Homework 4, Quantum Mechanics 501, Rutgers

October 28, 2016

1) Consider a harmonic oscillator which is in an initial state $a |n\rangle + b |n+1\rangle$ at t = 0, where a, b are real numbers with $a^2 + b^2 = 1$. Calculate the expectation values of X(t)and P(t) as a function of time. Compare your results to the classical motion x(t) of a harmonic oscillator with the same physical parameters (ω, m) and the same (average) energy $E \approx (n+1)\hbar\omega$.

Ans.: Time dependent wave function is

$$|\psi(t)\rangle = e^{-iE_n t/\hbar} (a |n\rangle + b e^{-i\omega t} |n+1\rangle)$$
(1)

The average of position operator gives

$$\langle X \rangle = \langle \psi | \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^{\dagger} + \hat{a}) | \psi \rangle =$$
 (2)

$$\sqrt{\frac{\hbar}{2m\omega}} \left(a \left\langle n \right| + be^{i\omega t} \left\langle n + 1 \right| \right) \left(\hat{a}^{\dagger} + \hat{a} \right) \left(a \left| n \right\rangle + be^{-i\omega t} \left| n + 1 \right\rangle \right) = \tag{3}$$

$$\sqrt{\frac{2\hbar(n+1)}{m\omega}}ab\cos(\omega t) \tag{4}$$

and similarly momentum is

$$\langle P \rangle = \langle \psi | i \sqrt{\frac{m\omega\hbar}{2}} (\hat{a}^{\dagger} - \hat{a}) | \psi \rangle = -\sqrt{2\hbar m\omega(n+1)} ab\sin(\omega t)$$
(5)

Clearly, the classical equations of motions are satisfied, since $d\langle X \rangle / dt = \langle P \rangle / m$. The frequency of oscilations is the same, however, the aplitudes are different. For the classical system, the position is given by

$$x = \sqrt{\frac{2E}{m\omega^2}}\cos(\omega t) \tag{6}$$

The quatum system satisfies

$$\langle X \rangle = \sqrt{\frac{2 \langle E \rangle}{m\omega^2}} ab \cos(\omega t) \tag{7}$$

Since a and b are some constants smaller than unity $(a^2 + b^2 = 1)$, the quantum amplitude is smaller for at least factor of 2. Clearly classical motion can not be properly described by only two eigenstates of quantum oscilator.

2) A particle of mass m is in a one-dimensional potential of form $V(x) = 1/2m\omega^2 x^2 + mgx$ with some real number g. (Think of this as an oscillator potential plus a constant force mg in -x direction acting on the particle).

Without doing much heavy math, can you write down the lowest energy eigenstate of this potential? (Think about the classical analog a weight hanging on a vertical spring. How does gravity affect the equations and solution for the harmonic spring potential energy?)

Ans.: The Hamiltonian can be cast into the following form

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2(x + \frac{g}{\omega^2})^2 - \frac{1}{2}m\frac{g^2}{\omega^2}$$
(8)

If we introduce a new variable $x_{new} = x + \frac{g}{\omega^2}$, the above Hamiltonian has a canonical form of H.O. apart from the energy shift. The solutions are then solutions of H.O. The ground state is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}(x+g/\omega^2)^2} \tag{9}$$

with energy $E_0 = \hbar \omega / 2 - \frac{1}{2} m \frac{g^2}{\omega^2}$.

What is the probability that a particle starting out in the ground state of the harmonic oscillator potential only (first part of V(x)) ends up in the new ground state once the force is "switched on"?

Ans.: If we denote the unshifted oscilator wave function by $\psi_0^0(x)$, then the probability is

$$P = |\langle \psi_0^0 | \psi_0 \rangle|^2 \tag{10}$$

which is

$$P = e^{-\frac{mg^2}{2\hbar\omega^3}}$$

and can also be written as $P = e^{-\frac{\Delta E}{\hbar\omega}}$ where ΔE is the change of the energy due to additional term in the Hamiltonian.

3) Find the eigenvalues and eigenstates of the one-dimensional Hamiltonian with potential

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & x < 0\\ \infty & x \ge 0 \end{cases}$$
(11)

Nearly no math is needed, only some clever argument.

Ans.: We know that the solutions must be the same as those for a the usual oscillator potential on the left side (x < 0), since they have to fulfill the same differential equation there. On the right hand side, the solutions must be of course simply equal to zero (infinitely high potential). All we have to do is match the l.h.s solution to the right hand one to get a continuous wave function. This is obviously only possible if the l.h.s. solution goes to zero as x goes to 0. This is the case for solutions with odd n, since

the corresponding Hermite polynomials have only odd powers of x. In other words, the eigenstates are $|n\rangle$, n = 1, 3, 5, ... and the eigenvalues are $E = \hbar\omega(n + 1/2)$.

Note that one also has to renormalize the wave functions (with an extra factor 2) since the integral in the spatial variable x now only goes from $-\infty...0$.

4) The wavefunction of a particle of mass m is in a 1D potential V(x) is

$$\psi(x) = \begin{cases} Axe^{-ax} & x \ge 0\\ 0 & x < 0 \end{cases}$$
(12)

a) Assuming the particle is in an eigenstate of the Hamiltonian, find the potential V(x) and the total energy E for this state.

Ans.: It needs to satisfy the Schroedinger Equation. The second derivative is

$$\psi''(x) = \psi(x)(a^2 - 2\frac{a}{x})$$
(13)

which gives for the Schroedinger equation

$$-\frac{\hbar^2}{2m}(a^2 - 2\frac{a}{x})\psi(x) + V(x)\psi(x) = E\psi(x)$$
(14)

For the equation to be satisfied, we need $V(x) = -\frac{\hbar^2 a}{m} \frac{1}{x} + C$. Without loss of generality, we can set C = 0, which gives $E = -\frac{\hbar^2 a^2}{2m}$. Note that this holds only for x > 0, as the wave function vanishes at x = 0 (with finite derivative) and potential is therefore infinite at x < 0.

b) Find the potential energy expectation value $\langle V \rangle$ for this state

Ans.:

$$\langle V \rangle = \int_0^\infty V(x)\psi(x)^2 = A^2 \int_0^\infty dx x^2 e^{-2ax} \left(-\frac{\hbar^2 a}{mx}\right) = -\frac{\hbar^2}{m} \frac{A^2}{4a}$$
(15)

and

$$1 = \int_0^\infty dx \psi(x)^2 = A^2 \int_0^\infty dx x^2 e^{-2ax} = \frac{A^2}{4a^3}$$
(16)

hence $\langle V \rangle = -\frac{\hbar^2 a^2}{m}$.

- c) Find the expectation value of the kinetic energy for this state. **Ans.:** $\langle K \rangle = E - \langle V \rangle = \frac{\hbar^2 a^2}{2m}$
- 5 The eigenstates, which are accesible to a single electron, have energies ε_0 , ε_1 and ε_2 and their states are $|0\rangle$, $|1\rangle$ and $|2\rangle$. When two electrons are introduced in such system, what are possible wave-functions of the system of two electrons, if we neglect interaction between the two electrons?

a) How many possible states can you write down, which have correct statistics? Write them down.

Ans.:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle) \tag{17}$$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |2\rangle - |2\rangle \otimes |0\rangle) \tag{18}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle) \tag{19}$$

b) What are the energies of these states?

Ans.: $\varepsilon_0 + \varepsilon_1$, $\varepsilon_0 + \varepsilon_2$, $\varepsilon_1 + \varepsilon_2$.

c) Is the state $|0\rangle \otimes |1\rangle$ a valid wave function of such system? Why (not)? Ans.: No. It does not satisfy fermionic statistics for identical particles.