PHYC20012 Thermal and Quantum Physics

Quantum Mechanics – Tutorial 4

1. ***Expectation values of the infinite well.***
   Suitable solutions of the TISE for an infinite square well in the region $0 \leq x \leq L$ are given by the family of functions $\psi_n(x) = A_n \sin\left(\frac{\pi n x}{L}\right)$, where $n \geq 1$.
   (a) By applying the normalisation condition, determine A_n.
   (b) Confirm that for the position operator, $\langle x \rangle_n = \frac{L}{2}$ and $\langle x^2 \rangle_n = \frac{L^2}{6}\left(2 - \frac{3}{\pi^2 n^2}\right)$.
   (c) Confirm that for the momentum operator, $\langle p \rangle_n = 0$ and $\langle p^2 \rangle_n = \frac{\hbar^2 \pi^2 n^2}{L^2}$.
   (d) What are the uncertainties in position and momentum, Δx_n and Δp_n?
   (e) Are these states consistent with the uncertainty principle?

2. ***Expectation values of the quantum harmonic oscillator.***
   The TISE for the quantum harmonic oscillator (QHO) is

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x) = E\psi(x).$$

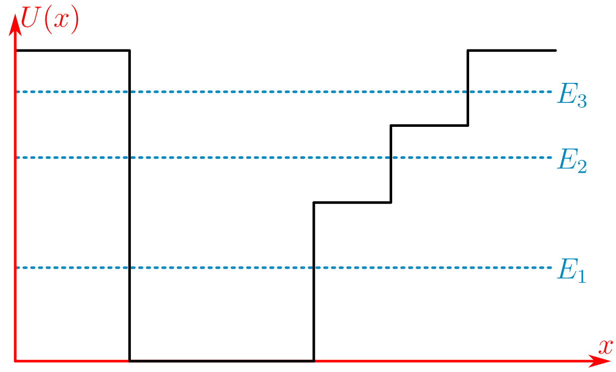
   We've already seen that the ground state of the QHO is $\psi_0(x) = C_0 \exp[-\alpha x^2]$ with $C_0 = (2\alpha/\pi)^{1/4}$, the first excited state is $\psi_1(x) = C_1 x \exp[-\alpha x^2]$ with $C_1 = (32\alpha^3/\pi)^{1/4}$, and the exponent has to be $\alpha = m\omega/2\hbar$ for all states.
   (a) Find the expectation values $\langle x \rangle_n$ and $\langle x^2 \rangle_n$ for the ground and first excited state.
   (b) Find the expectation values $\langle p \rangle_n$ and $\langle p^2 \rangle_n$ for the ground and first excited state.
   (c) What are the uncertainties Δx_n and Δp_n for the ground and first excited state?
   (d) Does the quantum harmonic oscillator satisfy the uncertainty principle? Is there anything interesting about your findings?
   (e) Are either of these wavefunctions in a position or momentum eigenstate? Explain.
   (f) What are the expectation values for the kinetic and potential energy in each of these states, $\langle K \rangle_n$ and $\langle U \rangle_n$? Does this agree with what you would expect for $\langle H \rangle_n$?

3. ***An oscillating harmonic oscillator...***
   A state $\Psi(x,t)$ is a linear superposition of two QHO solutions, $\psi_0(x)$ and $\psi_1(x)$:

$$\Psi(x,t) = a_0\psi_0(x)e^{-iE_0 t/\hbar} + a_1\psi_1(x)e^{-iE_1 t/\hbar},$$

   where a_0 and a_1 are real constants. The energies of the states $\psi_0(x)$ and $\psi_1(x)$ are E_0 and E_1 respectively, with $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$. Assume that the set $\{\psi_n(x)\}$ is pre-normalised.
   (a) Apply the normalisation condition to $\Psi(x,t)$ to unveil a constraint on a_0 and a_1.
   (b) Derive an expression for the expectation value of the energy $\langle E \rangle$ for this state.
   (c) Is energy a sharp observable for the state $\Psi(x,t)$?
   (d) Show that the time-dependence of $\langle x \rangle$ is given by $\cos(\omega t)$.
   (e) Given $\psi_0(x)$ and $\psi_1(x)$ as outlined in Q2, show that $\langle x \rangle = \alpha^{-1/2} a_0 \sqrt{1 - a_0^2}\cos(\omega t)$.
   (f) For what value of a_0 is the amplitude of $\langle x \rangle$ maximised? What is a_1 in this case?
   (g) What does this tell you about the linear superpositions of stationary states that lead to the most "interesting" behaviour?

4. ***Guess those wavefunctions!***
Sketch approximate wavefunctions $\psi_n(x)$ and probability densities $P_n(x)$ for the potential $U(x)$ as shown below, for the three energy levels indicated, assuming these are the first three allowed energies. Indicate (that is, annotate with comments) relative amplitudes, wavelengths, and all other salient features. Use separate diagrams for $\psi_n(x)$ and $P_n(x)$.



5. ***Why not work in reciprocal space?*** $(\star)$
Consider a particle of mass m under a potential $U(x)$. The particle is described in its ground state by the wavefunction $\psi(x) = Ax^2 \exp[-bx^2]$, where A and $b > 0$ are constants.

(a) Write down an expression for A.

(b) What are the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$ for this state?

(c) Is this wavefunction an eigenfunction of the momentum operator $[p]$? Justify your answer. Is the momentum a sharp or fuzzy observable in this case?

(d) Calculate the expectation value of the momentum operator, $\langle p \rangle$.

(e) What is the spectral function $a(k)$ for the ground state solution of $U(x)$? Recall that a momentum-space representation is accomplished by the Fourier transform

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x) e^{-ikx}\, \mathrm{d}x.$$

(f) In the context of the Heisenberg uncertainty principle between position and momentum, comment on the dependence of this expression on the constant b (that is, its role in *concentrating* the exponential behaviour) in the functions $\psi(x)$ and $a(k)$.

(g) Using the expression $a(k)$, and noting that $p = \hbar k$, confirm your result for $\langle p \rangle$ that you found in part (d) and also determine $\langle p^2 \rangle$.

(h) For this ground state $\psi(x)$, what are the uncertainties Δx and Δp?

(i) Are your findings consistent with the Heisenberg uncertainty principle?

(j) If the particle in its ground state was found to have $E = 5b\hbar^2/m$, then what must $U(x)$ have been? Sketch it, and indicate the ground-state energy level and its corresponding wavefunction on the same plot.

Answers: 1(a). $A_n = (2/L)^{1/2}$, 1(d). $\Delta x_n = L(\frac{1}{12} + \frac{1}{2\pi^2 n^2})^{1/2}$, $\Delta p_n = \frac{\hbar \pi n}{L}$, 1(e). $\Delta x_n \Delta p_n = \frac{\hbar}{2}(2 - \frac{\pi^2 n^2}{3})^{1/2} > \frac{\hbar}{2}$ so yes, 2(a). $\langle x \rangle_n = 0$, $\langle x^2 \rangle_n = (n + \frac{1}{2})\frac{\hbar}{m\omega}$, 2(b). $\langle p \rangle_n = 0$, $\langle p^2 \rangle_n = (n + \frac{1}{2}) m\omega\hbar$, 2(c). $\Delta x_n = [(n + \frac{1}{2})\frac{\hbar}{m\omega}]^{1/2}$, $\Delta p_n = [(n + \frac{1}{2}) m\hbar\omega]^{1/2}$, 2(d). $\Delta x_n \Delta p_n = (n + \frac{1}{2})\hbar$, 2(e). No, 2(f). $\langle K \rangle_n = (n + \frac{1}{2})\frac{\hbar\omega}{2}$, $\langle U \rangle_n = (n + \frac{1}{2})\frac{\hbar\omega}{2}$, $\langle H \rangle_n = (n + \frac{1}{2})\hbar\omega$, 3(a). $a_0^2 + a_1^2 = 1$, 3(b). $\langle E \rangle = a_0^2 E_0 + a_1^2 E_1$, 3(c). No, 3(f). $a_0 = \pm 1/\sqrt{2}$, $a_1 = \pm 1/\sqrt{2}$, 3(g). Similar coefficients a_n, 5(a). $A = \frac{4b}{3^{1/2}}(2b/\pi)^{1/4}$, 5(b). $\langle x \rangle = 0$, $\langle x^2 \rangle = \frac{5}{4b}$, 5(c). $[p]\psi(x) \neq p\psi(x)$ so no, must be fuzzy, 5(d). $\langle p \rangle = 0$, 5(e). $a(k) = \frac{A}{32^{1/2} b^{5/2}}(2b - k^2)e^{-k^2/4b}$, 5(f). Bigger b makes $\psi(x)$ narrower and $a(k)$ wider, 5(g). $\langle p^2 \rangle = \frac{7b\hbar^2}{3}$, 5(h). $\Delta x = \frac{1}{2}\sqrt{\frac{5}{b}}$, $\Delta p = \sqrt{\frac{7b}{3}}\hbar$, 5(i). $\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{35}{3}}$ so yes, 5(j). $U(x) = \frac{2b^2\hbar^2}{m}x^2 + \frac{\hbar^2}{m}\frac{1}{x^2}$.