PHYS852 Quantum Mechanics II, Spring 2010
HOMEWORK ASSIGNMENT 4: Solutions.

Topics covered: rotation with spin, exchange symmetry

1. A vector pointing in the θ, ϕ direction, can be formed by starting with a vector pointing along $\vec{e}_z$, then applying an active rotation by θ about the y-axis, followed by a rotation by ϕ about the z-axis.

   (a) Verify this for an ordinary vector, by starting with the vector $(0,0,1)^T$ and using

$$R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}; \qquad R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1}$$

   The vector $(0,0,1)^T$ is simply $\vec{e}_z$. Applying first the y rotation, and then the z rotation gives:

$$R_z(\phi)R_y(\theta)\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \tag{2}$$

   we can recognize this as the unit vector $\vec{e}_{\theta\phi}$ that points in the θ, ϕ direction.

   (b) Thus for a spin-1/2 system, the spin-up state with respect to the θ, ϕ direction can be found in the basis of S_z eigenstates, by starting with the spin-up state along $\vec{e}_z$, and applying unitary rotation operators, i.e.

$$|\uparrow_{\theta\phi}\rangle = e^{-\frac{i}{\hbar}\phi S_z} e^{-\frac{i}{\hbar}\theta S_y} |\uparrow_z\rangle. \tag{3}$$

   In this way, find the states $|\uparrow_{\theta\phi}\rangle$ and $|\downarrow_{\theta\phi}\rangle$.
   first we note that

$$e^{-\frac{i}{\hbar}\phi S_z} = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix} \tag{4}$$

   and

$$e^{-\frac{i}{\hbar}\theta S_y} = \cos(\theta/2)I - i\sin(\theta/2)\sigma_y = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \tag{5}$$

   this gives us

$$\begin{aligned} e^{-\frac{i}{\hbar}\phi S_z} e^{-\frac{i}{\hbar}\theta S_y} &= \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}\begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \\ &= \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix} \end{aligned} \tag{6}$$

   Thus we have

$$|\uparrow_{\theta\phi}\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} \end{pmatrix} \tag{7}$$

   and

$$|\downarrow_{\theta\phi}\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin(\theta/2)e^{-i\phi/2} \\ \cos(\theta/2)e^{i\phi/2} \end{pmatrix} \tag{8}$$

(c) Compute the operator $S_{\theta\phi}$ using unitary rotation operators to transform S_z, and compare it to the result using the 3×3 rotation matrices.
The operator $S_{\theta\phi}$ is given by definition as $S_{\theta\phi} = \vec{e}_{\theta\phi} \cdot \vec{S}$, which gives

$$\begin{aligned} S_{\theta\phi} &= \sin\theta\cos\phi S_x + \sin\theta\sin\phi S_y + \cos\theta S_z \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix} \end{aligned} \tag{9}$$

Note that we have computed this by rotating the unit vectors. According to the lecture, there are two additional equivalent transformations. We can apply the *inverse* transformation to each component of $\vec{S}$ via unitary operators, or we can apply the *inverse* transformation collectively to all three components via the 3×3 rotation matrix.

From part (b) we have

$$U = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix} \tag{10}$$

so that

$$\begin{aligned} S_{\theta\phi} &= \left(U^{-1}\right)^{\dagger} S_z U^{-1} \\ &= U S_z U^{\dagger} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \cos(\theta/2)e^{i\phi/2} & \sin(\theta/2)e^{-i\phi/2} \\ -\sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{-i\phi/2} \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix}\begin{pmatrix} \cos(\theta/2)e^{i\phi/2} & \sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & -\cos(\theta/2)e^{-i\phi/2} \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos^2(\theta/2) - \sin^2(\theta/2) & 2\cos(\theta/2)\sin(\theta/2)e^{-i\phi} \\ 2\cos(\theta/2)\sin(\theta/2)e^{i\phi} & \sin^2(\theta/2) - \cos^2(\theta/2) \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix} \end{aligned} \tag{11}$$

which remarkably gives the same result as Eq. (9).

The third approach gives

$$\begin{pmatrix} S'_x \\ S'_y \\ S'_z \end{pmatrix} = \left(R_z(\phi)R_y(\theta)\right)^{-1}\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} \tag{12}$$

$$= R_y(-\theta)R_z(-\phi)\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} \tag{13}$$

$$= \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}\begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} \tag{14}$$

$$= \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}\begin{pmatrix} \cos\phi S_x + \sin\phi S_y \\ -\sin\phi S_x + \cos\phi S_y \\ S_z \end{pmatrix}$$

$$= \left(\begin{array}{c} \cos\theta\cos\phi S_x + \cos\theta\sin\phi S)y - \sin\theta S_z \\ -\sin\phi S_x + \cos\phi S_y \\ \sin\theta\cos\phi S_x + \sin\theta\sin\phi S_y + \cos\theta S_z \end{array} \right) \tag{15}$$

identifying $S_{\theta\phi} = S_3'$ gives

$$S_{\theta\phi} = \sin\theta\cos\phi S_x + \sin\theta\sin\phi S_y + \cos\theta S_z \tag{16}$$

which again reproduces eq. (9).

(d) Using your results from parts (b) and (c), show explicitly that $S_{\theta\phi}|\uparrow_{\theta\phi}\rangle = \frac{\hbar}{2}|\uparrow_{\theta\phi}\rangle$ and $S_{\theta\phi}|\downarrow_{\theta\phi}\rangle = -\frac{\hbar}{2}|\downarrow_{\theta\phi}\rangle$.

$$\begin{aligned} S_{\theta\phi}|\uparrow_{\theta\phi}\rangle &= \frac{\hbar}{2} \left(\begin{array}{cc} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{array} \right) \left(\begin{array}{c} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} \end{array} \right) \\ &= \frac{\hbar}{2} \left(\begin{array}{c} \cos\theta\cos(\theta/2)e^{-i\phi/2} + \sin\theta\sin(\theta/2)e^{-i\phi/2} \\ \sin\theta\cos(\theta/2)e^{i\phi/2} - \cos\theta\sin(\theta/2)e^{i\phi/2} \end{array} \right) \end{aligned} \tag{17}$$

now we have

$$\cos^2(\theta) = \frac{1}{2}\left(1 + \cos(2\theta)\right) \tag{18}$$

so that

$$\cos\theta = 2\cos^2(\theta/2) - 1 \tag{19}$$

likewise

$$\sin\theta\cos\theta = \frac{1}{2}\sin(2\theta) \tag{20}$$

so that

$$\sin\theta = 2\sin(\theta/2)\cos(\theta/2) \tag{21}$$

this gives

$$\begin{aligned} S_{\theta\phi}|\uparrow_{\theta\phi}\rangle &= \frac{\hbar}{2} \left(\begin{array}{c} \left[2\cos^3(\theta/2) - \cos(\theta/2) + 2\sin^2(\theta/2)\cos(\theta/2)\right] e^{-i\phi/2} \\ \left[2\sin(\theta/2)\cos^2(\theta/2) - 2\cos^2(\theta/2)\sin(\theta/2) + \sin(\theta/2)\right] e^{i\phi/2} \end{array} \right) \\ &= \frac{\hbar}{2} \left(\begin{array}{c} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} \end{array} \right) \\ &= \frac{\hbar}{2}|\uparrow_{\theta\phi}\rangle \end{aligned} \tag{22}$$

and

$$\begin{aligned} S_{\theta\phi}|\downarrow_{\theta\phi}\rangle &= \frac{\hbar}{2} \left(\begin{array}{cc} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{array} \right) \left(\begin{array}{c} -\sin(\theta/2)e^{-i\phi/2} \\ \cos(\theta/2)e^{i\phi/2} \end{array} \right) \\ &= \frac{\hbar}{2} \left(\begin{array}{c} \left[-\cos\theta\sin(\theta/2) + \sin\theta\cos(\theta/2)\right] e^{-i\phi/2} \\ \left[-\sin\theta\sin(\theta/2) - \cos\theta\cos(\theta/2)\right] e^{-phi/2} \end{array} \right) \\ &= \frac{\hbar}{2} \left(\begin{array}{c} \sin(\theta/2)e^{-i\phi/2} \\ -\cos(\theta/2)e^{i\phi/2} \end{array} \right) \\ &= -\frac{\hbar}{2}|\downarrow_{\theta\phi}\rangle \end{aligned} \tag{23}$$

2. **The Bloch Sphere**: The most-general spin-1/2 state is

$$|\psi\rangle = c_\uparrow|\uparrow_z\rangle + c_\downarrow|\downarrow_z\rangle, \tag{24}$$

where $c_\uparrow$ and $c_\downarrow$ are c-numbers. This state is subject to the constraint $|c_\uparrow|^2 + |c_\downarrow|^2 = 1$, and is defined only up to a global phase-factor. This means that it only requires two real numbers to specify a spin-1/2 state. The state $|\uparrow_{\theta\phi}\rangle$ from problem 1 has two free real-valued parameters. This means that every possible spin-1/2 state must be spin-up with respect to some axis. Determine the axis angles, (θ, ϕ), for a state of the form (3).

The dynamical evolution of a spin-1/2 state can therefore be viewed as the motion of a single point on a sphere of unit radius, known as the Bloch sphere, i.e. the state $|\psi(t)\rangle = c_\uparrow(t)|\uparrow_z\rangle + c_\downarrow(t)|\downarrow_z\rangle$ maps onto the coordinate $(\theta(t), \phi(t))$. Describe the trajectory on the Bloch sphere of an arbitrary initial state, subject to the Hamiltonian

$$H = \omega S_z. \tag{25}$$

In addition, find the constant of motion, and express it in the form $f(\theta(t), \phi(t)) = f(\theta(0), \phi(0))$.
We have

$$|\uparrow_{\theta\phi}\rangle = \cos(\theta/2)e^{-i\phi/2}|\uparrow_z\rangle + \sin(\theta/2)e^{i\phi/2}|\downarrow_z\rangle \tag{26}$$

which means

$$\begin{aligned} c_\uparrow &= \cos(\theta/2)e^{-i\phi/2} && (27)\\ c_\downarrow &= \sin(\theta/2)e^{i\phi/2} && (28) \end{aligned}$$

inverting gives

$$\begin{aligned} \theta &= 2\arctan\frac{|c_\downarrow|}{|c_\uparrow|} && (29)\\ \phi &= \arg\left[c_\downarrow^2 + \left(c_\uparrow^*\right)^2\right] && (30) \end{aligned}$$

The Hamiltonian generates time evolution via the transformation

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle \\ &= U_R(\phi(t)\vec{e}_z)|\phi(0)\rangle && (31) \end{aligned}$$

where

$$\phi(t) = \omega t \tag{32}$$

This means that an initial point on the Bloch sphere orbits around the z-axis, forming a line of constant latitude. The constant of motion is therefore

$$\theta(t) = \theta(0) \tag{33}$$

3. Consider two identical spin-1/2 particles in a one-dimensional Harmonic oscillator potential, so that

$$H = H_1 + H_2 \tag{34}$$

with

$$H_j = \frac{P_j^2}{2M} + \frac{1}{2}M\omega^2 X_j^2 \tag{35}$$

(a) Show that H, H_1 and H_2 form a set of 3 commuting observables, so that simultaneous eigenstates of H, H_1 and H_2 exist. Label these states as $|n_1, n_2\rangle$ where $H_j|n_1, n_2\rangle = E_{n_j}|n_1, n_2\rangle$, and $H|n_1, n_2\rangle = (E_{n_1} + E_{n_2})|n_1, n_2\rangle$. Does the set $\{|n_1, n_2\rangle\}$ form a complete basis for the two-particle orbital Hilbert space?
H_1 and H_2 commute with each other and with H because $[X_j, P_k] = i\hbar\delta_{j,k}$ gives zero for $j \neq k$. The set $\{|n_1, n_2\rangle\}$ does form a complete basis.

(b) Switch to relative and center-of-mass coordinates, by expressing the operators X_1, X_2, P_1, and P_2, in terms of the operators X_{CM}, X, P_{CM} and P. Show that H separates as $H = H_{CM}(X_{CM}, P_{CM}) + H_r(X, P)$. Show that H, H_{CM} and H_r all commute, so that simultaneous eigenvalues of H, H_{CM} and H_r exist. Label these states as $|N, n\rangle$, where $H_{CM}|N, n\rangle = E_N|N, n\rangle$, $H_r|N, n\rangle = E_n|N, n\rangle$, and $H|N, n\rangle = (E_N + E_n)|N, n\rangle$. Does the set of states $\{|N, n\rangle\}$ form a compete basis for the two-particle orbital Hilbert space?
The transformation is

$$\begin{aligned} X_1 &= X_{CM} + \frac{1}{2}X && (36)\\ X_2 &= X_{CM} - \frac{1}{2}X && (37)\\ P_1 &= \frac{1}{2}P_{CM} + P && (38)\\ P_2 &= \frac{1}{2}P_{CM} - P && (39) \end{aligned}$$

The Hamiltonian becomes

$$H = H_{CM} + H_r \tag{40}$$

where

$$\begin{aligned} H_{CM} &= \frac{P_{CM}^2}{4M} + M\omega^2 X_{CM}^2 && (41)\\ H_r &= \frac{P^2}{M} + \frac{1}{4}M\omega^2 X^2 && (42) \end{aligned}$$

Because $[X, P_{CM}] = [X_{CM}, P] = 0$, it follows that H_{CM}, H_r, and H form a set of mutually commuting observables. Thus the set $\{|N, n\rangle\}$ is a complete basis.

(c) Let $X_j|x_1, x_2\rangle = x_j|x_1, x_2\rangle$, $X_{CM}|x_{CM}, x\rangle = x_{CM}|x_{CM}, x\rangle$, and $X|x_{CM}, x\rangle = x|x_{CM}, x\rangle$. The exchange operator is defined by $P_{1,2}|x_1, x_2\rangle = |x_2, x_1\rangle$. What is $P_{12}|x_{CM}, x\rangle$?
We start from the equivalence

$$|x_1, x_2\rangle^{(1,2)} = |\frac{x_1+x_2}{2}, x_1 - x_2\rangle^{(CM,r)} \tag{43}$$

so that

$$P_{1,2}|x_1, x_2\rangle^{(1,2)} = |x_1, x_1\rangle^{(1,2)} = |\frac{x_2+x_1}{2}, x_2 - x_1\rangle^{(CM,r)} = |x_{CM}, -x\rangle^{(CM,r)} \tag{44}$$

(d) Show that the states $|n_1, n_2\rangle$ are in general not eigenstates of the exchange operator, but that the states $|N, n\rangle$ are. What is the exchange eigenvalue of the state $|N, n\rangle$?

we have

$$\phi_{n_1,n_2}(x_1, x_2) = \frac{1}{\sqrt{2^{n_1+n_2} n_1! n_2! \pi\lambda}} H_{n_1}(x_1/\lambda) H_{n_2}(x_2/\lambda) e^{-\frac{1}{2}(x_1^2+x_2^2)/\lambda} \tag{45}$$

with $\phi'(x_1, x_2) = \phi(x_1, x_2)$, we see that unless $n_1 = n_2$, $|n_1, n_2\rangle$ is not an eigenstate of $P_{1,2}$.

In center-of-mass coordinates, we have

$$\phi_{N,n}(x_{CM}, x) = \frac{1}{\sqrt{2^{N+n} N! n! \pi\lambda}} H_N(\sqrt{2} x_{CM}/\lambda) H_n(x/(\sqrt{2}\lambda) e^{-(x_{CM}^2 + x^2/4)/\lambda^2} \tag{46}$$

but with $\phi'(x_{CM}, x) = \phi(x_{CM}, -x)$, we see that

$$\phi'_{N,n}(x_{CM}, x) = \frac{1}{\sqrt{2^{N+n} N! n! \pi\lambda}} H_N(\sqrt{2} x_{CM}/\lambda) H_n(-x/(\sqrt{2}\lambda) e^{-\frac{1}{2}(2x_{CM}^2 + x^2/2)/\lambda^2} \tag{47}$$

The Hermite polynomials have well-defined parity, so that $H_n(-x) = (-1)^n H_n(x)$.
Thus we have

$$P_{1,2}|N, n\rangle = (-1)^n |N, n\rangle \tag{48}$$

(e) If the two particles are in a spin-singlet state, which of the $|N, n\rangle$ states are forbidden? Which are forbidden for the spin-triplet state?

In the singlet state, the spatial wave function must be symmetric under exchange, which means that odd n states are forbidden. For the triplet state, the even n states are forbidden.

(f) Assume a zero-range interaction of the form $V(x_1, x_2) = g\delta(x_1 - x_2)$. For the 'repulsive' case, $g > 0$ will the true ground state be a singlet or triplet state? What about for 'attractive' interactions, i.e. $g < 0$?

For the repulsive case, the $n = 0$ state will have its energy increased, whereas the $n = 1$ state's energy will remain unchanged. While one might be tempted to say that for large enough g, the $n = 0$ state could have higher energy than the $n = 1$ state (which I will accept as a valid answer), in fact in the limit of $g \to \infty$, the singlet energy level assymptotically approaches the triplet level from below, a unique property of the 1D zero-range potential. Thus the singlet state will always be the ground state. For attractive interactions, the energy of the $n = 0$ state will decrease, while that of the $n = 1$ state remains unchanged, so that also, the singlet state remains the ground state.