{e/a_0^2} = \frac{B * \left(0.5 * 10^{-8}cm\right)^2}{4 * 137 * 4.8 * 10^{-10}esu} \tag{184}$$

$$R \approx \frac{B}{9 * 10^9 Guass} \tag{185}$$

$$B_* \sim 9 \times 10^9 Gauss \tag{186}$$

under typical conditions $B \ll B_*$, which means diamagnetic term is negligible in atomic physics.