Quantum Mechanics PHYS2B22
Problem Sheet 2
Work in by Monday February 14th

1) A particle is confined in a 1D box with walls of infinite height at $x = -a$ and $x = +a$. Suppose the particle is in the first excited state with wavefunction $\psi(x) = A\sin(\pi x/a)$ for $|x| \leq a$, $\psi(x) = 0$ otherwise.
(a) Find the value of A such that the wavefunction is correctly normalized. **[3]**
(b) If a measurement of the position of the particle is made, at what values of x is it **most likely** to be found? **[2]**
(c) What is the probability of finding the particle between $x = 0$ and $x = a/2$? **[3]**
(d) What would the average value of x be if many measurements were made on particles all in this same state? **[3]** What is the probability density of finding the particle at this particular value of x? **[1]**

2) Now consider the finite 1D square well of depth V_0 and width 2a, as discussed in the lectures. The potential is

$$\begin{aligned} V(x) &= 0 \qquad \text{for } -a \leq x \leq a \\ V(x) &= V_0 \quad \text{for } x < -a \text{ and } x > a. \end{aligned}$$

The condition for the occurrence of odd-parity bound-state solutions to the time-independent Schrödinger equation (i.e., odd-parity states with energy $E < V_0$) is

$$k\cot(ka) = -\sqrt{k_0^2 - k^2}. \tag{1}$$

(a) Define the quantities k and k_0 in this equation, and show with a sketch how it can be solved graphically. **[4]**
(b) Find the minimum value of k_0 necessary for there to be at least one solution to Eq. (1). Hence find, in terms of a, the minimum well depth V_0 needed to support an odd-parity bound state. **[4]**
(c) What are the solutions to Eq. (1) in the limit where k_0 becomes very large? [HINT: think about how your sketched graph would change as k_0 grows.] Compare your answer with the values of k found for the infinite square well solved in the lectures. **[4]**

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3) The lowest energy eigenfunction of the time-independent Schrödinger equation for a simple harmonic oscillator of angular frequency ω_0 is

$$\psi(y) = Ae^{-y^2/2},$$

where $y = (m\omega_0/\hbar)^{1/2}x$, x is the displacement of the oscillator from equilibrium, m is the mass, and A is a constant.

(a) Write the wavefunction in terms of x and verify, by explicit substitution in the time-independent Schrödinger equation, that the associated energy is $E = \hbar\omega_0/2$. **[4]**

(b) Find a value of the constant A which normalizes the wavefunction. Hence write down the probability density as a function of x. **[4]**

(c) What is the mean-squared displacement of the particle from the origin (i.e. what is the average value of x^2) in this state? Hence calculate the average potential energy. **[6]**

(d) Consider a carbon-hydrogen bond in a molecule. The stretching frequency of the bond is $\nu = 1.0 \times 10^{14}$ Hz and the mass is roughly that of the hydrogen atom, since the carbon atom remains nearly fixed. For the lowest vibrational energy eigenstate, find (i) the associated zero-point energy, and (ii) the mean-squared displacement of the hydrogen atom from equilibrium. **[2]**

You may use the following integrals in your answer:

$$\int_{-\infty}^{-\infty} e^{-x^2/a^2} = \sqrt{\pi}a, \qquad \int_{-\infty}^{-\infty} x^2 e^{-x^2/a^2} = \sqrt{\pi}a^3/2.$$