Problem Set 2

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Problem 1:
Solution:

(a)
$[\mathcal{T}_d, \mathcal{T}_{d'}] = 0$. We can show this as follows,

$$\mathcal{T}_d \mathcal{T}_{d'} = e^{-i\mathbf{d}\cdot\mathbf{p}/\hbar} e^{-i\mathbf{d}'\cdot\mathbf{p}/\hbar} = e^{-i\mathbf{d}'\cdot\mathbf{p}/\hbar} e^{-i\mathbf{d}\cdot\mathbf{p}/\hbar} = \mathcal{T}_{d'} \mathcal{T}_d$$

Hence, $\mathcal{T}_{d'}\mathcal{T}_d - \mathcal{T}_d\mathcal{T}_{d'} = 0$.

(b)
$[\mathcal{D}(\hat{n}, \phi), \mathcal{D}(\hat{n}', \phi)] \neq 0$. This is because rotation operators do not commute, as we have seen before.

(c)
$[\mathcal{T}, \Pi] \neq 0$. If we first operate the translation operator on a state, followed by the parity operator, the state will first be shifted then flipped. Clearly, this does not have the same effect of first flipping the state, followed by translation. Hence, the operators do not commute.

(d)
$[\mathcal{D}(\hat{n},\phi),\Pi] = 0$. Rotation of a state followed by flipping sign will have the same effect as first flipping the sign, then rotating. Hence, these operators commute.

Problem 2:
Solution:

Given that a state Ψ is an eigenstate of each A and B and that $\{A, B\} = 0$. Operating this on $|\Psi\rangle$,

$$\{A, B\}|\Psi\rangle = (AB + BA)|\Psi\rangle$$

Let a be an eigenvalue of A and b be an eigenvalue of B. Then the above becomes,

$$(AB+BA)|\Psi\rangle = AB|\Psi\rangle+BA|\Psi\rangle = bA|\Psi\rangle+aB|\Psi\rangle = ba|\Psi\rangle+ab|\Psi\rangle = 2ab|\Psi\rangle$$

Hence, for these to anti-commute we must have that a or b equal 0. We must have a state with - momentum given that the eigenstates of Π are ± 1. Here, A and B are general operators. These operators share the same property of Π and $\mathbf{p}$ in that the both anti-commute.

Problem 3:
Solution:

(a)
A plane wave wave function would have the form $\psi(\mathbf{x}, t) = e^{i\mathbf{p}\cdot\mathbf{x}}e^{-iEt/\hbar}$. Hence, $\psi^\star(\mathbf{x}, -t) = e^{-i\mathbf{p}\cdot\mathbf{x}}e^{-iEt/\hbar}$. Hence, under time reversal $\mathbf{p} \to -\mathbf{p}$. So, $\psi^\star(\mathbf{x}, -t) = \psi(\mathbf{p}, t)$.

(b)
We can take $\chi(\hat{n})$ to be an eigenspinor of $\sigma \cdot \hat{\mathbf{n}}$ with eigenvalue 1., If we write it in spherical coordinates, we get

$$\chi_+ = \begin{pmatrix} \cos\theta/2 \\ e^{i\phi}\sin(\theta/2) \end{pmatrix}$$

Now applying,

$$-i\sigma_y\chi_+^\star = -i\sigma_y \begin{pmatrix} \cos\theta/2 \\ e^{-i\phi}\sin(\theta/2) \end{pmatrix} = -i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \cos\theta/2 \\ e^{-i\phi}\sin(\theta/2) \end{pmatrix} = \begin{pmatrix} -e^{-i\phi}\sin(\theta/2) \\ \cos\theta/2 \end{pmatrix}$$

Hence, we have proved that $-i\sigma_y\chi_+^\star = \chi_-$.

Problem 4:
Solution:

(a)
If the Hamiltonian is invariant under time reversal, then $[\mathcal{H}, \Theta] = 0$. If we have a spinless nondegenerate particle, we can take its state to be

$$|\alpha\rangle = \int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle$$

Now applying Θ gives

$$\Theta|\alpha\rangle = K|\alpha\rangle = \int d^3x' K|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^\star = \int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^\star$$

Let the wave function be $\psi(\mathbf{x}) = \langle\mathbf{x}|\alpha\rangle$. Hence, we notice that the above result will always be satisfied when $\psi(\mathbf{x}) = \psi^\star(\mathbf{x})$. This would give us,

$$\Theta|\alpha\rangle = \int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle^\star$$

This implies that it would be fine to use a real wave function here.

(b)
If we have a plane wave state at $t = 0$ given by,

$$|\mathbf{x}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p' e^{i\mathbf{x}\cdot\mathbf{p}'/\hbar}|\mathbf{p}'\rangle$$

Hence,

$$\Theta|\mathbf{x}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p' e^{-i\mathbf{x}\cdot\mathbf{p}'/\hbar}|-\mathbf{p}'\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p' e^{i\mathbf{x}\cdot\mathbf{p}'/\hbar}|\mathbf{p}'\rangle = |\mathbf{x}\rangle$$

Hence, it does not matter if the wave function is complex. Time reversal invariance is still preserved. Another way to look at this is that both the plane wave and its complex conjugate have the same energy. Since we have this degeneracy, the Hamiltonian commutes with the time reversal operator so that it's still time reversal invariant.

Problem 5:
Solution:

(a)
Provided the Hamiltonian,

$$\mathcal{H} = E_0 - t(|1\rangle\langle 2| + |2\rangle\langle 3| + |4\rangle\langle 5| + |5\rangle\langle 6| + |6\rangle\langle 1| + h.c.) = E_0 - t\sum_{n=1}^{6}(|n\rangle\langle n+1| + |n+1\rangle\langle n|)$$

we can identify that the Hamiltonian has 6-fold rotational symmetry, as well as translational symmetry . Paying specific attention to the translation operator, we can obtain the eigenvalues and eigenstates. Here, we can let $\theta = \frac{2\pi}{6} = \frac{\pi}{3}$ since the molecule has a periodicity of 6 atoms.

$$\tau(a)|\theta\rangle = \sum_{n=1}^{6} e^{in\theta}|n+1\rangle = \sum_{n=1}^{6} e^{i(n-1)\theta}|n\rangle = e^{i\theta}|\theta\rangle$$

where θ is the eigenstate and $e^{i\theta}$ is the eigenvalue.

(b)
We can now find the eigenvalues and wave functions of the Hamiltonian by operating $\mathcal{H}|\theta\rangle$.

$$\mathcal{H}|\theta\rangle = \sum_{n=1}^{6} e^{i(n-1)\theta}\mathcal{H}|n\rangle$$

$$= \sum_{n=1}^{6} e^{i(n-1)\theta}[E_0 - t\sum_{n=1}^{6}(|n\rangle\langle n+1| + |n+1\rangle\langle n|)]|n\rangle$$

$$= \sum_{n=1}^{6} e^{i(n-1)\theta}[E_0 - t\sum_{n=1}^{6}(|n\rangle\langle n+1|n\rangle + |n+1\rangle\langle n|n\rangle)]$$

$$= \sum_{n=1}^{6} e^{i(n-1)\theta}[E_0 - t\sum_{n=1}^{6}|n+1\rangle)]$$

$$= \sum_{n=1}^{6} E_0 e^{i(n-1)\theta} - te^{i(n-1)\theta}\sum_{n=1}^{6}|n+1\rangle)$$

Giving us eigenvalues, $\epsilon = E_0 - t(e^{i\theta} + e^{-i\theta}) = E_0 - t\cos\theta$. The associated wave functions are given by $\psi_n = e^{i\theta n}$.