Homework #2

1 (Griffiths 6.1)

a) Show that the parity operator $\Pi\Psi(\vec{r}) = \Psi(-\vec{r})$ is equivalent to a mirror reflection followed by a rotation

$$\Pi\Psi(\vec{r}) = \Psi(-\vec{r})$$

is the same as, in Cartesian coordinates,

$$\Pi\Psi(x,y,z) = \Psi(-x,-y,-z)$$

A mirror reflection across the xy-plane changes $z \to -z$, i.e.

$$M\Psi(x,y,z) = \Psi(x,y,-z) \qquad \text{Eqn. 1}$$

where M is a mirror operator.

A rotation about the z-axis by π will change $x \to -x$ and $y \to -y$, i.e.

$$R_z(\pi)\Psi(x,y,z) = \Psi(-x,-y,-z) \qquad \text{Eqn. 2}$$

where $R_n(\varphi)$ is the operator for a rotation by φ about the $\hat{n}$ axis.

Putting Eqn.'s 1 & 2 together, we have

$$R_z(\pi)\left[M\Psi(x,y,z)\right] = \Psi(-x,-y,-z) \quad \text{Q.E.D.}$$

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b) Show that for $\psi(r,\theta,\phi)$,

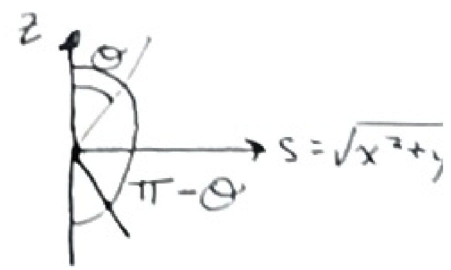
$$\Pi\,\psi(r,\theta,\phi) = \psi(r,\pi-\theta,\phi+\pi)$$

Let's look at the connection between polar and Cartesian coordinates.

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

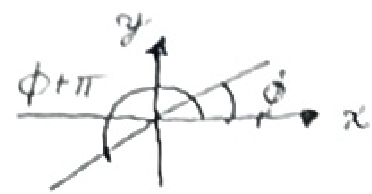
If $\theta \to \pi - \theta$:

$$\sin(\pi-\theta) = \sin\theta$$
$$\cos(\pi-\theta) = -\cos\theta$$



If $\phi \to \phi + \pi$:

$$\cos(\phi+\pi) = -\cos\phi$$
$$\sin(\phi+\pi) = -\sin\phi$$



Substituting these into our definitions of x, y, z:

$$x' = r\sin(\pi-\theta)\cos(\phi+\pi) = -r\sin\theta\cos\phi = -x$$
$$y' = r\sin(\pi-\theta)\sin(\phi+\pi) = -r\sin\theta\sin\phi = -y$$
$$z' = r\cos(\pi-\theta) = -r\cos\theta = -z$$

Q.E.D.

HW #2

c) Show that for hydrogenic orbitals

$$\Pi \psi_{n\ell m}(r, \theta, \phi) = (-1)^\ell \psi_{n\ell m}(r, \theta, \phi)$$

Hydrogenic orbitals have the form

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_\ell^m(\theta, \phi)$$

Now, r is unchanged by parity

$$\Pi R_{n\ell}(r) = R_{n\ell}(r)$$

so, all we need to look at is the $Y_\ell^m(\theta, \phi)$ terms (which is why this generalizes!).

$$Y_\ell^m(\theta, \phi) = C_\ell^m e^{im\phi} P_\ell^m(\cos\theta)$$

with C_ℓ^m being a normalization constant unaffected by parity. Thus, we have

$$\Pi\left(e^{im\phi} P_\ell^m(\cos\theta)\right)$$

From above, parity changes $\phi \to \pi + \phi$ and $\theta \to \pi - \theta$

$$\Pi\left(e^{im\phi} P_\ell(\cos\theta)\right) = e^{im(\phi+\pi)} P_\ell^m(\cos(\pi - \theta))$$

$$= e^{im\phi} e^{im\pi} P_\ell^m(-\cos\theta)$$

$$= (-1)^m e^{im\phi} P_\ell^m(-\cos\theta) \quad \text{Eqn. 1}$$

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HW #2 1D

The $P_\ell^m(-\cos\theta)$ are defined as (Eqn. 4.27 in text):

$$P_\ell^m(-x) = (-1)^m (1-x^2)^{m/2} \left(-\frac{d}{dx}\right)^m P_\ell(-x)$$

The $P_\ell(-x)$ are even functions if $\ell \in 2n$ and odd functions if $\ell \in 2n+1$ so

$$P_\ell(-x) = (-1)^\ell P_\ell(x)$$

$$\therefore P_\ell^m(-x) = (-1)^m (-1)^\ell P_\ell(x)$$

Which, substituting back into Eqn. 1

$$\Pi Y_\ell^m(\theta,\phi) = (-1)^m (-1)^m (-1)^\ell Y_\ell^m(\theta,\phi)$$

$$= (-1)^{2m} (-1)^\ell Y_\ell^m(\theta,\phi)$$

$$= (-1)^\ell Y_\ell^m(\theta,\phi)$$

Q.E.D.

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HW#2 2A

2. (Griffiths 6.2) Show that if $Q^{+} = Q$, then $U = \exp[iQ]$ is unitary.

$$U = \exp[iQ]$$

$$U = 1 + iQ + \frac{(iQ)^2}{2!} + \frac{(iQ)^3}{3!} + \dots$$

$$U = 1 + iQ - \frac{Q^2}{2!} - \frac{iQ^3}{3!}$$

$$U^{+} = 1 - iQ^{+} - \frac{1}{2!} Q^{+}Q^{+} + \frac{i}{3!} Q^{+}Q^{+}Q^{+} + \dots$$

$$U^{+} = 1 - iQ^{+} - \frac{1}{2!}(Q^{+})^2 + \frac{i}{3!}(Q^{+})^3 + \dots$$

$$U^{+} = \exp[-iQ^{+}]$$

Since $Q = Q^{+}$ by definition,

$$U^{+} = \exp[-iQ]$$

$$U^{+}U = e^{-iQ} e^{+iQ}$$

$$= e^{i(-Q+Q)}$$

True $\because [Q, Q] = 0$

$$= 1$$

Q.E.D.

HW #2

3A

3. (Griffiths 6.9) Show that for the "true" scalar s, $[\Pi, s] = 0$ while for the pseudoscalar p, $\{\Pi, p\} = 0$.

For the "true" scalar

$$\Pi^{+} s \Pi = s$$

by definition. Left multiply by Π:

$$\underbrace{\cancel{\Pi \Pi^{+}}}_{1} s \Pi = \Pi s$$

$$s \Pi = \Pi s$$

$$0 = \Pi s - s \Pi = [\Pi, s]$$

For the pseudoscalar p:

$$\Pi^{+} p \Pi = -p$$

Again, left multiply by Π

$$\underbrace{\cancel{\Pi \Pi^{+}}}_{1} p \Pi = -\Pi p$$

$$p \Pi = -\Pi p$$

$$0 = -\Pi p - p \Pi$$

$$0 = \Pi p + p \Pi = \{\Pi, p\}$$

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Homework #2 3B

b) Repeat for a vector $\vec{V}$ and axial vector $\vec{A}$

The proofs work just as before:

$$\Pi^{+}\vec{V}\Pi = -\vec{V} \rightarrow \{\Pi, \vec{V}\} = 0$$

and

$$\Pi^{+}\vec{A}\Pi = A \rightarrow [\Pi, \vec{A}] = 0$$

4. (Griffiths 6.10) Show that the position and momentum operators are odd under parity.

Let $|\psi'\rangle \equiv \Pi |\psi\rangle$

Now, the definition of parity is that $x \to -x$, $y \to -y$, $z \to -z$; i.e.

$$\langle \psi' | \vec{r} | \psi' \rangle = -\langle \psi | \vec{r} | \psi \rangle$$

You can see this from the fact that expectation values must match the classical results.

Substituting back:

$$(\langle \psi | \Pi^\dagger) \vec{r} (\Pi | \psi \rangle) = -\langle \psi | \vec{r} | \psi \rangle$$

Moving the parentheses around, we see that the quantity inside the parentheses on the LHS is the transformation of $\vec{r}$:

$$\langle \psi | (\Pi^\dagger r \Pi) | \psi \rangle = \langle \psi | (-\vec{r}) | \psi \rangle$$

$\therefore \Pi^\dagger \vec{r} \Pi = -\vec{r}$ Q.E.D.

For momentum, we only need do a bit more work. Since parity takes $v_x \Rightarrow -v_x$, $v_y \Rightarrow -v_y$, $v_z \Rightarrow -v_z$, we again have

$$\langle \psi' | \vec{p} | \psi' \rangle = -\langle \psi | p | \psi \rangle$$

where ψ' is again defined as

$$|\psi'\rangle \equiv \Pi |\psi\rangle$$

$$\left(\langle \psi | \Pi^{+}\right) \vec{p} \left(\Pi |\psi\rangle\right) = -\langle \psi | \vec{p} | \psi \rangle$$

$$\langle \psi | \left(\Pi^{+} \vec{p}\, \Pi\right) | \psi \rangle = \langle \psi | (-\vec{p}) | \psi \rangle$$

$$\therefore \; \Pi^{+} \vec{p}\, \Pi = -\vec{p} \quad \text{Q.E.D.}$$

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5A

HW #2

4. (Griffiths 6.11) Under what conditions is the matrix element $\langle n'l'm'|\vec{L}|nlm\rangle$ guaranteed to vanish?

Angular momentum is an axial vector which means that

$$\Pi^{+}\vec{L}\,\Pi = \vec{L}$$

Which means I can replace $\vec{L}$ in

$$\langle n'l'm'|\vec{L}|nlm\rangle$$

with

$$\langle n'l'm'|\Pi^{+}\vec{L}\,\Pi|nlm\rangle$$

From Griffiths 6.1 (problem 1 in this HW):

$$\langle n'l'm'|(-1)^{l'}\vec{L}(-1)^{l}|nlm\rangle$$

which, again because $\Pi^{+}\vec{L}\Pi = \vec{L}$,

$$\langle n'l'm'|(-1)^{l'}\vec{L}(-1)^{l}|nlm\rangle = \langle n'l'm'|\vec{L}|nlm\rangle$$

$$(-1)^{l'+l}\langle n'l'm'|\vec{L}|nlm\rangle = \langle n'l'm'|\vec{L}|nlm\rangle$$

which is not true unless $l'+l \in 2n$, ie. the two states must have the same parity.

6A

6. (Griffiths 6.13) Consider an e^- in an H-atom.

a) Show that if the electron is in the ground state, then

$$\langle P_e \rangle = 0$$

NO CALCULATION!

Again, using our definition of parity from 6.10,

$$\langle \psi_1' | \vec{P}_e | \psi_2' \rangle = -\langle \psi_1 | \vec{P}_e | \psi_2 \rangle$$

$$\langle \psi_1 | \Pi^\dagger \vec{P}_e \Pi | \psi_2 \rangle = -\langle \psi_1 | \vec{P}_e | \psi_2 \rangle$$

In the case of hydrogen,

$$|\psi\rangle = |n l m\rangle$$

$$\langle n_1 l_1 m_1 | \Pi^\dagger \vec{P}_e \Pi | n_2 l_2 m_2 \rangle = \langle n_1 l_1 m_1 | (-\vec{P}_e) | n_2 l_2 m_2 \rangle$$

In a prior problem, you showed

$$\Pi |n l m\rangle = (-1)^l |n l m\rangle$$

6B

$$\therefore \langle n_1 l_1 m_1 | (-1)^{l_1} \vec{R}_e (-1)^{l_2} | n_2 l_2 m_2 \rangle = \langle n_1 l_1 m_1 | -\vec{R}_e | n_2 l_2 m_2 \rangle$$

Combining the $(-1)^{l_i}$ (they are numbers) and rewriting $(-1) = (-1)^{2j+1}$, we have

$$\langle n_1 l_1 m_1 | (-1)^{l_1+l_2} \vec{R}_e | n_2 l_2 m_2 \rangle = \langle n_1 l_1 m_1 | (-1)^{2j+1} R_e | n_2 l_2 m_2 \rangle$$

The only ways this can be true are if either

$$(-1)^{l_1+l_2} = (-1)^{2j+1} \rightarrow l_1 + l_2 = 2j+1$$

or if $\langle P_e \rangle = 0$

In the case of the ground state:

$l_1 = l_2 = 0 \neq$ an odd number

$\therefore \langle P_e \rangle = 0$ Q.E.D.

6C

b) Show that if $n=2$, $\langle p_e \rangle \neq 0$ necessarily. Give an example and compute $\langle p_e \rangle$.

The only way to get $l_1 + l_2 \in$ odd is to do a superposition:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_{200}\rangle + |\psi_{210}\rangle\right)$$

Then

$$\langle p_e \rangle = \frac{1}{2}\left[\langle \psi_{200}| + \langle \psi_{210}|\right] p_e \left[|\psi_{200}\rangle + |\psi_{210}\rangle\right]$$

$$= \frac{1}{2}\Big[\cancel{\langle \psi_{200}|p_e|\psi_{200}\rangle} + \cancel{\langle \psi_{210}|p_e|\psi_{210}\rangle} + \langle \psi_{200}|p_e|\psi_{210}\rangle + \langle \psi_{210}|p_e|\psi_{200}\rangle\Big]$$

These terms $\to 0$ because $l_1 + l_2 \in$ even

$$\langle \psi_{200}|p_e|\psi_{210}\rangle + \langle \psi_{210}|p_e|\psi_{200}\rangle = 2\,\mathrm{Re}\left[\langle \psi_{210}|p_e|\psi_{200}\rangle\right]$$

$$\therefore \langle p_e \rangle = \mathrm{Re}\left[\langle 210|p_e|200\rangle\right]$$

Now, to compute the matrix element, recall

$$\vec{p}_e = q\vec{r}$$

6D

$$\therefore \langle p_e \rangle = \mathrm{Re}\{ -e\langle 210|x|200\rangle \hat{x} - e\langle 210|y|200\rangle \hat{y} - e\langle 210|z|200\rangle \hat{z} \}$$

$$= -e\,\mathrm{Re}\{ \int \psi_{210}^{*} (r\sin\theta\cos\phi)\psi_{200}\, d^3r\, \hat{x} + \int \psi_{210}^{*} (r\sin\theta\sin\phi)\psi_{200}\, d^3r\, \hat{y} + \int \psi_{210}^{*} (r\cos\theta)\psi_{200}\, d^3r\, \hat{z} \}$$

When you put in the actual functions:

$$\psi_{200} = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2}} \frac{1}{2\sqrt{2}\, a_0^{3/2}} \left[2 - \frac{r}{a_0}\right] e^{-r/2a_0}$$

$$\psi_{210} = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{6}}{2} \cos\theta \frac{1}{2\sqrt{6}\, a^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$$

and calculate the integrals with Mathematica, you see that only the $\hat{z}$ term remains and

$$\langle p_e \rangle = 3ea\,\hat{z}$$