Homework Set 3 — Symmetries 2

Due April 13, 2020

1. (a) The plane wave is

$$\psi(\mathbf{x},t) = e^{i(\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar} - \omega t)} \tag{1}$$

Reversing the direction of momentum $\mathbf{p} \to -\mathbf{p}$ gives

$$\begin{aligned}\psi(\mathbf{x},t) &\to e^{i(-\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar} - \omega t)} && (2)\\ &= e^{-i(\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar} + \omega t)} && (3)\\ &= \psi^*(\mathbf{x},-t) && (4)\end{aligned}$$

(b) From Sakurai (3.2.52):

$$\chi(\hat{\mathbf{n}}) = \begin{pmatrix} \cos\frac{\beta}{2}e^{-i\alpha/2} \\ \sin\frac{\beta}{2}e^{i\alpha/2} \end{pmatrix}, \tag{5}$$

Note that this is defined so that

$$\sigma\cdot\hat{\mathbf{n}}\chi = \chi. \tag{6}$$

It has spin in the direction of $\hat{\mathbf{n}}$. (E.g., the usual spin up state for $\hat{\mathbf{n}} = \hat{z}$).

We then have

$$\begin{aligned}\chi^*(\hat{\mathbf{n}}) &= \begin{pmatrix} \cos\frac{\beta}{2}e^{i\alpha/2} \\ \sin\frac{\beta}{2}e^{-i\alpha/2} \end{pmatrix}, && (7)\\ -i\sigma_2\chi^*(\hat{\mathbf{n}}) &= -i\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} \cos\frac{\beta}{2}e^{i\alpha/2} \\ \sin\frac{\beta}{2}e^{-i\alpha/2} \end{pmatrix}, && (8)\\ &= \begin{pmatrix} -\sin\frac{\beta}{2}e^{-i\alpha/2} \\ \cos\frac{\beta}{2}e^{i\alpha/2} \end{pmatrix} && (9)\end{aligned}$$

But this has opposite eigenvalue:

$$\sigma \cdot \hat{\mathbf{n}}[-i\sigma_2\chi^*(\hat{\mathbf{n}})] = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \begin{pmatrix} -\sin\frac{\beta}{2}e^{-i\alpha/2} \\ \cos\frac{\beta}{2}e^{i\alpha/2} \end{pmatrix} \tag{10}$$

$$= \begin{pmatrix} \cos\beta & \sin\beta\cos\alpha - i\sin\beta\sin\alpha \\ \sin\beta\cos\alpha + i\sin\beta\sin\alpha & -\cos\beta \end{pmatrix} \begin{pmatrix} -\sin\frac{\beta}{2}e^{-i\alpha/2} \\ \cos\frac{\beta}{2}e^{i\alpha/2} \end{pmatrix} \tag{11}$$

$$= -\begin{pmatrix} -\sin\frac{\beta}{2}e^{-i\alpha/2} \\ \cos\frac{\beta}{2}e^{i\alpha/2} \end{pmatrix} \tag{12}$$

$$= -[-i\sigma_2\chi^*(\hat{\mathbf{n}})] \tag{13}$$

$\implies$ it is the two-component eigenspinor with spin direction reversed. (E.g., spin down for $\hat{\mathbf{n}} = \hat{z}$, or spin up for $\hat{\mathbf{n}} = -\hat{z}$)

2. (a) Time reversal commutes with the rotation operator:

$$\Theta\mathcal{D}\Theta^{-1} = \Theta e^{-iJ\cdot\hat{n}\theta/\hbar}\Theta^{-1} \tag{14}$$

$$= e^{-(\Theta iJ\Theta^{-1})\cdot\hat{n}\theta/\hbar} \tag{15}$$

$$= e^{-(\Theta i\Theta^{-1}\Theta J\Theta^{-1})\cdot\hat{n}\theta/\hbar} \tag{16}$$

$$= e^{-iJ\cdot\hat{n}\theta/\hbar} = \mathcal{D} \tag{17}$$

since $\Theta i\Theta^{-1} = -1$ and $\Theta J\Theta^{-1} =$ -J.

$\implies \Theta\mathcal{D} = \mathcal{D}\Theta$

So we have

$$\Theta\mathcal{D}(R)|j,m\rangle = \mathcal{D}(R)\Theta|j,m\rangle \tag{18}$$

$$= i^{2m}\mathcal{D}(R)|j,-m\rangle \tag{19}$$

(b) Consider

$$\langle j,-m'|\Theta\mathcal{D}(R)|j,-m\rangle = i^{-2m}\langle j,-m'|\mathcal{D}(R)|j,-m\rangle \tag{20}$$

$$= i^{-2m}\mathcal{D}^{(j)}_{-m'-m}(R) \tag{21}$$

(see part 2a).

But we also have

$$\langle j,-m'|\Theta\mathcal{D}(R)|j,-m\rangle = \sum_{m''}\langle j,-m'|\Theta\Big[|j,m''\rangle\langle j,m''|\mathcal{D}(R)|j,m\rangle\Big], \tag{22}$$

$$= \sum_{m''}\Big[\langle j,-m'|\Theta|j,m''\rangle\Big]\langle j,m''|\mathcal{D}(R)|j,m\rangle^*, \tag{23}$$

$$= i^{2m''}\sum_{m''}\langle j,-m'|j,-m''\rangle\langle j,m''|\mathcal{D}(R)|j,m\rangle^* \tag{24}$$

$$= i^{2m''}\sum_{m''}\delta_{m',m''}\langle j,m''|\mathcal{D}(R)|j,m\rangle^* \tag{25}$$

$$= i^{2m''}\langle j,m'|\mathcal{D}(R)|j,m\rangle^* \tag{26}$$

$$= i^{2m''}\mathcal{D}^{(j)*}_{m'm}(R) \tag{27}$$

(Note that Θ acts on everything to the right, and hence the complex conjugation in the second line.)

Comparing the two results, we have:

$$\mathcal{D}^{(j)*}_{m'm}(R) = i^{-2(m'+m)}\mathcal{D}^{(j)}_{-m'-m}(R), \tag{28}$$

3. Since both $\mathbf{p}^2$ and $\mathbf{x}$ are invariant under time reversal, so is H: $[H,\Theta]=0$. If there is no degeneracy, any energy eigenstate $|\alpha\rangle$ must also be an eigenstate of Θ:

$$\Theta|\alpha\rangle = |\tilde{\alpha}\rangle = e^{-\delta}|\alpha\rangle \tag{29}$$

The expectation $\langle\mathbf{L}\rangle$ is real, since $\mathbf{L}$ is Hermitian:

$$\langle\mathbf{L}\rangle = \langle\mathbf{L}^\dagger\rangle^* \tag{30}$$

$$= \langle\mathbf{L}\rangle^* \tag{31}$$

If we define $|\beta\rangle \equiv \mathbf{L}|\alpha\rangle$, then by the antiunitarity of time reversal:

$$\begin{aligned}
\langle\alpha|\mathbf{L}|\alpha\rangle &= \langle\alpha|\beta\rangle && (32)\\
&= \langle\tilde{\alpha}|\tilde{\beta}\rangle^* && (33)\\
&= \langle\tilde{\alpha}|\tilde{\beta}\rangle && (34)\\
&= \langle\tilde{\alpha}|\Theta\mathbf{L}|\alpha\rangle && (35)\\
&= \langle\tilde{\alpha}|\Theta\mathbf{L}\Theta^{-1}\Theta|\alpha\rangle && (36)\\
&= -\langle\tilde{\alpha}|\mathbf{L}\Theta|\alpha\rangle && (37)\\
&= -\langle\tilde{\alpha}|\mathbf{L}|\tilde{\alpha}\rangle && (38)\\
&= -e^{-i\delta}\langle\alpha|\mathbf{L}|\alpha\rangle e^{i\delta} && (39)\\
&= -\langle\alpha|\mathbf{L}|\alpha\rangle && (40)\\
\implies \langle\mathbf{L}\rangle &= 0 && (41)
\end{aligned}$$

If we expand the wavefunction in spherical harmonics:

$$\begin{aligned}
\psi_\alpha(\mathbf{x}) &\equiv \langle\mathbf{x}|\alpha\rangle && (42)\\
&= \sum_{l,m}\langle\mathbf{x}|l,m\rangle\langle l,m|\alpha\rangle && (43)\\
&= \sum_{l,m} F_{l,m}(r)Y_l^m(\theta,\phi), && (44)
\end{aligned}$$

then

$$\begin{aligned}
\langle\mathbf{x}|\tilde{\alpha}\rangle &= \langle\mathbf{x}|\Theta|\alpha\rangle && (45)\\
&= e^{i\delta}\langle\mathbf{x}|\alpha\rangle && (46)\\
\implies \langle\mathbf{x}|\alpha\rangle &= e^{-i\delta}\langle\mathbf{x}|\tilde{\alpha}\rangle && (47)\\
&= e^{-i\delta}\psi_\alpha^*(\mathbf{x}) && (48)\\
&= e^{-i\delta}\sum_{l,m} F_{l,m}^*(r)[Y_l^m(\theta,\phi)]^* && (49)\\
&= e^{-i\delta}\sum_{l,m} F_{l,m}^*(r)(-1)^m Y_l^{-m}(\theta,\phi) && (50)\\
&= e^{-i\delta}\sum_{l,m} F_{l,-m}^*(r)(-1)^{-m} Y_l^{m}(\theta,\phi) && (51)
\end{aligned}$$

Comparing the coefficients to Y_l^m:

$$F_{l,m} = (-1)^{-m} e^{-i\delta} F^*_{l,-m}(r) \tag{52}$$

4. The Hamiltonian for a spin 1 system is given by

$$H = AS_z^2 + B(S_x^2 - S_y^2). \tag{53}$$

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 this Hamiltonian invariant under time reversal? How do the normalized eigenstates you obtained transform under time reversal?

For a spin 1 system the spin operators have the form

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{54}$$

$$S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \tag{55}$$

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{56}$$

And so the Hamiltonian is:

$$H = AS_z^2 + B(S_x^2 - S_y^2) \tag{57}$$

$$= \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix} \tag{58}$$

The eigenvalues are 0, $A \pm B$, with eigenvectors (0,1,0), (1,0,1)/$\sqrt{2}$, (1,0,-1)/$\sqrt{2}$, respectively.

Or, in terms of $|s, s_z\rangle$:

$$\begin{cases} |1,0\rangle & 0 \\ \frac{1}{\sqrt{2}}\left(|1,1\rangle + |1,-1\rangle\right) & A+B \\ \frac{1}{\sqrt{2}}\left(|1,1\rangle - |1,-1\rangle\right) & A-B \end{cases} \tag{59}$$

Assume A and B are real (otherwise H is not Hermitian). Then:

$$\Theta H \Theta^{-1} = A\Theta S_z \Theta^{-1}\Theta S_z \Theta^{-1} + B(\Theta S_x \Theta^{-1}\Theta S_x \Theta^{-1} - \Theta S_y \Theta^{-1}\Theta S_y \Theta^{-1}) \tag{60}$$

$$= A(-S_z)^2 + B[(-S_x)^2 - (-S_y)^2] \tag{61}$$

$$= H \tag{62}$$

The Hamiltonian is invariant under time reversal.

We know that $\Theta|lm\rangle = (-1)^m|l, -m\rangle$, so the first and third eigenstates (eigenvalues 0 and $A - B$) are invariant under time reversal, while the other (eigenvalue $A + B$) is odd under time reversal

$$\begin{cases} \Theta|1,0\rangle = |1,0\rangle \\ \Theta\frac{1}{\sqrt{2}}\left(|1,1\rangle + |1,-1\rangle\right) = -\frac{1}{\sqrt{2}}\left(|1,1\rangle + |1,-1\rangle\right) \\ \Theta\frac{1}{\sqrt{2}}\left(|1,1\rangle - |1,-1\rangle\right) = \frac{1}{\sqrt{2}}\left(|1,1\rangle - |1,-1\rangle\right) \end{cases} \tag{63}$$