HW1 solution[1] - Phys487 Spring 2015

Problem 1 (6 points)

The permutation matrices are:

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad P_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad P_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$P_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad P_4 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad P_5 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Indeed

$$I \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad P_1 \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} \quad P_2 \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix}$$

$$P_3 \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix} \quad P_4 \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \\ 1 \end{pmatrix} \quad P_5 \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix}$$

The permutation matrices satisfy $I^2 = P_1^2 = P_2^2 = P_3^2 = I$, $P_4^3 = P_4 P_4^2 = P_4 P_5 = I$ and $P_5^3 = P_5 P_5^2 = P_5 P_4 = I$. This means that $\{I, P_1\}, \{I, P_2\}, \{I, P_3\}$ and $\{I, P_4, P_5\}$ form subgroups of the larger permutation matrix group $\{I, P_1, P_2, P_3, P_4, P_5\}$.

Griffiths 5.1 (9 points)

(a)

$$\mathbf{R} + \frac{\mu}{m_1}\mathbf{r} = \frac{m_1\mathbf{r_1} + m_2\mathbf{r}_2}{m_1 + m_2} + \frac{m_2}{m_1 + m_2}(\mathbf{r}_1 - \mathbf{r}_2) = \mathbf{r}_1$$
$$\mathbf{R} - \frac{\mu}{m_2}\mathbf{r} = \frac{m_1\mathbf{r_1} + m_2\mathbf{r}_2}{m_1 + m_2} - \frac{m_1}{m_1 + m_2}(\mathbf{r}_1 - \mathbf{r}_2) = \mathbf{r}_2$$

Considering $\mathbf{R} = \mathbf{R}(\mathbf{r}_1, \mathbf{r}_2)$ and $\mathbf{r} = \mathbf{r}(\mathbf{r}_1, \mathbf{r}_2)$

$$\nabla_1 = \frac{\partial}{\partial \mathbf{r}_1} = \frac{\partial \mathbf{R}}{\partial \mathbf{r}_1}\frac{\partial}{\partial \mathbf{R}} + \frac{\partial \mathbf{r}}{\partial \mathbf{r}_1}\frac{\partial}{\partial \mathbf{r}} = \frac{\mu}{m_2}\nabla_R + \nabla_r$$
$$\nabla_2 = \frac{\partial}{\partial \mathbf{r}_2} = \frac{\partial \mathbf{R}}{\partial \mathbf{r}_2}\frac{\partial}{\partial \mathbf{R}} + \frac{\partial \mathbf{r}}{\partial \mathbf{r}_2}\frac{\partial}{\partial \mathbf{r}} = \frac{\mu}{m_1}\nabla_R - \nabla_r$$

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(b)

$$\begin{aligned}
\nabla_{1,2}^2\psi &= \nabla_{1,2}\left(\frac{\mu}{m_{2,1}}\nabla_R\psi + \nabla_r\psi\right) \\
&= \frac{\mu}{m_{2,1}}\nabla_R\left(\frac{\mu}{m_{2,1}}\nabla_R\psi + \nabla_r\psi\right) + \nabla_r\left(\frac{\mu}{m_{2,1}}\nabla_R\psi + \nabla_r\psi\right) \\
&= \left(\frac{\mu}{m_{2,1}}\right)^2\nabla_R^2\psi + 2\frac{\mu}{m_{2,1}}(\nabla_R\nabla_r)\psi + \nabla_r^2\psi
\end{aligned}$$

Therefore,

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2\right]\psi = -\frac{\hbar^2}{2}\left[\frac{\mu^2}{m_1m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\nabla_R^2 + \left(\frac{1}{m_1}+\frac{1}{m_2}\right)\nabla_r^2\right]\psi$$

and since $\mu = m_1m_2/(m_1+m_2)$, then

$$-\frac{\hbar^2}{2(m_1+m_2)}\nabla_R^2\psi - \frac{\hbar^2}{2\mu}\nabla_r^2\psi + V(\mathbf{r})\psi = E\psi$$

(c) Put in $\psi_r(\mathbf{r})\psi_R(\mathbf{R})$ and divide by $\psi_r\psi_R$

$$\underbrace{\left[-\frac{\hbar^2}{2(m_1+m_2)\psi_R}\nabla^2\psi_R\right]}_{E_R} + \underbrace{\left[-\frac{\hbar^2}{2\mu\psi_r}\nabla^2\psi_r + V(\mathbf{r})\right]}_{E_r} = E$$

The first term depends only on $\mathbf{R}$ and the second only on $\mathbf{r}$, so each must be a constant; call them E_R and E_r respectively. Then $E_R + E_r = E$.

Griffiths 5.4 (6 points)

(a) The (anti)symmetrized wavefunction is $\psi_\pm(r_1,r_2) = \psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_1)\psi_a(r_2)$

$$\begin{aligned}
1 &= \int |\psi_\pm(r_1,r_2)|^2 d^3r_1 d^3r_2 \\
&= |A|^2\left[\int |\psi_a(r_1)|^2 d^3r_1 \int |\psi_b(r_2)|^2 d^3r_2 + \int |\psi_b(r_1)|^2 d^3r_1 \int |\psi_a(r_2)|^2 d^3r_2\right. \\
&\left.\pm \int \psi_a(r_1)^*\psi_b(r_1)d^3r_1 \int \psi_b(r_2)^*\psi_a(r_2)d^3r_2 \pm \int \psi_b(r_1)^*\psi_a(r_1)d^3r_1 \int \psi_a(r_2)^*\psi_b(r_2)d^3r_2\right] \\
&= |A|^2(1+1\pm 0\pm 0)
\end{aligned}$$

Therefore $A = 1/\sqrt{2}$.
(b) In this case $\psi_+(r_1,r_2) = 2\psi_a(r_1)\psi_a(r_2)$

$$1 = 4|A|^2\int |\psi_a(r_1)|^2 d^3r_1 \int |\psi_a(r_2)|^2 d^3r_2$$

Therefore $A = 1/2$.

Griffiths 5.6 (9 points)

(a) From Griffiths 5.19, $\langle (x_1 - x_2)^2 \rangle = \langle x^2 \rangle_n + \langle x^2 \rangle_m - 2\langle x \rangle_n \langle x \rangle_m$, where the terms on the right-hand side are given by $\langle x \rangle_n = \frac{2}{a}\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a}{2}$ and $\langle x^2 \rangle_n = \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = a^2(1/3 - 1/(2n^2\pi^2))$. We have used the following *Mathematica* codes for computing the integrals:
'Simplify[Integrate[$x \sin^2[n\pi x/a], \{x, 0, a\}$], $n \in$Integers]' and
'Simplify[Integrate[$x^2 \sin^2[n\pi x/a], \{x, 0, a\}$], $n \in$Integers]'. Therefore

$$\langle (x_1 - x_2)^2 \rangle = a^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right) + a^2\left(\frac{1}{3} - \frac{1}{2m^2\pi^2}\right) - \frac{a^2}{2} = a^2\left[\frac{1}{6} - \frac{1}{2\pi^2}\left(\frac{1}{n^2} + \frac{1}{m^2}\right)\right]$$

(b,c) Because of (anti)symmetrization of the wavefunctions (Griffiths 5.21), we have $\langle (x_1 - x_2)^2 \rangle = \langle x^2 \rangle_n + \langle x^2 \rangle_m - 2\langle x \rangle_n \langle x \rangle_m \mp 2|\langle x \rangle_{nm}|^2$ ($-$ for bosons and $+$ for fermions). We only have to calculate the last term: $\langle x \rangle_{nm} = \frac{2}{a}\int_0^a x \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right) dx = [-1 + (-1)^{m+n}]\frac{4anm}{\pi^2(n^2-m^2)^2}$. We have used 'Simplify[Integrate[$x \sin[n\pi x/a]\sin[m\pi x/a], \{x, 0, a\}$], $\{n, m\} \in$ Integers]'. Therefore

$$\langle (x_1 - x_2)^2 \rangle = a^2\left[\frac{1}{6} - \frac{1}{2\pi^2}\left(\frac{1}{n^2} + \frac{1}{m^2}\right)\right] \mp [-1 + (-1)^{m+n}]^2 \frac{32a^2n^2m^2}{\pi^4(n^2 - m^2)^4}$$

Griffiths 5.11 (6 points)

(a) Considering $\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a}$, then

$$\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \left(\frac{8}{\pi a^3}\right)^2 \int d^3r_1 \left[2\pi \int_0^\infty dr_2\, r_2^2 e^{-4(r_1+r_2)/a} \int_0^\pi d\theta_2 \frac{\sin\theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\theta_2}}\right]$$

Using 'Simplify[Integrate[$\sin[\theta_2]/\sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos[\theta_2]}, \{\theta_2, 0, \pi\}$], $\{r_1, r_2\} \in$ Reals && $r_1 > 0$ && $r_2 > 0$]', we have

$$\int_0^\pi d\theta_2 \frac{\sin\theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\theta_2}} = \begin{cases} 2/r_1 & \text{if } r_2 < r_1 \\ 2/r_2 & \text{if } r_2 > r_1 \end{cases}$$

Therefore

$$\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = 4\pi \left(\frac{8}{\pi a^3}\right)^2 \int d^3r_1 e^{-4r_1/a} \left[\frac{1}{r_1}\int_0^{r_1} dr_2\, r_2^2 e^{-4r_2/a} + \int_{r_1}^\infty dr_2\, r_2 e^{-4r_2/a}\right]$$

Using 'Simplify[Integrate[r_2^2/r_1 Exp[$-4r_2 a$], $\{r_2, 0, r_1\}$] +Integrate[r_2 Exp[$-4r_2 a$], $\{r_2, r_1, \infty\}$], $\{a, r_1\} \in$ Reals && $a > 0$ && $r_1 > 0$]', the term enclosed in brakets is equal to $\frac{a^2}{32r_1}[a - (2r_1 + a)e^{-4r_1/a}]$. Then

$$\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \frac{32}{a^4}\int_0^\infty dr_1\, r_1 e^{-4r_1/a}[a - (2r_1 + a)e^{-4r_1/a}] = \frac{32}{a^4} \cdot \frac{5a^3}{128} = \frac{5a}{4}$$

where we have used 'Simplify[Integrate[r_1 Exp[$-4r_1/a$]($a - (2r_1 + a)$Exp[$-4r_1/a$]), $\{r_1, 0, \infty\}$], $a \in$ Reals && $a > 0$]' for the last integral.

(b) Using Bohr radius $a = 4\pi\epsilon_0\hbar^2/(me^2)$, we conclude that

$$V_{ee} \approx \frac{e^2}{4\pi\epsilon_0}\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \frac{5}{4}\frac{e^2}{4\pi\epsilon_0}\frac{1}{a} = \frac{5m}{4\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = \frac{5}{2}(13.6 \text{ eV})$$

and $E_0 + V_{ee} = (-109 + 34)$ eV $= -75$ eV, which is close to the experimental value -79 eV.

Problem 3 **(6 points)**

A spin-1 system in the basis of S_z satisfies

$$S_z|m\rangle = \hbar|m\rangle \quad \text{and} \quad S_\pm|m\rangle = \hbar\sqrt{2 - m(m \pm 1)}|m \pm 1\rangle$$

with $m = 1, 0, -1$. The matrix representation of S_z and $S_\pm$ are

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad S_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \quad S_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

Now, using that $S_x = (S_+ + S_-)/2$ and $S_y = (S_+ - S_-)/(2i)$ we obtain

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad S_y = \frac{i\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

Let us choose the particular state $|1\rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}^T$

$$\langle 1|S_z|1\rangle = \hbar \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \hbar$$

$$\langle 1|S_{x,y}|1\rangle \propto \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$\langle 1|S_z^2|1\rangle = \frac{\hbar^2}{2}\langle 1| \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} |1\rangle = \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{\hbar^2}{2}$$

$$\langle 1|S_y^2|1\rangle = -\frac{\hbar^2}{2}\langle 1| \begin{pmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{pmatrix} |1\rangle = -\frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = \frac{\hbar^2}{2}$$

Therefore,

$$\sigma_x \sigma_y = \sqrt{(\langle S_x^2\rangle - \langle S_x\rangle^2)(\langle S_y^2\rangle - \langle S_y\rangle^2)} = \frac{\hbar^2}{2} \geq \frac{\hbar}{2}\langle S_z\rangle$$