Assignment 4

Due: 8:30 am, 3 November 2022 (Thursday)

Course: Quantum Mechanics - 1
Tata Institute of Fundamental Research Hyderabad, India
Instructor: ramakrishnan@tifrh.res.in

Problem 1

In the dimensionless coordinate, q, the position and momentum operators are denoted $\hat{q}$ and $\hat{p}_q$. These are related to the usual position and momentum operators through the transformation

$$\hat{q} = \sqrt{\frac{m\omega}{\hbar}}\hat{x}$$

a) By dimensional analysis, ensure that $\hat{q}$ is dimensionless
b) Derive an expression for $\hat{p}_q$ in terms of q. What is the dimension of this operator?
c) Show that annihilation and creation ladder operators can be written in terms of the dimensionless variables as

$$\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2}}\left[q + \frac{d}{dq}\right] \\ \hat{a}^{\dagger} &= \frac{1}{\sqrt{2}}\left[q - \frac{d}{dq}\right] \end{aligned}$$

d) Show that the ground state wavefunction of a quantum harmonic oscillator is

$$\begin{aligned} \psi_0(q) &= \langle q|0\rangle \\ &= \left[\frac{1}{\pi}\right]^{1/4} e^{-q^2/2} \end{aligned}$$

e) Prove that

$$\left(q - \frac{d}{dq}\right)^n e^{-q^2/2} = e^{-q^2/2}\left((-1)^n e^{q^2}\frac{d^n}{dq^n}e^{-q^2}\right)$$

f) Show that for the n-state of a quantum harmonic oscillator, the wavefunction is

$$\begin{aligned} \psi_n(q) &= \langle q|n\rangle \\ &= \frac{1}{\sqrt{n!}}\left(\hat{a}^{\dagger}\right)^n \psi_0(q) \\ &= \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-q^2/2} H_n(q), \end{aligned}$$

where $H_n(q)$ is the Hermite's polynomial in q of degree n, defined using Rodrigue's formula

$$H_n(q) \quad = \quad (-1)^n e^{q^2} \frac{d^n}{dq^n} e^{-q^2}$$

g) Start with $H_0(q) = 1$ and $H_1(q) = 2q$, and derive expressions for $H_2(q), H_3(q), \ldots, H_6(q)$ using the recurrence relation

$$H_{n+1}(q) = 2qH_n(q) - 2nH_{n-1}(q)$$

Problem 2

Quantum harmonic oscillator is a model for diatomic molecules vibrating about their equilibrium bond length. In spectroscopy, vibrational energy levels are determined by probing a molecule with infra-red radiation. The resulting intensity-vs.-wavelengths graph shows us the wavelength where absorption has happened and the molecule has been 'excited' from the ground state.

In the dipole approximation of light-matter interaction, we say that the operator which couples light to matter is proportional to the position operator $\hat{x}$. The dipole allowed transitions for a quantum harmonic oscillator is determined by the spectroscopic selection rule

$$\begin{aligned} \langle m|\hat{x}|n\rangle &\neq 0;\ \text{when}\, m = n \pm 1 \\ &= 0;\ \text{otherwise} \end{aligned}$$

which will tell us whether a photon of a certain wavelength will be absorbed or not. A transition (excitation or deexcitation) from the n-th state to m-th state is dipole-allowed only when the matrix element $\langle m|\hat{x}|n\rangle$ does not vanish. Derive this selection rule using results from Problem 1.

Problem 3

Show that there is at least one bound state for a quantum particle trapped in a one-dimensional finite-rectangular-well.

Problem 4

Derive an expression for the transmission coefficient of a finite-rectangular-well as a function of the energy of the incident beam (E), well-depth ($-|V|$), and well-width ($2a$). Explain your result with a diagram.

Problem 5

The result of Problem 4 can be used to understand a scattering experiment where electrons are scattered by noble gas atoms. The influence of a noble gas atom on the motion of electrons can be approximated with a rectangular well potential. Let us say, the first maximum of the transmission coefficient occurs at 1 eV. Assume the diameter of the noble gas atoms to be 1 Å, and estimate the well-depth.