Chapter 5 Problems

PHY 852 Quantum Mechanics

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Problem 1: Show whether or not the following terms are invariant under parity and time reversal.
(Proving statements from lecture notes pg. 91)

a) $\frac{\vec{p}^2}{2m}$

b) $\vec{p} \cdot \vec{r}$

c) $\vec{L} \cdot \vec{p}$

d) $\vec{S} \cdot \vec{B}$

e) $\vec{p} \cdot \vec{A}$

Parity $\Rightarrow$ Space inversion

$$\vec{r} \Rightarrow -\vec{r}$$

Time Reversal $\Rightarrow$ Reversal of Motion

$$t \Rightarrow -t$$

Analyize how an operator depends on $\vec{r}$ or t.

Recall: Momentum goes like

$$m\frac{d\vec{r}}{dt}$$

Both the coordinate and momentum operators should flip sign under parity. Momentum also flips sign under time reversal, but coordinate does not. The first three terms can be solved with this in mind.

a)

$$\frac{1}{2m}\Pi(\vec{p} \cdot \vec{p})\Pi^{-1} = \frac{1}{2m}(\Pi(\vec{p})\Pi^{-1} \cdot \Pi(\vec{p})\Pi^{-1}) = \frac{1}{2m}(-\vec{p}) \cdot (-\vec{p}) = \frac{\vec{p}^2}{2m}$$

$$\frac{1}{2m}\Theta(\vec{p} \cdot \vec{p})\Theta^{-1} = \frac{1}{2m}(\Theta(\vec{p})\Theta^{-1} \cdot \Theta(\vec{p})\Theta^{-1}) = \frac{1}{2m}(-\vec{p}) \cdot (-\vec{p}) = \frac{\vec{p}^2}{2m}$$

Therefore, invariant under both.

b)

$$\Pi(\vec{p}\cdot\vec{r})\Pi^{-1} = \Pi(\vec{p})\Pi^{-1}\cdot\Pi(\vec{r})\Pi^{-1} = \vec{-p}\cdot\vec{-r} = \vec{p}\cdot\vec{r}$$
$$\Theta(\vec{p}\cdot\vec{r})\Theta^{-1} = \Theta(\vec{p})\Theta^{-1}\cdot\Theta(\vec{r})\Theta^{-1} = \vec{-p}\cdot\vec{r}$$

Therefore, invariant under parity, not invariant under time reversal.

c)Angular momentum come from the relation

$$\vec{L} = \vec{r}\times\vec{p}$$

$$\Pi(\vec{L}\cdot\vec{p})\Pi^{-1} = \Pi[(\vec{r}\times\vec{p})\cdot\vec{p}]\Pi^{-1} = \Pi\vec{r}\Pi^{-1}\times\Pi\vec{p}\Pi^{-1}\cdot\Pi\vec{p}\Pi^{-1} =$$
$$((-\vec{r})\times(-\vec{p}))\cdot(\vec{-p}) = -\vec{L}\cdot\vec{p}$$

$$\Theta(\vec{L}\cdot\vec{p})\Theta^{-1} = \Theta[(\vec{r}\times\vec{p})\cdot\vec{p}]\Theta^{-1} = \Theta\vec{r}\Theta^{-1}\times\Theta\vec{p}\Theta^{-1}\cdot\Theta\vec{p}\Theta^{-1} =$$
$$((\vec{r})\times(-\vec{p}))\cdot(\vec{-p}) = \vec{L}\cdot\vec{p}$$

Therefore, not invariant under parity, invariant under time reversal.

Now consider how $\vec{B}$, $\vec{A}$, and $\vec{S}$ behave, based on if they are even or odd operators under parity or time reversal.

A kind of shorthand is to remember that $\vec{J}$ and $\vec{S}$ both transform like $\vec{L}$. On a test, this is a fast (non-rigorous) way to think of what they will do here.

For $\vec{A}$ and $\vec{B}$, we know the potential $\vec{A}$ depends on both coordinate and time, so it will be odd under both. $\vec{B} = \nabla\times\vec{A}$, and nabla is coordinate dependent, therefore it is odd under parity and even under time reversal. For $\vec{B}$ the whole thing will end up odd-odd for parity (so even) and odd-even for time reversal (so odd).

$$\Pi\vec{B}\Pi^{-1} = \vec{B} \qquad \Pi\vec{A}\Pi^{-1} = -\vec{A} \qquad \Pi\vec{S}\Pi^{-1} = \vec{S}$$
$$\Theta\vec{B}\Theta^{-1} = -\vec{B} \qquad \Theta\vec{A}\Theta^{-1} = -\vec{A} \qquad \Theta\vec{S}\Theta^{-1} = -\vec{S}$$

d)

$$\Pi(\vec{S}\cdot\vec{B})\Pi^{-1} = \Pi\vec{S}\Pi^{-1}\cdot\Pi\vec{B}\Pi^{-1} = \vec{S}\cdot\vec{B}$$
$$\Theta(\vec{S}\cdot\vec{B})\Theta^{-1} = \Theta\vec{S}\Theta^{-1}\cdot\Theta\vec{B}\Theta^{-1} = (-\vec{S})\cdot(-\vec{B}) = \vec{S}\cdot\vec{B}$$

Invariant under both.

e)

$$\Pi(\vec{p}\cdot\vec{A})\Pi^{-1} = \Pi\vec{p}\Pi^{-1}\cdot\Pi\vec{A}\Pi^{-1} = (-\vec{p})\cdot(-\vec{A}) = \vec{p}\cdot\vec{A}$$
$$\Theta(\vec{p}\cdot\vec{A})\Theta^{-1} = \Theta\vec{p}\Theta^{-1}\cdot\Theta\vec{A}\Theta^{-1} = (-\vec{p})\cdot(-\vec{A}) = \vec{p}\cdot\vec{A}$$

Invariant under both.

Problem 2: Question 4.12 Sakurai

The Hamiltonian for a system is given by:

$$H = AS_z^2 + B(S_x^2 - S_y^2) \tag{1}$$

Solve this problem exactly to find the normalized energy eigenstates and eigenvalues. (A spin-dependent Hamiltonian of this kind actually appears in crystal physics.) Is the Hamiltonian invariant under time reversal? How do the normalized eigenstates you obtained transform under time reversal?

Solution:

First, we are dealing with a spin 1 system, $l = 1$, $m = -1, 0, 1$. We also have,

$$S_z\left|l,m\right\rangle = \hbar m\left|l,m\right\rangle \longrightarrow \left\langle l,n\right| S_z \left|l,m\right\rangle = \hbar m\left\langle n|m\right\rangle \tag{2}$$

So,

$$(S_z)_{nm} = \hbar m\delta_{nm} \tag{3}$$

$$S_z = \hbar\begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{bmatrix} \tag{4}$$

$$S_z^2 = \hbar^2\begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{bmatrix} \tag{5}$$

Now to get S_x^2 and S_y^2, recall that we define the raising and lowering operators in the following way:

$$S_\pm = S_x \pm iS_y \tag{6}$$

Since we know the effect of the lowering and raising operators on a spin state, we can now calculate the matrix elements of the rest of the relevant operators:

$$\langle 1, m| S_x |1, n\rangle = \langle 1, m| \frac{1}{2}(S_+ + S_-) |1, n\rangle \tag{7}$$

$$\frac{1}{2} \langle 1, m| S_+ |1, n\rangle + \frac{1}{2} \langle 1, m| S_- |1, n\rangle = \\ \frac{1}{2}\hbar\sqrt{(1-m)(1+m+1)}\delta_{n,m+1} + \frac{1}{2}\hbar\sqrt{(1+m)(1-m+1)}\delta_{n,m-1}$$

In matrix representation:

$$S_x = \hbar\frac{\sqrt{2}}{2} \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} + \hbar\frac{\sqrt{2}}{2} \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{8}$$

$$S_x^2 = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{9}$$

Similarly for S_y:

$$S_y = \frac{S_+ - S_-}{2i} \tag{10}$$

$$\langle 1, m| S_y |1, n\rangle = \langle 1, m| \frac{1}{2i}(S_+ - S_-) |1, n\rangle \tag{11}$$

$$\frac{1}{2i} \langle 1, m| S_+ |1, n\rangle - \frac{1}{2i} \langle 1, m| S_- |1, n\rangle = \\ \frac{1}{2i}\hbar\sqrt{(1-m)(1+m+1)}\delta_{n,m+1} - \frac{1}{2i}\hbar\sqrt{(1+m)(1-m+1)}\delta_{n,m-1}$$

Which gives us the matrix:

$$S_y = \hbar\frac{\sqrt{2}}{2i} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} \tag{12}$$

$$S_y^2 = \frac{\hbar^2}{2} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix} \tag{13}$$

After all of that, we can now write our Hamiltonian as:

$$H = AS_z^2 + B(S_x^2 - S_y^2) \doteq \hbar^2 \begin{bmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{bmatrix} \tag{14}$$

To find the eigenvalues and eigenvectors, we have to solve the equation:

$$det(H - \lambda I) = 0 \tag{15}$$

Just use Mathematica to get,

$$\begin{aligned}\lambda_1 &= 0\\ \lambda_2 &= A - B\\ \lambda_3 &= A + B\end{aligned}$$

And the eiegenstates,

$$|\lambda_1\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix} \tag{16}$$

$$|\lambda_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\1\end{pmatrix} \tag{17}$$

$$|\lambda_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix} \tag{18}$$

Now we answer the question, "Is the Hamiltonian invariant under time reversal?" We must note that $\Theta\mathbf{J}\Theta^{-1} = -\mathbf{J}$ from Sakurai. The $\mathbf{J}$ must be odd under time reversal to preserve the commutation relation:

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k \tag{19}$$

From this it is quick to find that:

$$\begin{aligned}\Theta H\Theta^{-1} &= \Theta(AS_z^2 + B(S_x^2 - S_y^2))\Theta^{-1}\\ &= A\Theta S_z^2\Theta^{-1} + B\Theta S_x^2\Theta^{-1} - B\Theta S_y^2\Theta^{-1}\\ &= A\Theta S_z\Theta^{-1}\Theta S_z\Theta^{-1} + B\Theta S_x\Theta^{-1}\Theta S_x\Theta^{-1} - B\Theta S_y\Theta^{-1}\Theta S_y\Theta^{-1}\\ &= AS_z^2 + B(S_x^2 - S_y^2) = H\end{aligned}$$

So we find that this specific spin-dependent Hamiltonian is invariant under time reversal. What about the eigenstates? We start with fact that,

$$\Theta\,|j, m\rangle = (-1)^m\,|j, -m\rangle \tag{20}$$

which can be found in Sakurai (4.4.78) or Scott's lecture notes (5.20 in the Time Reversal and Angular Momentum section). We also must keep in mind that the basis we are using for spin-1 particles is:

$$|1, m = 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; |1, m = 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; |1, m = -1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Now we can rewrite our eigenvectors in terms of the basis vectors,

$$\begin{aligned}
|\lambda_1\rangle &= |1, 0\rangle \\
|\lambda_2\rangle &= \frac{1}{\sqrt{2}}(-|1, 1\rangle + |1, -1\rangle) \\
|\lambda_3\rangle &= \frac{1}{\sqrt{2}}(|1, 1\rangle + |1, -1\rangle)
\end{aligned}$$

which makes checking the time reversal much simpler.

$$\begin{aligned}
\Theta |\lambda_1\rangle &= \Theta |1, 0\rangle \\
&= |1, 0\rangle \\
&= |\lambda_1\rangle
\end{aligned}$$

$$\begin{aligned}
\Theta |\lambda_2\rangle &= \frac{1}{\sqrt{2}}(-\Theta |1, 1\rangle + \Theta |1, -1\rangle) \\
&= \frac{1}{\sqrt{2}}(|1, -1\rangle - |1, 1\rangle) \\
&= |\lambda_2\rangle
\end{aligned}$$

$$\begin{aligned}
\Theta |\lambda_3\rangle &= \frac{1}{\sqrt{2}}(\Theta |1, 1\rangle + \Theta |1, -1\rangle) \\
&= \frac{1}{\sqrt{2}}(-|1, -1\rangle - |1, 1\rangle) \\
&= -|\lambda_3\rangle
\end{aligned}$$

So we find that $|\lambda_3\rangle$ is odd under time reversal where the others are even. This exercise also shows that these combinations of states are eigenstates of the time reversal operator, as mentioned at the end of Section 5.4 of Scott's notes.