1 Problem 1

A particle of mass m is moving on a sphere of radius a. Its wave function is given by $\psi(\theta, \phi)$ where θ and ϕ parameterize the sphere $(x, y, z) = a(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. The Hamiltonian of the system is $H = \mathbf{L}^2/2ma^2$, where \mathbf{L}^2 is the square of the angular momentum operator, and is given by

$$\mathbf{L}^{2} = -\hbar^{2} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} \right).$$

The eigenfunctions of H are spherical harmonics Y_m^l with energies

$$E_l = \frac{\hbar^2 l(l+1)}{2ma^2}. (1)$$

1.1 The wave function of the system at t = 0 is given by

$$\psi(\theta, \phi, 0) = A\sin^2\theta \cos^2\phi,$$

where A is a constant. This wave function can be expanded in spherical harmonics:

$$\psi(\theta, \phi, 0) = \sum_{l,m} a_m^l Y_m^l(\theta, \phi).$$

Find all nonzero a_m^l .

Solution. We will look for nonzero a_m^l by comparing the θ and ϕ dependence of Y_m^l and $\psi(\theta, \phi, 0)$. From (3.6.36) and (3.6.37) in Sakurai, the spherical harmonic functions are given by

$$Y_{m}^{l}(\theta,\phi) = \frac{(-1)^{l}}{2^{l} l!} \sqrt{\frac{(2l+1)}{4\pi} \frac{(l+m)!}{(l-m)!} \frac{e^{im\phi}}{\sin^{m} \theta} \frac{d^{l-m} (\sin \theta)^{2l}}{d(\cos \theta)^{l-m}}}, \qquad Y_{-m}^{l}(\theta,\phi) = (-1)^{m} Y_{m}^{l*}(\theta,\phi)$$

for $m \geq 0$. Beginning with the ϕ dependence of $\psi(\theta, \phi, 0)$, note that

$$\psi(\theta, \phi, 0) \propto \cos^2 \phi = \left(\frac{e^{i\phi} + e^{-i\phi}}{2}\right)^2 = \frac{1}{2} + \frac{e^{i2\phi}}{4} + \frac{e^{-i2\phi}}{4},$$
 (2)

which implies that the only nonzero a_m^l correspond to $m \in \{0, \pm 2\}$.

For the θ dependence, we have $\psi(\theta, \phi, 0) \propto \sin^2 \theta$. Looking at Y_m^l , note that $(\sin \theta)^{2l} = (1 - \cos^2 \theta)^l$, so

$$Y_m^l \propto \frac{1}{\sin^m \theta} \frac{d^{l-m} (1 - \cos^2 \theta)^l}{d(\cos \theta)^{l-m}}.$$

Plugging in m = 0 and the first few values of l,

$$\begin{split} Y_0^0 &\propto \frac{d^0 (1-\cos^2\theta)^0}{d(\cos\theta)^0} = 1, \\ Y_0^1 &\propto \frac{d(1-\cos^2\theta)}{d(\cos\theta)} = -2\cos\theta, \\ Y_0^2 &\propto \frac{d^2 (1-2\cos^2\theta+\cos^4\theta)}{d(\cos\theta)^2} = \frac{d(-4\cos\theta+4\cos^3\theta)}{d(\cos\theta)} = -4+12\cos^2\theta = 8-12\sin^2\theta, \end{split}$$

so we know $a_0^1=0$. Inspecting the above, we deduce that Y_0^l with l>2 contain mixed terms of $\sin\theta$ and $\cos\theta$ and higher powers of $\sin\theta$, so $a_0^l=0$ for l>2.

Plugging in $m = \pm 2$ and l = 2,

$$Y_{\pm 2}^2 \propto \frac{1}{\sin^2 \theta} \frac{d^0 (1 - \cos^2 \theta)^2}{d(\cos \theta)^0} = \frac{\sin^4 \theta}{\sin^2 \theta} = \sin^2 \theta.$$

Again, by inspection $Y_{\pm 2}^l$ with l>2 contain terms that are not in $\psi(\theta,\phi,0)$, so $a_{\pm 2}^l=0$ for l>2 as well.

Thus, only a_0^0, a_0^2 , and $a_{\pm 2}^2$ are nonzero; that is,

$$\psi(\theta,\phi,0) = a_0^0 Y_0^0 + a_0^2 Y_0^2 + a_2^2 Y_2^2 + a_{-2}^2 Y_{-2}^2$$

The relevant spherical harmonics are

$$Y_0^0 = \sqrt{\frac{1}{4\pi}}, \qquad Y_0^2 = \sqrt{\frac{5}{16\pi}}(2 - 3\sin^2\theta), \qquad Y_{\pm 2}^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi}.$$
 (3)

Expanding out $\psi(\theta, \phi, 0)$ as in (2),

$$\psi(\theta, \phi, 0) = \frac{A}{2}\sin^2\theta + \frac{A}{4}\sin^2\theta e^{i2\phi} + \frac{A}{4}\sin^2\theta e^{-i2\phi}.$$

Then we can deduce the nonzero a_m^l :

$$\frac{A}{4}\sin^2\theta e^{\pm i2\phi} = a_{\pm 2}^2 \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi} \implies a_{\pm 2}^2 = A\sqrt{\frac{2\pi}{15}},$$

$$\frac{A}{2}\sin^2\theta = a_0^0 \sqrt{\frac{1}{4\pi}} + a_0^2 \sqrt{\frac{5}{16\pi}}(2 - 3\sin^2\theta) \implies a_0^2 = -\frac{2}{3}A\sqrt{\frac{\pi}{5}}, \ a_0^0 = \frac{2}{3}A\sqrt{\pi}.$$

1.2 Now consider the wave function at nonzero time t. Use your results from 1.1 and the expressions for spherical harmonics to derive an explicit expression in terms of sines and cosines of θ and ϕ for $\psi(\theta, \phi, t)$.

Solution. From 1.1, we have

$$\psi(\theta,\phi,0) = \frac{2}{3}A\sqrt{\pi}Y_0^0 - \frac{2}{3}A\sqrt{\frac{\pi}{5}}Y_0^2 + A\sqrt{\frac{2\pi}{15}}Y_2^2 + A\sqrt{\frac{2\pi}{15}}Y_{-2}^2.$$
 (4)

We can evaluate the time evolution for each spherical harmonic term in (4) individually, and sum them up to find $\psi(\theta, \phi, t)$:

$$\psi(\theta,\phi,t) = U(t)\psi(\theta,\phi,0) = \frac{2}{3}A\sqrt{\pi}\,U(t)Y_0^0 - \frac{2}{3}A\sqrt{\frac{\pi}{5}}\,U(t)Y_0^2 + A\sqrt{\frac{2\pi}{15}}\,U(t)Y_2^2 + A\sqrt{\frac{2\pi}{15}}\,U(t)Y_{-2}^2$$

The time evolution operator is given by $U(t) = e^{-iHt/\hbar}$. From (1), the relevant eigenvalues are

$$E_0 = 0,$$
 $E_2 = 3\frac{\hbar^2}{ma^2},$

SO

$$U(t)Y_0^0 = \exp\left(-\frac{i}{\hbar}E_0t\right)Y_0^0 = Y_0^0, \qquad U(t)Y_m^2 = \exp\left(-\frac{i}{\hbar}E_2t\right)Y_m^2 = \exp\left(-3i\frac{\hbar}{ma^2}t\right)Y_m^2.$$

Then, using the explicit Y_m^l from (3),

$$\psi(\theta,\phi,t) = \frac{2}{3}A\sqrt{\pi}\sqrt{\frac{1}{4\pi}} - \frac{2}{3}A\sqrt{\frac{\pi}{5}}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sqrt{\frac{5}{16\pi}}(2-3\sin^2\theta) + A\sqrt{\frac{2\pi}{15}}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{2i\phi} + A\sqrt{\frac{2\pi}{15}}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{-2i\phi}$$

$$= \frac{A}{3} - \frac{A}{6}\exp\left(-3i\frac{\hbar}{ma^2}t\right)(2-3\sin^2\theta) + \frac{A}{4}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sin^2\theta e^{2i\phi} + \frac{A}{4}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sin^2\theta e^{-2i\phi}$$

$$= \frac{A}{3} - \frac{A}{3}\exp\left(-3i\frac{\hbar}{ma^2}t\right) + \frac{A}{2}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sin^2\theta + \frac{A}{2}\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sin^2\theta\cos 2\phi$$

$$= \frac{A}{3}\left[1-\exp\left(-3i\frac{\hbar}{ma^2}t\right)\right] + A\exp\left(-3i\frac{\hbar}{ma^2}t\right)\sin^2\theta\cos^2\phi. \tag{5}$$

1.3 Use your results from 1.2 to derive expressions for the expected values of L_x , L_y , and L_z as functions of time.

Solution. From (3.6.23) in Sakurai, $\langle \theta, \phi | l, m \rangle = Y_m^l(\theta, \phi)$ and therefore $\psi(\theta, \phi, t) = \langle \theta, \phi | \psi(t) \rangle$. Using the result of 1.2, this implies

$$|\psi(t)\rangle = a_0^0 |0,0\rangle + a_0^2 \exp\left(-3i\frac{\hbar}{ma^2}t\right) |2,0\rangle + a_2^2 \exp\left(-3i\frac{\hbar}{ma^2}t\right) |2,2\rangle + a_{-2}^2 \exp\left(-3i\frac{\hbar}{ma^2}t\right) |2,-2\rangle.$$

Then the time-dependent expectation value of an operator O is given by

$$\begin{split} \langle \psi(t)|O|\psi(t)\rangle &= a_0^{0^2} \, \langle 0,0|O|0,0\rangle + a_0^0 a_0^2 U(t) \, \langle 0,0|O|2,0\rangle + a_0^0 a_2^2 U(t) \, \langle 0,0|O|2,2\rangle + a_0^0 a_{-2}^2 U(t) \, \langle 0,0|O|2,-2\rangle \\ &\quad + a_0^0 a_0^2 U^\dagger(t) \, \langle 2,0|O|0,0\rangle + a_0^{2^2} \, \langle 2,0|O|2,0\rangle + a_0^2 a_2^2 \, \langle 2,0|O|2,2\rangle + a_0^2 a_{-2}^2 \, \langle 2,0|O|2,-2\rangle \\ &\quad + a_0^0 a_2^2 U^\dagger(t) \, \langle 2,2|O|0,0\rangle + a_0^2 a_2^2 \, \langle 2,2|O|2,0\rangle + a_2^{2^2} \, \langle 2,2|O|2,2\rangle + a_2^2 a_{-2}^2 \, \langle 2,2|O|2,-2\rangle \\ &\quad + a_0^0 a_{-2}^2 U^\dagger(t) \, \langle 2,-2|O|0,0\rangle + a_0^2 a_{-2}^2 \, \langle 2,-2|O|2,0\rangle + a_2^2 a_{-2}^2 \, \langle 2,-2|O|2,2\rangle + a_{-2}^2 \, \langle 2,-2|O|2,-2\rangle \,, \end{split}$$

where $U(t) = e^{-3i\hbar t/ma^2}$ and $U^{\dagger}(t) = e^{3i\hbar t/ma^2}$.

From the results of 3.3 on the previous homework.

$$0 = \langle 2, -2|L_i|2, -2 \rangle = \langle 2, -2|L_i|2, 0 \rangle = \langle 2, -2|L_i|2, 2 \rangle$$

= $\langle 2, 0|L_i|2, -2 \rangle = \langle 2, 0|L_i|2, 0 \rangle = \langle 2, 0|L_i|2, 2 \rangle$
= $\langle 2, 2|L_i|2, -2 \rangle = \langle 2, 2|L_i|2, 0 \rangle = \langle 2, 2|L_i|2, 2 \rangle$

for $i \in \{x, y, z\}$. For (l, m) = (0, 0), a similar procedure to the one used for 3.3 yields

$$\langle l', m' | L_x | 0, 0 \rangle = \langle 0, 0 | L_x | l', m' \rangle = \frac{\hbar}{2} \delta_{0, l'} \, \delta_{1, m'} \sqrt{l^2 + l} = 0,$$

$$\langle l', m' | L_y | 0, 0 \rangle = \langle 0, 0 | L_y | l', m' \rangle = -\frac{i\hbar}{2} \delta_{0, l'} \, \delta_{1, m'} \sqrt{l^2 + l} = 0,$$

$$\langle l', m' | L_z | 0, 0 \rangle = \langle 0, 0 | L_z | l', m' \rangle = 0,$$

where the last result comes from the eigenvalues of L_z being $\hbar m$. Thus, we find

$$\langle \psi(t)|L_x|\psi(t)\rangle = \langle \psi(t)|L_y|\psi(t)\rangle = \langle \psi(t)|L_z|\psi(t)\rangle = 0.$$

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2 Problem 2

In this problem, we are working in the basis that diagonalizes the z component of the spin.

2.1 Consider $\mathbf{n} \cdot \boldsymbol{\sigma}$, where \mathbf{n} is a three-dimensional unit vector and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ represents the Pauli matrices. Compute the eigenvalues λ_1, λ_2 and the corresponding eigenvectors $|\lambda_1\rangle, |\lambda_2\rangle$ of $\mathbf{n} \cdot \boldsymbol{\sigma}$. Use them to obtain the spectrum decomposition of $\mathbf{n} \cdot \boldsymbol{\sigma}$.

Solution. From (3.2.32) in Sakurai, the Pauli matrices are

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{6}$$

Let $\mathbf{n} = (n_x, n_y, n_z)$. Then

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \begin{bmatrix} 0 & n_x \\ n_x & 0 \end{bmatrix} + i \begin{bmatrix} 0 & -n_y \\ n_y & 0 \end{bmatrix} + \begin{bmatrix} n_z & 0 \\ 0 & -n_z \end{bmatrix} = \begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix}. \tag{7}$$

The eigenvalues of $\mathbf{n} \cdot \boldsymbol{\sigma}$ are the solutions to the characteristic polynomial equation

$$0 = \det(\mathbf{n} \cdot \boldsymbol{\sigma} - \lambda I) = \begin{vmatrix} n_z - \lambda & n_x - in_y \\ n_x + in_y & -(n_z + \lambda) \end{vmatrix} = -(n_z - \lambda)(n_z + \lambda) - (n_x - in_y)(n_x + in_y) = \lambda^2 - n_x^2 - n_y^2 - n_z^2.$$

Since $|\mathbf{n}|^2 = n_x^2 + n_y^2 + n_z^2$, we have $\lambda = \pm |\mathbf{n}| = \pm 1$. Let $\lambda_1 = 1$ and $\lambda_2 = -1$.

For the eigenvectors, let $|\lambda_{+}\rangle$ and $|\lambda_{-}\rangle$ be the non-normalized eigenkets corresponding to $|\lambda_{1}\rangle$ and $|\lambda_{2}\rangle$, respectively. Let the elements of $|\lambda_{+}\rangle$ be $\lambda_{+1}, \lambda_{+2}$ and the elements of $|\lambda_{-}\rangle$ be $\lambda_{-1}, \lambda_{-2}$. Then

$$\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix} \begin{bmatrix} \lambda_{\pm 1} \\ \lambda_{\pm 2} \end{bmatrix} = \pm \begin{bmatrix} \lambda_{\pm 1} \\ \lambda_{\pm 2} \end{bmatrix},$$

which is equivalent to the system of equations

$$n_z \lambda_{\pm 1} + (n_x - in_y)\lambda_{\pm 2} = \pm \lambda_{\pm 1}, \qquad (n_x + in_y)\lambda_{\pm 1} - n_z \lambda_{\pm 2} = \pm \lambda_{\pm 2}.$$

We may fix $\lambda_{\pm 2} = n_x + i n_y$ without loss of generality. Then $\lambda_{\pm 1} = n_z \pm 1$, so

$$|\lambda_{+}\rangle = \begin{bmatrix} n_z + 1 \\ n_x + in_y \end{bmatrix}, \qquad |\lambda_{-}\rangle = \begin{bmatrix} n_z - 1 \\ n_x + in_y \end{bmatrix}.$$

For the normalization,

$$\langle \lambda_+ | \lambda_+ \rangle = (n_z + 1)^2 + (n_x - in_y)(n_x + in_y) = n_z^2 + 2n_z + 1 + n_x^2 + n_y^2 = 2(1 + n_z),$$

$$\langle \lambda_- | \lambda_- \rangle = (n_z - 1)^2 + (n_x - in_y)(n_x + in_y) = n_z^2 - 2n_z + 1 + n_x^2 + n_y^2 = 2(1 - n_z),$$

so the normalized eigenkets are

$$|\lambda_1\rangle = \frac{1}{\sqrt{2(1+n_z)}} \begin{bmatrix} n_z+1\\ n_x+in_y \end{bmatrix}, \qquad |\lambda_2\rangle = \frac{1}{\sqrt{2(1-n_z)}} \begin{bmatrix} n_z-1\\ n_x+in_y \end{bmatrix}.$$

Finally, the spectrum decomposition of $\mathbf{n} \cdot \boldsymbol{\sigma}$ is

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \sum_{i} \lambda_{i} |\lambda_{i} \rangle \langle \lambda_{i}| = |\lambda_{1} \rangle \langle \lambda_{1}| - |\lambda_{2} \rangle \langle \lambda_{2}|$$

$$= \frac{1}{2(1+n_{z})} \begin{bmatrix} n_{z}+1 \\ n_{x}+in_{y} \end{bmatrix} \begin{bmatrix} n_{z}+1 & n_{x}-in_{y} \end{bmatrix} - \frac{1}{2(1-n_{z})} \begin{bmatrix} n_{z}-1 \\ n_{x}+in_{y} \end{bmatrix} \begin{bmatrix} n_{z}-1 & n_{x}-in_{y} \end{bmatrix}. \tag{8}$$

2.2 Express the matrix $e^{i\alpha \mathbf{n}\cdot\boldsymbol{\sigma}}$ in terms of σ_x , σ_y , and σ_z and the 2×2 unit matrix.

Solution. Denote the 2×2 unit matrix as I. From (7), note that

$$(\mathbf{n} \cdot \boldsymbol{\sigma})^2 = \begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix}^2 = \begin{bmatrix} n_x^2 + n_y^2 + n_z^2 & (n_z - n_z)(n_x - in_y) \\ (n_z - n_z)(n_x + in_y) & n_x^2 + n_y^2 + n_z^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I.$$
 (9)

Using the power series expansion,

$$e^{i\alpha\mathbf{n}\cdot\boldsymbol{\sigma}} = \sum_{n=0}^{\infty} \frac{(i\alpha\mathbf{n}\cdot\boldsymbol{\sigma})^n}{n!} = i\alpha \ \mathbf{n}\cdot\boldsymbol{\sigma} - \frac{\alpha^2}{2}I - \frac{i\alpha^3}{6}\mathbf{n}\cdot\boldsymbol{\sigma} + \frac{\alpha^4}{24}I + \dots = i\mathbf{n}\cdot\boldsymbol{\sigma}\sum_{n=1}^{\infty} \frac{(-1)^{n-1}\alpha^{2n-1}}{(2n-1)!} + I\sum_{n=0}^{\infty} \frac{(-1)^n\alpha^{2n}}{(2n)!}$$
$$= i\sin\alpha \ \mathbf{n}\cdot\boldsymbol{\sigma} + \cos\alpha I = i\sin\alpha(n_x\sigma_x + n_y\sigma_y + n_z\sigma_z) + \cos\alpha I.$$

2.3 Consider two spin 1/2 degrees of freedom. The total spin is $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$. Consider the state $|j,m\rangle = |1,1\rangle$, where j is the total spin and m is the z component of the total spin. Compute $e^{-i\theta S_y/\hbar} |1,1\rangle$ and express it as a linear superposition of $|j,m\rangle$.

Solution. In the S_z eigenbasis, which we will call $\{|s_z\rangle\}$ where $s_z \in \{\uparrow = 1/2, \downarrow = -1/2\}$,

$$S_{y_1} \sim S_{y_2} = \frac{\hbar}{2} \sigma_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

In the basis $\{|s_{z1} s_{z2}\rangle\}$,

$$S_y = S_{y2} \otimes I + I \otimes S_{y2} = \frac{\hbar}{2} \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} + \frac{\hbar}{2} \begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} \uparrow \uparrow & \uparrow \downarrow & \downarrow \uparrow & \downarrow \downarrow \\ 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix},$$

where we have labeled the columns corresponding to (s_{z1}, s_{z2}) .

We will solve the problem in the basis $\{|s_{z_1}s_{z_2}\rangle\}$, and then express it in terms of $|j,m\rangle$. Proceeding similarly to 2.2, note that

$$\begin{split} S_y^2 &= \frac{\hbar^2}{4} \begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix}^2 = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix} \equiv \hbar K, \\ S_y^3 &= \frac{\hbar^3}{8} \begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix}^3 = \frac{\hbar^3}{2} \begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix} = \hbar^2 S_y, \\ S_y^4 &= \frac{\hbar^4}{16} \begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix}^4 = \frac{\hbar^4}{2} \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix} = \hbar^3 K, \end{split}$$

where we have defined K.

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Then, once more using the power series expansion,

$$e^{-i\theta S_y/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\theta S_y}{\hbar} \right)^n = -\frac{i\theta}{\hbar} S_y - \frac{\theta^2}{2\hbar} K + \frac{i\theta^3}{6\hbar} S_y + \frac{\theta^4}{24\hbar} K + \cdots$$

$$= -\frac{i}{\hbar} S_y \sum_{n=1}^{\infty} \frac{(-1)^{n-1} \theta^{2n-1}}{(2n-1)!} + \frac{1}{\hbar} K \sum_{n=0}^{\infty} \frac{(-1)^n \theta^{2n}}{(2n)!} = \frac{1}{\hbar} \left(-i \sin \theta S_y + \cos \theta K \right).$$

From (3.7.15) in Sakurai,

$$|1,1\rangle = |\uparrow\uparrow\rangle = \begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}, \quad |1,0\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0\\1\\1\\0 \end{bmatrix}, \quad |0,0\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0\\1\\-1\\0 \end{bmatrix}, \quad |1,-1\rangle = |\downarrow\downarrow\rangle = \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}.$$

Note also that

$$|\uparrow\downarrow\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix} = \frac{1}{2}\begin{bmatrix}0\\1\\1\\0\end{bmatrix} + \frac{1}{2}\begin{bmatrix}0\\1\\-1\\0\end{bmatrix} = \frac{|1,0\rangle + |0,0\rangle}{\sqrt{2}}, \qquad |\downarrow\uparrow\rangle = \begin{bmatrix}0\\0\\1\\0\end{bmatrix} = \frac{1}{2}\begin{bmatrix}0\\1\\1\\0\end{bmatrix} - \frac{1}{2}\begin{bmatrix}0\\1\\-1\\0\end{bmatrix} = \frac{|1,0\rangle - |0,0\rangle}{\sqrt{2}}.$$

Finally,

$$\begin{split} e^{-i\theta S_y/\hbar} \left| 1, 1 \right\rangle &= -\frac{i}{\hbar} \sin\theta \, S_y \left| 1, 1 \right\rangle + \frac{1}{\hbar} \cos\theta \, K \left| 1, 1 \right\rangle \\ &= -\frac{i}{2} \sin\theta \begin{bmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \frac{1}{2} \cos\theta \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = -\frac{i}{2} \sin\theta \begin{bmatrix} 0 \\ i \\ i \\ 0 \end{bmatrix} + \frac{1}{2} \cos\theta \begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} \cos\theta \\ \sin\theta \\ \sin\theta \\ -\cos\theta \end{bmatrix} = \frac{1}{2} \left(\cos\theta \left| 1, 1 \right\rangle + \sin\theta \frac{\left| 1, 0 \right\rangle + \left| 0, 0 \right\rangle}{\sqrt{2}} + \sin\theta \frac{\left| 1, 0 \right\rangle - \left| 0, 0 \right\rangle}{\sqrt{2}} - \cos\theta \left| 1, -1 \right\rangle \right) \\ &= \frac{\cos\theta}{2} \left| 1, 1 \right\rangle + \frac{\sin\theta}{\sqrt{2}} \left| 1, 0 \right\rangle - \frac{\cos\theta}{2} \left| 1, -1 \right\rangle. \end{split}$$

3 Problem 3

Consider a spin 1/2 state $|\psi\rangle = c_1 |\uparrow\rangle + c_2 |\downarrow\rangle$, where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the S_z eigenstates with eigenvalues $+\hbar/2$ and $-\hbar/2$, respectively.

3.1 Consider the operator $\rho = |\psi\rangle\langle\psi|$. Write down the matrix elements of ρ in the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$.

Solution. From the definition of $|\psi\rangle$,

$$\langle \uparrow | \psi \rangle = c_1,$$
 $\langle \psi | \uparrow \rangle = c_1^*,$ $\langle \downarrow | \psi \rangle = c_2,$ $\langle \psi | \downarrow \rangle = c_2^*.$

Using these,

$$\langle \uparrow | \rho | \uparrow \rangle = \langle \uparrow | \psi \rangle \langle \psi | \uparrow \rangle = c_1 c_1^* = |c_1|^2, \qquad \langle \uparrow | \rho | \downarrow \rangle = \langle \uparrow | \psi \rangle \langle \psi | \downarrow \rangle = c_1 c_2^*,$$

$$\langle \downarrow | \rho | \uparrow \rangle = \langle \downarrow | \psi \rangle \langle \psi | \uparrow \rangle = c_1^* c_2, \qquad \langle \downarrow | \rho | \downarrow \rangle = \langle \downarrow | \psi \rangle \langle \psi | \downarrow \rangle = c_2 c_2^* = |c_2|^2.$$

In matrix form,

$$\rho = \begin{bmatrix} |c_1|^2 & c_1 c_2^* \\ c_1^* c_2 & |c_2|^2 \end{bmatrix}. \tag{10}$$

3.2 In the S_z eigenbasis, express ρ by using the Pauli matrices. That is, write ρ as

$$\rho = \frac{s_0}{2}I + \frac{1}{2}\mathbf{s} \cdot \boldsymbol{\sigma},\tag{11}$$

and express s_0, s_1, s_2, s_3 in terms of c_1 and c_2 .

Solution. Expanding (11) using the Pauli matrices given by (6),

$$\rho = \frac{1}{2} \begin{bmatrix} s_0 & 0 \\ 0 & s_0 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 0 & s_1 \\ s_1 & 0 \end{bmatrix} + \frac{i}{2} \begin{bmatrix} 0 & -s_2 \\ s_2 & 0 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} s_3 & 0 \\ 0 & -s_3 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} s_0 + s_3 & s_1 - is_2 \\ s_1 + is_2 & s_0 - s_3 \end{bmatrix}.$$

Matching up the matrix elements with those in (10), we have a system of four equations:

$$\frac{s_0 + s_3}{2} = |c_1|^2 \qquad \qquad \frac{s_1 - is_2}{2} = c_1 c_2^* \qquad \qquad \frac{s_1 + is_2}{2} = c_1^* c_2 \qquad \qquad \frac{s_0 - s_3}{2} = |c_2|^2.$$

Solving these for s_0, s_1, s_2, s_3 ,

$$s_0 = \frac{s_0 + s_3}{2} + \frac{s_0 - s_3}{2} = |c_1|^2 + |c_2|^2, \qquad s_1 = \frac{s_1 - is_2}{2} + \frac{s_1 + is_2}{2} = c_1 c_2^* + c_1^* c_2, \qquad (12)$$

$$s_2 = i\left(\frac{s_1 - is_2}{2} - \frac{s_1 + is_2}{2}\right) = i(c_1c_2^* - c_1^*c_2), \qquad s_3 = \frac{s_0 + s_3}{2} - \frac{s_0 - s_3}{2} = |c_1|^2 - |c_2|^2.$$
 (13)

Note that s_0 is the norm of $|\psi\rangle$, so $s_0=1$ assuming $|\psi\rangle$ is normalized. Then (11) can be written

$$\begin{split} \rho &= \frac{|c_1|^2 + |c_2|^2}{2} I + \frac{c_1 c_2^* + c_1^* c_2}{2} \sigma_x + i \frac{c_1 c_2^* - c_1^* c_2}{2} \sigma_y + \frac{|c_1|^2 - |c_2|^2}{2} \sigma_z \\ &= \frac{1}{2} I + \frac{c_1 c_2^* + c_1^* c_2}{2} \sigma_x + i \frac{c_1 c_2^* - c_1^* c_2}{2} \sigma_y + \frac{|c_1|^2 - |c_2|^2}{2} \sigma_z. \end{split}$$

3.3 Compute ρ^2 and \mathbf{s}^2 .

Solution. Using the representation of ρ in (11),

$$\rho^2 = \frac{s_0^2}{4}I^2 + \frac{s_0}{4}I(\mathbf{s} \cdot \boldsymbol{\sigma}) + \frac{s_0}{4}(\mathbf{s} \cdot \boldsymbol{\sigma})I + \frac{1}{4}(\mathbf{s} \cdot \boldsymbol{\sigma})^2 = \frac{1}{4}(s_0^2 + |\mathbf{s}|^2)I + \frac{s_0}{2}\mathbf{s} \cdot \boldsymbol{\sigma} = \frac{1}{4}(1 + |\mathbf{s}|^2)I + \frac{1}{2}\mathbf{s} \cdot \boldsymbol{\sigma},$$

where $\mathbf{s} = (s_1, s_2, s_3)$, and in the final equality we have assumed $|\psi\rangle$ is normalized. Using (12) and (13),

$$\mathbf{s}^{2} = \mathbf{s} \cdot \mathbf{s} = s_{1}^{2} + s_{2}^{2} + s_{3}^{2} = (c_{1}c_{2}^{*} + c_{1}^{*}c_{2})^{2} - (c_{1}c_{2}^{*} - c_{1}^{*}c_{2})^{2} + (|c_{1}|^{2} - |c_{2}|^{2})^{2}$$

$$= c_{1}^{2}c_{2}^{*2} + 2|c_{1}|^{2}|c_{2}|^{2} + c_{1}^{*2}c_{2}^{2} - c_{1}^{2}c_{2}^{*2} + 2|c_{1}|^{2}|c_{2}|^{2} - c_{1}^{*2}c_{2}^{2} + |c_{1}|^{4} - 2|c_{1}|^{2}|c_{2}|^{2} + |c_{2}|^{4}$$

$$= |c_{1}|^{4} + 2|c_{1}|^{2}|c_{2}|^{2} + |c_{2}|^{4} = (|c_{1}|^{2} + |c_{2}|^{2})^{2}$$

$$= s_{0}^{2} = 1.$$

We can use this result to simplify the expression for ρ^2 :

$$\rho^2 = \frac{1}{2}s_0^2 I + \frac{s_0}{2}\mathbf{s} \cdot \boldsymbol{\sigma} = \rho.$$

3.4 Using the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle,$$
 (14)

derive the equation of motion obeyed by ρ .

Solution. The adjoint of (14) is

$$-i\hbar\frac{\partial}{\partial t}\left\langle \psi\right| = \left\langle \psi\right| H \iff i\hbar\frac{\partial}{\partial t}\left\langle \psi\right| = -\left\langle \psi\right| H.$$

Then

$$i\hbar \frac{d\rho}{dt} = i\hbar \frac{d}{dt} |\psi\rangle\langle\psi| = H |\psi\rangle\langle\psi| - |\psi\rangle\langle\psi| H = H\rho - \rho H = [H, \rho],$$

so the equation of motion is

$$\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, H].$$

3.5 When the Hamiltonian is given by

$$H = \frac{\hbar}{2} \mathbf{\Omega} \cdot \mathbf{\sigma},\tag{15}$$

write down the equation of motion obeyed by $(\psi_{\uparrow}(t), \psi_{\downarrow}(t))$, where $\psi_{\uparrow}(t), \psi_{\downarrow}(t)$ are the (complex) expansion coefficients of the state ket

$$|\psi(t)\rangle = \psi_{\uparrow}(t) |\uparrow\rangle + \psi_{\downarrow}(t) |\downarrow\rangle.$$

Solution. Using (14),

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \frac{\hbar}{2} \mathbf{\Omega} \cdot \boldsymbol{\sigma} |\psi(t)\rangle \iff i\hbar \frac{d}{dt} (\psi_{\uparrow}(t) |\uparrow\rangle + \psi_{\downarrow}(t) |\downarrow\rangle) = \frac{\hbar}{2} \mathbf{\Omega} \cdot \boldsymbol{\sigma} (\psi_{\uparrow}(t) |\uparrow\rangle + \psi_{\downarrow}(t) |\downarrow\rangle),$$

which can be separated into two equations:

$$\frac{d}{dt}\psi_{\uparrow}(t)|\uparrow\rangle = -\frac{i}{2}\psi_{\uparrow}(t)\,\mathbf{\Omega}\cdot\boldsymbol{\sigma}|\uparrow\rangle\,,\qquad\qquad \frac{d}{dt}\psi_{\downarrow}(t)|\downarrow\rangle = -\frac{i}{2}\psi_{\downarrow}(t)\,\mathbf{\Omega}\cdot\boldsymbol{\sigma}|\downarrow\rangle\,.$$
(16)

Generalizing the results of 2.1, let $\Omega = \Omega \mathbf{n}$ where \mathbf{n} is a unit vector. Using (7),

$$\mathbf{\Omega} \cdot \boldsymbol{\sigma} \left| \uparrow \right\rangle = \Omega \begin{bmatrix} n_z \\ n_x + i n_y \end{bmatrix} = \Omega_z \left| \uparrow \right\rangle + (\Omega_x + i \Omega_y) \left| \downarrow \right\rangle, \quad \mathbf{\Omega} \cdot \boldsymbol{\sigma} \left| \downarrow \right\rangle = \Omega \begin{bmatrix} n_x - i n_y \\ -n_z \end{bmatrix} = (\Omega_x - i \Omega_y) \left| \uparrow \right\rangle - \Omega_z \left| \downarrow \right\rangle,$$

where $\Omega = (\Omega_x, \Omega_y, \Omega_z)$. Then, explicitly, we have the equations of motion

$$\frac{d}{dt}\psi_{\uparrow}(t)|\uparrow\rangle = -\frac{i}{2}\psi_{\uparrow}(t)\left[\Omega_{z}|\uparrow\rangle + (\Omega_{x} + i\Omega_{y})|\downarrow\rangle\right], \qquad \frac{d}{dt}\psi_{\downarrow}(t)|\downarrow\rangle = -\frac{i}{2}\psi_{\downarrow}(t)\left[(\Omega_{x} - i\Omega_{y})|\uparrow\rangle - \Omega_{z}|\downarrow\rangle\right]. \tag{17}$$

This can also be written in matrix form in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis:

$$\frac{d}{dt} \begin{bmatrix} \psi_{\uparrow}(t) \\ \psi_{\downarrow}(t) \end{bmatrix} = -\frac{i}{2} \begin{bmatrix} \Omega_z & \Omega_x - i\Omega_y \\ \Omega_x + i\Omega_y & -\Omega_z \end{bmatrix} \begin{bmatrix} \psi_{\uparrow}(t) \\ \psi_{\downarrow}(t) \end{bmatrix}.$$

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3.6 When the Hamiltonian is given by (15), write down the (Heisenberg) equation of motion obeyed by the spin operators S.

Solution. From (3.2.35) in Sakurai,

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k.$$

Let $\mathbf{S} = (S_1, S_2, S_3)$ and $\mathbf{\Omega} = (\Omega_1, \Omega_2, \Omega_3)$. Then the Heisenberg equation of motion is

$$\frac{dS_i}{dt} = -\frac{i}{\hbar}[S_i, H] = -\frac{i\hbar}{4}[\sigma_i, \mathbf{\Omega} \cdot \boldsymbol{\sigma}] = -\frac{i\hbar}{4} \sum_{j=1}^3 \Omega_j[\sigma_i, \sigma_j] = \frac{\hbar}{2} \sum_{j=1}^3 \Omega_j \varepsilon_{ijk} \sigma_k.$$

Explicitly, the equations of motion are

$$\frac{dS_x}{dt} = \frac{\hbar}{2}(\Omega_y \sigma_z - \Omega_z \sigma_y), \qquad \frac{dS_y}{dt} = \frac{\hbar}{2}(\Omega_z \sigma_x - \Omega_x \sigma_z), \qquad \frac{dS_z}{dt} = \frac{\hbar}{2}(\Omega_x \sigma_y - \Omega_y \sigma_x).$$

While writing up these solutions, I consulted Sakurai's *Modern Quantum Mechanics* and Shankar's *Principles of Quantum Mechanics*.