F2014

PROBLEM 4: Two Particles in a 1D Box

Consider two noninteracting particles of mass m inside a 1D box,

$$V(x) = \begin{cases} 0 & , 0 < |x| < a \\ \infty & , \text{otherwise} \end{cases} .$$

Make sure to consider the spin part of the wavefunction in this problem.

a) Let n_1 and n_2 be the quantum numbers of particle 1 and 2 respectively. What are the wavefunctions of the single particle states for the each particle in the box? What are the single particle energies? (2 Points)

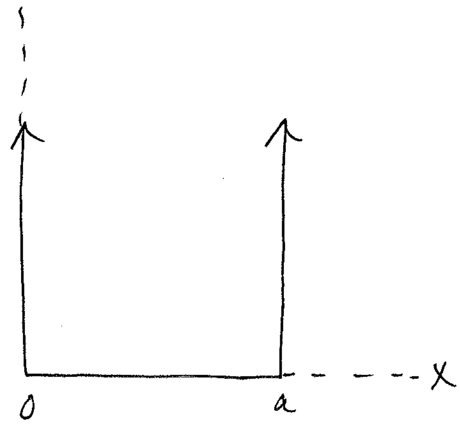
b) If the particles are distinguishable what is the two-particle wavefunction that describes the state? What is the energy? Write out explicitly the state (or states) and energies for the ground state and first excited states of the system. (2 Points)

c) If the two particles are identical spin 0 bosons what are the ground state and first excited state wavefunctions and energies? (2 Points)

d) If the two particles are identical spin 1/2 fermions what are the ground state and first excited state wavefunctions and energies? (2 Points)

e) Write down the Hamiltonian for the two particles in the box and show that when the particles are identical H commutes with the exchange operator. (2 Points)

(a)



The single particle wavefunctions are

$$\boxed{\begin{aligned}\psi_{n_1}(x_1) &= \sqrt{\frac{2}{a}}\sin\left(\frac{n_1\pi x_1}{a}\right)\\ \psi_{n_2}(x_2) &= \sqrt{\frac{2}{a}}\sin\left(\frac{n_2\pi x_2}{a}\right)\end{aligned}}$$

In general, we know Schrödinger's equation for a single particle in this potential well is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+0\right]\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

and if

$$k = \frac{\sqrt{2mE}}{\hbar},$$

then we have

$$\frac{d^2\psi}{dx^2} = -k^2\psi.$$

(a), cont'd...

Solutions are then, generally, of the form

$$\psi(x) = A\sin(kx) + B\cos(kx).$$

The wavefunction must be equal to $\emptyset$ at $x=0$ and $x=a$ based on our boundary conditions, so

$$\psi(0) = A\sin(0) + B\cos(0) = 0$$
$$B = 0$$

and thus

$$\psi(a) = A\sin(ka) = 0.$$

This can only be the case if

$$ka = n\pi$$

or

$$k = \frac{n\pi}{a}.$$

but we said

$$k = \frac{\sqrt{2mE}}{\hbar}.$$

So our single particle energies are

$$\boxed{\begin{aligned} E_1 &= \frac{n_1^2\pi^2\hbar^2}{2ma^2} \\ E_2 &= \frac{n_2^2\pi^2\hbar^2}{2ma^2} \end{aligned}}$$

NOTE: The total single particle wavefunctions are the product of the spatial wavefunction (on the previous page) and the spin wavefunction, which will be discussed in more detail in part (b).

(b)

We are told that the particles are distinguishable, so the total wavefunction is

$$\boxed{\psi(x_1, x_2) = \frac{2}{a}\sin\left(\frac{n_1 \pi x_1}{a}\right)\sin\left(\frac{n_2 \pi x_2}{a}\right)} \quad \text{(spatial)}$$

and the energy is

$$E = E_1 + E_2$$

$$\boxed{E = \frac{(n_1^2 + n_2^2)\pi^2 \hbar^2}{2ma^2}}$$

The ground state wavefunction and energy occur at $n_1 = n_2 = 1$, so

$$\boxed{\psi_{ground}(x_1, x_2) = \frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)} \quad \text{(spatial)}$$

$$\boxed{E = \frac{\pi^2 \hbar^2}{ma^2}}.$$

The first excited states occur when $n_1 = 1$ and $n_2 = 2$ or $n_1 = 2$ and $n_2 = 1$. So

$$\boxed{\begin{aligned} \psi_{exc}(x_1, x_2) &= \frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) \\ \psi_{exc}(x_1, x_2) &= \frac{2}{a}\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) \end{aligned}} \quad \text{(spatial)}$$

and

$$\boxed{E = \frac{5\pi^2 \hbar^2}{2ma^2}}$$

(b), cont'd...

The wavefunctions on the previous page are only the spatial wavefunctions. The total wavefunction, including spin, is given by

$$\psi = \psi_{spatial} \cdot \psi_{spin} .$$

Assuming $\uparrow$ corresponds to a spin up particle and $\downarrow$ to a spin down particle, and there are two particles, we can have the following spin wavefunctions:

<u>Antisymmetric</u>

$$\psi_{spin} = \frac{1}{\sqrt{2}} \left[|\uparrow_1 \downarrow_2\rangle - |\downarrow_1 \uparrow_2\rangle \right]$$

<u>Symmetric</u>

$$\psi_{spin} = |\uparrow_1 \uparrow_2\rangle$$

$$\psi_{spin} = |\downarrow_1 \downarrow_2\rangle$$

$$\psi_{spin} = \frac{1}{\sqrt{2}} \left[|\uparrow_1 \downarrow_2\rangle + |\downarrow_1 \uparrow_2\rangle \right]$$

These will become important in parts (c) and (d).

(c)

Bosons must have symmetric wavefunctions. Assuming the particles are indistinguishable, the spatial wavefunction is

$$\psi_{spatial}(x_1, x_2) = K\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right].$$

To keep the total wavefunction symmetric, the spin wavefunction must be symmetric, as well. So

$$\psi = K\left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right] \cdot \psi_{spin}^{S}$$

where ψ_{spin}^{S} is one of the symmetric triplet states listed on page 4.

The ground state corresponds to $n_1 = n_2 = 1$, so we have

$$\psi_{ground} = K\left[\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) + \frac{2}{a}\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{\pi x_1}{a}\right)\right] \cdot \psi_{spin}^{S}$$

$$\psi_{ground} = 2K\,\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) \cdot \psi_{spin}^{S},$$

where K is a normalization factor. In the excited state, $n_1 = 1$ and $n_2 = 2$, or vice versa. So

$$\psi_{exc} = K\left[\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \frac{2}{a}\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{2\pi x_1}{a}\right)\right] \cdot \psi_{spin}^{S}$$

or

$$\psi_{exc} = K\left[\frac{2}{a}\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) + \frac{2}{a}\sin\left(\frac{2\pi x_2}{a}\right)\sin\left(\frac{\pi x_1}{a}\right)\right] \cdot \psi_{spin}^{S}.$$

(c), cont'd...

The ground state energy is then

$$E_{ground} = \frac{\pi^2 \hbar^2}{ma^2}$$

and the excited energy is

$$E_{exc} = \frac{5\pi^2\hbar^2}{2ma^2}.$$

(d)

Fermions must have antisymmetric wavefunctions. This means the spatial wavefunction is symmetric and the spin wavefunction is antisymmetric, or vice versa. We must consider both cases.

$\underline{\psi = \psi^S_{spatial} \cdot \psi^A_{spin}}$

In this case, our energies are the same because the ground state corresponds to $n_1 = n_2 = 1$, and the excited state corresponds to either $n_1 = 1$ and $n_2 = 2$ or $n_1 = 2$ and $n_2 = 1$. The wavefunctions are also the same as in the boson case, except the spin wavefunction is antisymmetric.

$\underline{\psi = \psi^A_{spatial} \cdot \psi^S_{spin}}$

Our spatial wavefunction is

$$\psi(x_1, x_2) = K\left[\frac{2}{a}\sin\left(\frac{n_1\pi x_1}{a}\right)\sin\left(\frac{n_2\pi x_2}{a}\right) - \frac{2}{a}\sin\left(\frac{n_1\pi x_2}{a}\right)\sin\left(\frac{n_2\pi x_1}{a}\right)\right]$$

(d), cont'd ...

In this case, the ground state no longer corresponds to $n_1 = n_2 = 1$ because of the Pauli Exclusion Principle. So the ground state must be $n_1 = 1$ and $n_2 = 2$, or vice versa, and the wavefunction is

$$\psi(x_1, x_2) \cdot \psi^S_{spin}$$
$$= K\left[\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \frac{2}{a}\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{2\pi x_1}{a}\right)\right] \cdot \psi^S_{spin}$$

or vice versa. The energy is then

$$E_{ground} = \frac{5\pi^2\hbar^2}{2ma^2}.$$

The first excited state is $n_1 = 1$ and $n_2 = 3$, or vice versa and

$$\psi = K\left[\frac{2}{a}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right) - \frac{2}{a}\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{3\pi x_1}{a}\right)\right] \cdot \psi^S_{spin}$$

or vice versa. The energy is then

$$E_{exc} = \frac{5\pi^2\hbar^2}{ma^2}.$$

(e) The Hamiltonian, given that the potential is zero between $0 < x < a$, is

$$H = \underbrace{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx_1^2}\right)}_{\text{particle 1}} + \underbrace{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx_2^2}\right)}_{\text{particle 2}}$$