HW #7 (due Wed. 11/29)
(Physics 115B, Fall 2017)

1. Two identical particles, each of mass m, move in one dimension in the potential

$$V(x_1, x_2) = \frac{1}{2}A(x_1^2 + x_2^2) + \frac{1}{2}B(x_1 - x_2)^2$$

where A and B are positive constants and x_1 and x_2 denote the positions of the particles.

(a) Show that the Schrodinger equation is separable in the variables x_1+x_2 and x_1-x_2. Find the eigenvalues and the corresponding eigenfunctions.

(b) Discuss the symmetry of the eigenfunctions with respect to particle exchange.

2. At $t = 0$, the wave function of a two particle system of unequal mass m_1 and m_2, respectively, in one-dimensional impenetrable box is given as

$$\psi(x_1, x_2, 0) = \frac{1}{\sqrt{5}}\{2\psi_1(x_1)\psi_3(x_2) + \psi_5(x_1)\psi_7(x_2)\}$$

(a) Suppose we measure the energy of this system, what values will we find? With what probability?

(b) Let the measurement give the value E_{13}. What is the wave function of the system at time t in this case?

3-6. Griffiths 5.6, 5.11, 5.12 and 5.13.

1 (20')

2 (20)

5.6 (10)

5.11 (20)

5.12 (10)

5.13 (20)

HW#7 Solution

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1.

(a) $$H = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + \frac{A}{2}(x_1^2 + x_2^2) + \frac{B}{2}(x_1 - x_2)^2$$

do change of variables:

$$\begin{cases} x = x_1 + x_2 \\ y = x_1 - x_2 \end{cases} \Rightarrow \begin{array}{l} x_1 = \frac{1}{2}(x+y) \\ x_2 = \frac{1}{2}(x-y) \end{array}$$

Then:

$$x_1^2 + x_2^2 = \frac{1}{4}(x+y)^2 + \frac{1}{4}(x-y)^2$$

$$= \frac{1}{4}\left(x^2 + 2xy + y^2\right) + \frac{1}{4}\left(x^2 - 2xy + y^2\right)$$

$$= \frac{1}{2}(x^2 + y^2)$$

Then potential becomes:

$$\tilde{V}(x,y) = \frac{A}{2}\,\frac{1}{2}(x^2+y^2) + \frac{B}{2}y^2$$

$$= \frac{A}{4}x^2 + \frac{A}{4}y^2 + \frac{B}{2}y^2$$

$$= \frac{A}{4}x^2 + \frac{A+2B}{4}y^2$$

Now, work out how kinetic terms transform:

$$\hat{p}_1 = -i\hbar\frac{\partial}{\partial x_1} = -i\hbar\left[\frac{\partial}{\partial x}\frac{\partial x}{\partial x_1} + \frac{\partial}{\partial y}\frac{\partial y}{\partial x_1}\right]$$

$$= -i\hbar\left[\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right]$$

$$\hat{P}_2 = -i\hbar \frac{\partial}{\partial x_2} = -i\hbar \left[\frac{\partial}{\partial x}\frac{\partial x}{\partial x_2} + \frac{\partial}{\partial y}\frac{\partial y}{\partial x_2} \right]$$

$$= -i\hbar \left[\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right]$$

$$\hat{P}_1^2 + \hat{P}_2^2 = -\hbar^2 \left[\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right]^2 + (-\hbar^2) \left[\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right]^2$$

$$= -2\hbar^2 \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right]$$

So, in new coordinate:

$$H = \frac{\hat{P}_1^2 + \hat{P}_2^2}{2m} + V(\hat{x}_1, \hat{x}_2)$$

$$= \frac{1}{2m}(-2\hbar^2)\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] + \frac{A}{4}x^2 + \frac{A+2B}{4}y^2$$

$$= \frac{P_x^2 + P_y^2}{2\frac{m}{2}} + \frac{A}{4}x^2 + \frac{A+2B}{4}y^2$$

$$= \frac{P_x^2}{2\frac{m}{2}} + \frac{A}{4}x^2 + \frac{P_y^2}{2\frac{m}{2}} + \frac{A+2B}{4}y^2$$

$$= H_x + H_y$$

set $\tilde{m} = \frac{m}{2}$

$$\frac{\tilde{m}\omega_1^2}{2} = \frac{A}{4} \Rightarrow \frac{m\omega_1^2}{4} = \frac{A}{4} \Rightarrow \omega_1 = \sqrt{\frac{A}{m}}$$

$$\frac{\tilde{m}\omega_2^2}{2} = \frac{A+2B}{4} \Rightarrow \frac{m\omega_2^2}{4} = \frac{A+2B}{4} \Rightarrow \omega_2 = \sqrt{\frac{A+2B}{m}}$$

Then: the eigenvalues & eigenfunctions:

$$H = \frac{\hat{P}_x^2}{2\tilde{m}} + \frac{\tilde{m}}{2}\omega_1^2 x^2 + \frac{\hat{P}_y^2}{2\tilde{m}} + \frac{\tilde{m}}{2}\omega_2^2 y^2$$

Two harmonic osciallator :

we assume:

$$\left(\frac{\hat{p}_x^2}{2\tilde{m}} + \frac{\tilde{m}}{2}\omega_1^2 x^2\right)|n_1\rangle = \hbar\omega_1\left(n_1+\frac{1}{2}\right)\ |n_1\rangle$$

$n_1 = 0, 1, 2, \dots$

$$\left(\frac{\hat{p}_y}{2\tilde{m}} + \frac{\tilde{m}}{2}\omega_2^2 y^2\right)|n_2\rangle = \hbar\omega_2\left(n_2+\frac{1}{2}\right)|n_2\rangle$$

$n_2 = 0, 1, 2, \dots$

Then:

The eigenfunction

$$\psi_{n_1 n_2}(x, y) = |n_1\rangle \otimes |n_2\rangle = |n_1\, n_2\rangle$$

eigenvalues:

$$E_{n_1 n_2} = \hbar\omega_1\left(n_1+\frac{1}{2}\right) + \hbar\omega_2\left(n_2+\frac{1}{2}\right)$$

$$\omega_1 = \sqrt{\frac{A}{m}}\ , \quad \omega_2 = \sqrt{\frac{A+2B}{m}}$$

(b) when we exchange particles:

$$x \longrightarrow x$$
$$y \longrightarrow -y$$

Then:

$|n_1, n_2 = 2k\rangle$ is even under exchange of particles.

where: $n_1 = 0, 1, 2, \dots$

$k = 0, 1, 2, \dots$

$|n_1, n_2 = 2k+1\rangle$ is odd ...

where $n_1 = 0, 1, 2, \dots$

$k = 0, 1, 2, \dots$

2.

$$\psi(x_1, x_2, 0) = \frac{1}{\sqrt{5}} \left\{ 2\psi_1(x_1)\psi_3(x_2) + \psi_5(x_1)\psi_7(x_2) \right\}$$

(a) when we measure the energy: we can get

$$E_{13} \longrightarrow \left|\frac{2}{\sqrt{5}}\right|^2 = \frac{4}{5}$$

$$E_{57} \longrightarrow \left|\frac{1}{\sqrt{5}}\right|^2 = \frac{1}{5}$$

(b) when we get E_{13}, we have:

$$\tilde{\psi}(x_1, x_2, 0) = \psi_1(x_1)\psi_3(x_2)$$

Then: at time t:

$$\tilde{\psi}(x_1, x_2, t) = e^{-\frac{i\hat{H}_1 t}{\hbar}} e^{-\frac{i\hat{H}_2 t}{\hbar}} \psi_1(x_1)\psi_3(x_2)$$

$$= e^{-\frac{iE_1 t}{\hbar}} e^{-\frac{i\mathcal{E}_3 t}{\hbar}} \psi_1(x_1)\psi_3(x_2)$$

Remark: I assume Hamiltonian of first particle is $\hat{H}(x_1)$

second is $\hat{H}'(x_2)$

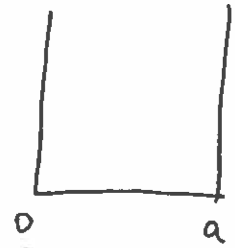
and: $\hat{H}(x_1)\psi_i(x_1) = E_i(x_1)$

$\hat{H}'(x_2)\psi_i(x_2) = \mathcal{E}_i(x_2)$

and $E_{ij} = E_i + \mathcal{E}_j$.

5.6

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$



Before starting, we compute:

$$\langle x^2 \rangle_n = \int_0^a \psi_n^*(x)\, x^2\, \psi_n(x)\, dx$$

$$= \frac{2}{a} \int_0^a x^2 \sin^2\left(\frac{n\pi}{a}x\right) dx$$

$$= \frac{2}{a} \int_0^a x^2 \frac{1-\cos\left(\frac{2n\pi}{a}x\right)}{2} dx$$

$$= \frac{1}{a} \int_0^a x^2\, dx - \frac{1}{a} \int_0^a x^2 \cos\left(\frac{2n\pi}{a}x\right) dx$$

$$= \frac{1}{a}\frac{a^3}{3} - \frac{1}{a} \int_0^a x^2 \cos\left(\frac{2n\pi}{a}x\right) dx$$

$$= \frac{a^2}{3} - \frac{1}{a} \int_0^a x^2 \cos\left(\frac{2n\pi}{a}x\right) dx$$

$$\int_0^a x^2 \cos\left(\frac{2n\pi}{a}x\right) dx = \frac{a}{2n\pi} \int_0^a x^2\, d\sin\left(\frac{2n\pi}{a}x\right)$$

$$= \frac{a}{2n\pi} x^2 \sin\left(\frac{2n\pi}{a}x\right)\Bigg|_0^a - \frac{a}{2n\pi} \int_0^a \sin\left(\frac{2n\pi}{a}x\right) \cdot 2x\, dx$$

$$= -\frac{a}{n\pi} \int_0^a x \sin\left(\frac{2n\pi}{a}x\right) dx$$

$$= \frac{a}{n\pi} \frac{a}{2n\pi} \int_0^a x\, d\cos\left(\frac{2n\pi}{a}x\right)$$

$$= \frac{1}{2}\left(\frac{a}{n\pi}\right)^2 \left[x\cos\left(\frac{2n\pi}{a}x\right)\Big|_0^a - \int_0^a \cos\left(\frac{2n\pi}{a}x\right)dx \right]$$

$$= \frac{1}{2}\left(\frac{a}{n\pi}\right)^2 \cdot a \cos(2n\pi)$$

$$= \frac{a}{2}\left(\frac{a}{n\pi}\right)^2$$

Then: $\boxed{\langle x^2\rangle_n = \frac{a^2}{3} - \frac{1}{a}\cdot\frac{a}{2}\left(\frac{a}{n\pi}\right)^2 = \frac{a^2}{3} - \frac{1}{2}\left(\frac{a}{n\pi}\right)^2}$

$$\boxed{\langle x^2\rangle_l = \frac{a^2}{3} - \frac{1}{2}\left(\frac{a}{l\pi}\right)^2}$$

$$\langle x\rangle_n = \langle n|\hat{x}|n\rangle = \int_0^a \psi_n^*(x)\, x\, \psi(x)\, dx$$

$$= \frac{2}{a}\int_0^a x \sin^2\left(\frac{n\pi}{a}x\right) dx \qquad\qquad x - \frac{a}{2} = y$$

$$= \frac{2}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} \left(y + \frac{a}{2}\right)\sin^2\left(\frac{n\pi}{a}y + \frac{n\pi}{2}\right) dy$$

$$= \int_{-\frac{a}{2}}^{\frac{a}{2}} \sin^2\left(\frac{n\pi}{a}y + \frac{n\pi}{2}\right) dy \qquad\qquad x = \frac{a}{2}+y$$

$$= \int_0^a \sin^2\left(\frac{n\pi}{a}x\right) dx$$

$$= \int_0^a \frac{1-\cos\left(\frac{2n\pi}{a}x\right)}{2} dx$$

$$= \frac{a}{2}$$

Then :

$$\boxed{\langle x \rangle_n = \langle x \rangle_l = \frac{a}{2}}$$

$$\begin{aligned}
\langle x \rangle_{nl} &= \langle n | \hat{x} | l \rangle \\
&= \frac{2}{a} \int_0^a \sin\left(\frac{n\pi}{a} x\right) \sin\left(\frac{l\pi}{a} x\right) x \, dx \\
&= \frac{a}{\pi^2} \left[(-1)^{n+l} - 1 \right] \left(\frac{1}{(n-l)^2} - \frac{1}{(n+l)^2} \right) \\
&= \begin{cases} \dfrac{a(-8nl)}{\pi^2 (n^2 - l^2)^2} & \text{if } n, l \text{ have opposite parity} \\ 0 & \text{if } n, l \text{ have same parity.} \end{cases}
\end{aligned}$$

(a) Distinguishable particles :

$$\begin{aligned}
\langle (x_1 - x_2)^2 \rangle &= \langle x^2 \rangle_n + \langle x^2 \rangle_l - 2 \langle x \rangle_n \langle x \rangle_l \\
&= a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{l^2} \right) \right]
\end{aligned}$$

(b) Identical Bosons:

$$\begin{aligned}
\langle (x_1 - x_2)^2 \rangle &= \langle x^2 \rangle_n + \langle x^2 \rangle_l - 2 \langle x \rangle_n \langle x \rangle_l - 2 \left| \langle x \rangle_{nl} \right|^2 \\
&= a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{l^2} \right) \right] - \frac{128 a^2 n^2 l^2}{\pi^4 (l^2 - n^2)^4}
\end{aligned}$$

The last term is present only when n, l have opposite parity.

(c). Identical Fermion:

$$\langle (x_1 - x_2)^2 \rangle = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{l^2} \right) \right] + \frac{128\, a^2\, l^2 n^2}{\pi^4 (l^2 - n^2)^4}$$

the last term is present only when n, l have opposite parity.

Problem 5.11

(a)

$$\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \left(\frac{8}{\pi a^3}\right)^2 \int \Bigg(\underbrace{\int \frac{e^{-4(r_1+r_2)/a}}{\sqrt{r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta_2}}\, d^3 r_2}_{\text{denote as } I_1} \Bigg)\, d^3 r_1$$

$$I_1 = 2\pi \int_0^{+\infty} r_2^2 e^{-4(r_1+r_2)/a} \left(\int_0^{\pi} \frac{\sin\theta_2}{\sqrt{r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta_2}}\, d\theta_2 \right) dr_2$$

integration by parts:

$$= \frac{1}{r_1 r_2}\left[\sqrt{r_1^2 + r_2^2 + 2 r_1 r_2} - \sqrt{r_1^2 + r_2^2 - 2 r_1 r_2}\right]$$

$$= \begin{cases} \dfrac{2}{r_1} & (r_2 < r_1) \\ \dfrac{2}{r_2} & (r_1 < r_2) \end{cases}$$

$$= 4\pi e^{-4r_1/a}\left[\frac{1}{r_1}\int_0^{r_1} r_2^2 e^{-4r_2/a}\, dr_2 + \int_{r_1}^{\infty} r_2 e^{-4r_2/a}\, dr_2\right]$$

$$\cancel{= 4\pi \left(\frac{a^3}{32 r_1}\right) e^{-4r_1/a}}$$

$$= \frac{\pi a^2}{8}\left\{\frac{a}{r_1} e^{-4r_1/a} - \left(2 + \frac{a}{r_1}\right) e^{-8r_1/a}\right\}$$

Then:

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

$$= \frac{32}{a^4}\left\{ a\int_0^{\infty} r_1 e^{-4r_1/a}\, dr_1 - 2\int_0^{\infty} r_1^2 e^{-8r_1/a}\, dr_1 - a\int_0^{\infty} r_1 e^{-8r_1/a}\, dr_1 \right.$$

$$= \frac{32}{a}\left(\frac{1}{16} - \frac{1}{128} - \frac{1}{64}\right) = \frac{5}{4a}$$

(b)

$$V_{ee} \approx \frac{e^2}{4\pi\epsilon_0}\left\langle \frac{1}{|r_1 - r_2|} \right\rangle = \frac{5}{2}(-E_1) = \frac{5}{2}(13.6\ eV) = 34\ eV$$

$$E_0 + V_{ee} = (-109 + 24)\ eV = -75\ eV$$

which is pretty close to the experimental value (−79 eV)

Problem 5.12

(a) Hydrogen $(1s)$ helium $(1s)^2$ lithium $(1s)^2(2s)$

beryllium $(1s)^2(2s)^2$ boron $(1s)^2(2s)^2(2p)$ carbon $(1s)^2(2s)^2(2p)^2$

nitrogen $(1s)^2(2s)^2(2p)^3$ oxygen $(1s)^2(2s)^2(2p)^4$ fluorine $(1s)^2(2s)^2(2p)^5$

neon $(1s)^2(2s)^2(2p)^6$

(b)

Hydrogen: $\quad {}^2S_{\frac{1}{2}}$

Helium: $\quad {}^1S_0$

Lithium: $\quad {}^2S_{\frac{1}{2}}$

Beryllium $\quad {}^1S_0$

Boron: orbital $l = 1$,

spin $s = \frac{1}{2}$ $\quad \Rightarrow \quad j = \frac{1}{2}, \frac{3}{2}$

so:

maybe:

$${}^2P_{3/2}, \quad {}^2P_{1/2}$$

Carbon: For orbital:

$$l_1 = 1 \otimes l_2 = 1$$

we have:

total ~~..~~ orbital angular momentum: 0, 1, 2 spin can be 0, 1, so:

$^1S_0$, $^3S_1$, $^1P_1$, $^3P_2$, $^3P_0$, $^1D_2$, $^3D_3$, $^3D_2$, $^3D_1$

Nitrogen,

$l_1 = 1$ $\quad l_2 = 1$ $\quad l_3 = 1$

$\tilde{l}_1 = 0$ $\quad \tilde{l}_2 = 1$, $\tilde{l}_3 = 2$

$\tilde{l}_1 = 0$ $\quad l_3 = 1$

$l_{tot} = 1$

$\tilde{l}_2 = 1$ $\quad l_3 = 1$

$l_{tot} = 0, 1, 2$

$\tilde{l}_3 = 2$ $\quad l_3 = 1$

$l_{tot} = 1, 2, 3$

so: $\boxed{l_{total} = 0, 1, 2, 3}$

$\boxed{\text{total spin can be: } \frac{1}{2}, \frac{3}{2}}$

$^2S_{\frac{1}{2}}$ $\quad ^4S_{3/2}$ $\quad ^2P_{1/2}$ $\quad ^2P_{3/2}$ $\quad ^4P_{1/2}$ $\quad ^4P_{3/2}$

$^4P_{5/2}$ $\quad ^2D_{3/2}$ $\quad ^2D_{5/2}$ $\quad ^4D_{1/2}$ $\quad ^4D_{3/2}$ $\quad ^4D_{5/2}$

$^4D_{7/2}$ $\quad ^2F_{5/2}$ $\quad ^2F_{3/2}$ $\quad ^4F_{3/2}$ $\quad ^4F_{5/2}$ $\quad ^4F_{7/2}$ $\quad ^4F_{9/2}$

5.13.

a) Orthohelium should have lower energy than parahelium.

b) Hund's first rule: $S=1$ for the ground state of carbon which is symmetric. So the orbital state will have to be antisymmetric.

Hund's second rule: $L=2$, but this is symmetric:

$|22\rangle = |11\rangle_1 \, |11\rangle_2$

So: the ground state of carbon will be

$S=1, \; L=1$

so, there are three possibilities:

${}^3P_2, \; {}^3P_1, \; {}^3P_0$

c) boron, only one elctron in 2P subsell.

so: we'll have $J = |L-S|$

${}^2P_{\frac{1}{2}}$

For carbon, from Hund's third rule: $J = 0$

$$^3P_0$$

For nitrogen:

1^{st} rule: $S = \frac{3}{2}$, symmetric

so the orbital part is antisymmetric which is $L = 0$

3^{rd} rule: $J = |L - S| = \frac{3}{2}$

So:

ground state of nitrogen: $^4S_{3/2}$