PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 15, March 23, 2021 (Tuesday)

- Handouts:
  (a) Midterm Exam Solutions, and
  (b) Harmonic Oscillator
- Reading: Harmonic Oscillator, My Notes and Griffiths 2.3
- Assignment: Problem Set 7 due March 24 (Wednesday).
  Submit your homework assignments to Canvas.

Topics for Today: Harmonic Oscillator [Griffiths 2.3]

3.8 Equation of continuity

4.1 Introduction

4.2 Energy Eigenstates of the Harmonic Oscillator [Griffiths 2.3.1]

Topics for Next Lecture: Harmonic Oscillator

4.2 Energy Eigenstates of the Harmonic Oscillator [Griffiths 2.3.1]

4.3 The Harmonic Oscillator in the Coordinate Basis [Griffiths 2.3.2]

PROBLEM 2 in Midterm Exam

(b) We can easily make the D operator Hermitian by defining

$$K \equiv -iD \quad \text{and} \quad K|k\rangle = k|k\rangle \,.$$

The operator K has the eigenvector $|k\rangle$ and the eigenvalue k.

In the x basis, we have

$$\langle x|K|k\rangle = k\langle x|k\rangle \quad \text{and} \quad \int \langle x|K|y\rangle\langle y|k\rangle \, dy = k\langle x|k\rangle \,.$$

Let us apply the matrix element of K

$$\langle x|K|y\rangle = -i\langle x|D|y\rangle = -i\frac{d}{dx}\delta(x-y)$$

and define $\langle x|k\rangle = \psi_k(x)$, then we have

$$\begin{aligned} \int -i\frac{d}{dx}\delta(x-y)\psi_k(y)\,dy &= k\psi_k(x) \quad \text{or} \\ -i\frac{d}{dx}\psi_k(x) &= k\psi_k(x)\,. \end{aligned}$$

(c) This is a linear first order differential equation that has the standard form

$$\frac{d}{dx}\psi_k(x) - ik\psi_k(x) = 0\,,$$

with the characteristic equation

$$\lambda - ik = 0$$

and the root $\lambda = ik$.

Therefore, the general solution is

$$\psi_k(x) = Ae^{\lambda x} = Ae^{ikx}$$

where A is a normalization constant, k is an eigenvalue with $\psi_k(x)$ as the eigenfunction of the operator K.

(d) Here A is an arbitrary constant and we can choose A so that the vector $|k\rangle$ is normalized:

$$\begin{aligned}
\langle k|q\rangle &= \int \langle k|x\rangle\langle x|q\rangle\, dx \\
&= \int \psi_k^*(x)\psi_q(x)\, dx \\
&= |A|^2 \int e^{-ikx}e^{iqx}\, dx \\
&= |A|^2 \int e^{-i(k-q)x}\, dx \\
&= \delta(k-q)
\end{aligned}$$

Bonus (3 points):

The integral in the previous equation is the Gaussian representation of the Dirac delta function

$$\int e^{-i(k-q)x}\, dx = (2\pi)\delta(k-q)\,.$$

Choosing $A \in \mathcal{R}$, and $A > 0$, we obtain

$$|A|^2(2\pi) = 1 \quad \text{and} \quad A = \frac{1}{\sqrt{2\pi}}\,.$$

(e) Any state vector $|\psi\rangle$ can be expanded in the x basis

$$|\psi\rangle = \int |x\rangle\langle x|\psi\rangle\, dx = \int \psi(x)|\psi\rangle\, dx$$

with the wave function

$$\psi(x) \equiv \langle x|\psi\rangle\,.$$

Expanding the state vector in the k basis

$$|\psi\rangle = \int |k\rangle\langle k|\psi\rangle\, dk = \int \phi(k)|k\rangle\, dk$$

we then have the wave function $\phi(k)$

$$\phi(k) \quad \equiv \quad \langle k|\psi\rangle$$

$$
\begin{aligned}
&= \int dx \langle k|x\rangle\langle x|\psi\rangle \quad \text{(completeness relation)} \\
&= \int \psi_k^*(x)\psi(x) \\
&= A^* \int dx e^{-ikx}\psi(x)\,.
\end{aligned}
$$

This is just the Fourier transform.

Bonus (2 points): In part (d), we have found $A = A^* = 1/\sqrt{2\pi}$. Thus

$$
\begin{aligned}
\phi(k) &= A^* \int e^{-ikx}\psi(x)\,dx \\
&= \frac{1}{\sqrt{2\pi}} \int e^{-ikx}\psi(x)\,dx\,.
\end{aligned}
$$

3.8 Equation of continuity

In electrodynamics the total charge (Q) of a system is a constant

$$Q(t) = \int \rho \, d^3x \; = \; \text{constant} \, , \quad \rho(\vec{r}) \; = \; \text{charge density} \, ,$$

which is often described as the conservation of charge.

- Such a relation is known as a global conservation law.
- Global conservation laws allow charges to disappear at some place and to appear suddenly at some other place in an isolated system.

Divergence Theorem:

For a simple solid region V with the boundary surface S, if $\vec{A}$ is a vector field with continuous components and first order derivative, then

$$\int \vec{A} \cdot d\vec{S} = \int \nabla \cdot \vec{A} \, dV$$

where $\nabla \cdot \vec{A} =$ the divergence of $\vec{A}$.

However, in electrodynamics, we also know of a continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{J} \quad \text{or} \quad \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0\,,$$

where ρ is the electric charge density and $\vec{J}$ is the current density at some point. Integrating this over a volume we have

$$\frac{\partial}{\partial t}\int_V \rho(\vec{x},t)\; d^3x = -\int_V \nabla \cdot \vec{J}\, d^3x = -\int_S \vec{J} \cdot d\vec{S}$$

- This shows that any decrease in the charge in a volume must be accompanied by an electric flux out of the volume.
- In other words, charge has to be locally conserved.

In quantum mechanics there are globally conserved quantities as well. For example,

$$\langle \Psi(t) | \Psi(t) \rangle = \langle \Psi(0) | U^\dagger(t) U(t) | \Psi(0) \rangle = \langle \Psi(0) | \Psi(0) \rangle \, .$$

If the states are normalized this implies that the probability of finding a particle anywhere is unity. For example,

$$\begin{aligned} \langle \Psi(0) | \Psi(0) \rangle \; = \; 1 \quad &= \quad \langle \Psi(t) | \Psi(t) \rangle \\ &= \quad \int \langle \Psi(t) | x \rangle \langle x | \Psi(t) \rangle \, dx \\ &= \quad \int \Psi^*(x,t) \Psi(x,t) \, dx \\ &= \quad \int \rho(x,t) \, dx \, . \end{aligned}$$

We also have local conservation laws in quantum mechanics. Let us consider the Schrödinger equation in the coordinate basis:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{x},t) = H\Psi(\vec{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]\Psi(\vec{x},t)\,.$$

The conjugate equation reads

$$-i\hbar\frac{\partial}{\partial t}\Psi^*(\vec{x},t) = H\Psi^*(\vec{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]\Psi^*(\vec{x},t)\,.$$

Multiplying the first equation with $\Psi^*(\vec{x},t)$ and the second with $\Psi(\vec{x},t)$ and subtracting the two, we have

$$\begin{aligned} & i\hbar\left[\Psi^*(\vec{x},t)\frac{\partial}{\partial t}\Psi(\vec{x},t) + \Psi^{(}\vec{x},t)\frac{\partial}{\partial t}\Psi^*(\vec{x},t)\right] \\ = \quad & -\frac{\hbar^2}{2m}\left[\Psi^*(\vec{x},t)\nabla^2\Psi(\vec{x},t) - \Psi(\vec{x},t)\nabla^2\Psi^*(\vec{x},t)\right]\,. \end{aligned}$$

That leads to

$$\frac{\partial}{\partial t}\left[\Psi^*(\vec{x},t)\Psi(\vec{x},t)\right] = -\frac{\hbar}{2im}\nabla\cdot\left[\Psi^*(\vec{x},t)\nabla\Psi(\vec{x},t) - \nabla\Psi^*(\vec{x},t)\Psi(\vec{x},t)\right]$$

where ∇^2 is the Laplacian

$$\nabla^2 f(\vec{r}) = \nabla\cdot\nabla f(\vec{r})$$

with the gradient of $f(\vec{r})$

$$\nabla f(\vec{r}) = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}\,.$$

Note that $\vec{r} = \vec{x}$.

- We know that $\Psi^*(\vec{x},t)\Psi(\vec{x},t)d^3x = \rho(\vec{x},t)d^3x$ is the probability of finding a particle between $\vec{x}$ and $\vec{x}+d\vec{x}$ at t.
- Thus $\Psi^*(\vec{x},t)\Psi(\vec{x},t) = \rho(\vec{x},t)$ is the probability density.

We can define a probability density

$$\rho(\vec{x},t) \equiv \Psi^*(\vec{x},t)\Psi(\vec{x},t)$$

and a probability current density

$$\vec{J} \equiv +\frac{\hbar}{2im}\left[\Psi^*(\vec{x},t)\left(\nabla\Psi(\vec{x},t)\right) - \left(\nabla\Psi^*(\vec{x},t)\right)\Psi(\vec{x},t)\right] .$$

So that the equation of continuity becomes

$$\frac{\partial}{\partial t}\rho(\vec{x},t) + \nabla \cdot \vec{J} = 0 .$$

- This again leads to a local conservation law, namely, locally the charge in the probability density must be equal to the negative of the probability flux out of that volume.

- This continuity equation further emphasizes that the solutions to Schrödinger equation must be such that both $\Psi(\vec{x},t)$ and $\nabla\Psi(\vec{x},t)$ are continuous for proper potentials.

4 The Harmonic Oscillator

4.1 Introduction

The harmonic oscillator is very important in both classical mechanics and quantum mechanics because it is

(a) a system that can be exactly solved,

(b) a system of great relevance in physics, and

(c) a superb pedagogical tool.

The Hamiltonian for a classical harmonic oscillator in one dimension is given by

$$H = T + V = \frac{P^2}{2m} + \frac{1}{2}kX^2 = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\,,$$

where k = spring constant, and ω = angular frequency.

Any system fluctuating by small amounts near a configuration of stable equilibrium may be described either by an oscillator or by a collection of decoupled harmonic oscillators.

Let us consider a particle moving in a potential $V(x)$. If the particle is placed at one of its minima at x_0, it will remain there in a state of stable static equilibrium. The potential it experiences can be expanded in a Taylor series:

$$V(x) = V(x_0 + \Delta x) = V(x_0) + \left.\frac{dV}{dx}\right|_{x_0} (x - x_0) + \frac{1}{2} \left.\frac{d^2V}{dx^2}\right|_{x_0} (x - x_0)^2 + \ldots$$

where $\Delta x = x - x_0$,

(i) $V(x_0) =$ constant $=$ arbitrary reference potential, and

(ii) $-(dV/dx)_{x=x_0} =$ force $= 0$, at an equilibrium position.

If we shift the origin of coordinates to x_0, the potential becomes

$$V(x) = \frac{1}{2!} \left.\frac{d^2V}{dx^2}\right|_{x=0} x^2 + \frac{1}{3!} \left.\frac{d^3V}{dx^3}\right|_{x=0} x^3 + \cdots$$

For small oscillations, we may consider the leading term as the harmonic oscillator potential with $(d^2V/dx^2)|_{x=0} = m\omega^2$.

Let us consider a system with N degrees of freedom and a Hamiltonian

$$\begin{aligned}
H &= \sum_{i}^{n} \frac{p_i^2}{2m} + V(x_1, \ldots, x_N) \quad \text{and} \\
V(x_1, \ldots, x_N) &= V(\vec{x}^0) + \frac{1}{2!} \sum_{i,j}^{N} \left. \frac{\partial^2 V}{\partial x_i \partial x_j} \right|_{\vec{x}=\vec{x}_0} (x_i - x_i^0)(x_j - x_j^0) + \cdots \\
&= V(\vec{x}^0) + \sum_{i,j} \frac{1}{2!} \sum_{i,j}^{N} (x_i - x_i^0) S_{ij} (x_j - x_j^0) + \mathcal{O}(\Delta x^3) \\
&\simeq V(\vec{x}^0) + \frac{1}{2}(x - x^0)^T S (x - x^0) \,,
\end{aligned}$$

near an equilibrium point $\vec{x}^0 = (x_1^0, \ldots, x_N^0)$.

The $N \times N$ matrix S is real and symmetric and can be diagonalized by some orthogonal matrix O

$$\frac{1}{2}(x - x^0)^T S (x - x^0) = \frac{1}{2} y^T O^T S O y = \frac{1}{2} y^T S_D y.$$

Let us express

$$\begin{aligned} (x - x^0) &= O \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}, \text{ and} \\ O^T S O &= S_D = \begin{pmatrix} k_1 & & \\ & \ddots & \\ & & k_N \end{pmatrix}. \end{aligned}$$

In this new basis of y, the Hamiltonian becomes

$$\begin{aligned} H &= \sum_{i}^{N} \frac{p_i^2}{2m} + V_0 + \frac{1}{2}\sum_{i}^{N} k_i y_i^2 \\ &= V_0 + \sum_{i}^{N} (\frac{p_i^2}{2m} + \frac{1}{2} k_i y_i^2) \\ &= V_0 + \sum_{i}^{N} H_i \end{aligned}$$

is the sum of N independent harmonic oscillators in one dimension.

The total energy is given by

$$E = E_1 + E_2 + \cdots + E_N + V_0.$$

The eigenfunction in the coordinate basis can be expressed as

$$\psi_E(y_1, \ldots, y_N) = \psi_{E_1}(y_1)\psi_{E_2}(y_2)...\psi_{E_N}(y_N).$$

4.1 Energy Eigenstates of the Harmonic Oscillator

The energy eigenvalue equation for the harmonic oscillator is

$$H|E_n\rangle = \left(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2\right)|E_n\rangle = E_n|E_n\rangle\,.$$

Apart from scaling factors, the Hamiltonian has the following form

$$H \sim X^2 + P^2 = (X+iP)(X-iP) \quad \text{N.B.} \quad A^2 - B^2 = (A+B)(A-B)\,.$$

Let us define two new operators

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(X + \frac{i}{m\omega}P\right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(X - \frac{i}{m\omega}P\right)\,.$$

The operator $a^\dagger a$ is related to the Hamiltonian

$$\begin{aligned} a^\dagger a &= \frac{1}{\hbar\omega}(\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2) + \frac{i}{2\hbar}[X,P] \\ &= \frac{1}{\hbar\omega}H - \frac{1}{2} \quad \text{with} \quad [X,P] = i\hbar\,. \end{aligned}$$

The Hamiltonian becomes

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) .$$

The operators a and $a^\dagger$ has the following commutation relation

$$\begin{aligned} [a, a^\dagger] &= \left(\frac{m\omega}{2\hbar}\right) \left(-\frac{i}{m\omega}[X,P] + \frac{i}{m\omega}[P,X] \right) \\ &= \left(\frac{m\omega}{2\hbar}\right) \left(\frac{2\hbar}{m\omega} \right) \\ &= 1\,. \end{aligned}$$

That is

$$[a, a^\dagger] = 1\,.$$

Let us define the operator $a^\dagger a$ as the number operator

$$N \equiv a^\dagger a$$

and the Hamiltonian can be expressed as

$$H = \hbar\omega(N + \frac{1}{2}).$$

Applying the commutation relations

$$[a, a^\dagger] = 1\,,$$

and

$$[a, a] = 0\,, \quad \text{and} \quad [a^\dagger, a^\dagger] = 0\,,$$

we obtain

- $[N, a] = ?$ and $[N, a^\dagger] = ?$
- $[H, a] = ?$ and $[H, a^\dagger] = ?$
- $[H, N] = ?$

Applying the commutation relations among a and $a^\dagger$, we obtain

$$\begin{aligned}
\left[N, a^\dagger\right] &= \left[a^\dagger a, a^\dagger\right] = a^\dagger \,, \\
[N, a] &= \left[a^\dagger a, a\right] = -a \,, \\
\left[H, a^\dagger\right] &= (\hbar\omega)\left[(N + \frac{1}{2}), a^\dagger\right] = (\hbar\omega) a^\dagger \,, \\
[H, a] &= (\hbar\omega)\left[(N + \frac{1}{2}), a\right] = -(\hbar\omega) a \,,
\end{aligned}$$

and

$$[H, N] = 0.$$

This implies that H and N can be simultaneous diagonalized or that they have a common set of eigenvectors.

Let us denote the eigenvector by $|n\rangle$ such that

$$N|n\rangle = n|n\rangle$$

where n is the eigenvalue and the eigenvectors $|n\rangle$ form a complete set of orthonormal basis vectors

$$\langle m|n\rangle = \delta_{mn} \quad \text{and} \quad \sum_n |n\rangle\langle n| = \mathrm{I}\,.$$

Then we have

$$\begin{aligned} H|n\rangle &= \hbar\omega(N + \frac{1}{2})|n\rangle \\ &= \hbar\omega(n + \frac{1}{2})|n\rangle \\ &= E_n|n\rangle \end{aligned}$$

The energy associate with the state $|n\rangle$ us

$$E_n = (n + \frac{1}{2})\hbar\omega.$$

Now let us consider $|n'\rangle = a|n\rangle$, and

$$\begin{aligned} H(a|n\rangle) &= aH|n\rangle + [H,a]|n\rangle \\ &= E_n(a|n\rangle) - \hbar\omega(a|n\rangle) \\ &= (E_n - \hbar\omega)(a|n\rangle) \\ &= E_{n-1}(a|n\rangle) \\ H|n'\rangle &= E_{n-1}|n'\rangle\,, \end{aligned}$$

where we have applied

$$[H,a] \equiv Ha - aH \quad \text{and} \quad Ha = aH + [H,a] = aH - (\hbar\omega)a\,.$$

The state $a|n\rangle$ is an eigenstate of the Hamiltonian with the eigenvalue

$$E_n - \hbar\omega = E_{n-1}$$

The effect of the operator a on a state is to lower its energy by one unit of $\hbar\omega$. Therefore, the operator a is called the lowering operator.

The state with energy

$$E_n - \hbar\omega = [(n-1) + \frac{1}{2}]\hbar\omega = E_{n-1}$$

must correspond to to $|n-1\rangle$. We can write

$$\begin{aligned} a|n\rangle &= c_n|n-1\rangle \\ \langle n|a^\dagger &= c_n^*\langle n-1| \end{aligned}$$

Multiplying by the adjoint, we have

$$\begin{aligned} |c_n|^2 &= c_n^* c_n \\ &= c_n^* c_n \langle n-1|n-1\rangle \\ &= \langle n|a^\dagger a|n\rangle \\ &= \langle n|N|n\rangle \\ &= n\langle n|n\rangle \\ &= n, \end{aligned}$$

that is $|c_n|^2 = n$. We may choose c_n to be real and obtain

$$c_n = c_n^* = \sqrt{n}\,, \quad a|n\rangle = \sqrt{n}|n-1\rangle\,, \quad \text{and} \quad |n-1\rangle = \frac{1}{\sqrt{n}}a|n\rangle\,.$$

Similarly, we have $|n''\rangle = a^\dagger|n\rangle$, and

$$\begin{aligned} H(a^\dagger|n\rangle) &= a^\dagger H|n\rangle - [a^\dagger, H]|n\rangle \\ &= E_n a^\dagger|n\rangle - (-\hbar\omega a^\dagger)|n\rangle \\ &= (E_n + \hbar\omega)a^\dagger|n\rangle \\ &= E_{n+1}(a^\dagger|n\rangle) \\ H|n''\rangle &= E_{n+1}|n''\rangle\,, \end{aligned}$$

where we have applied

$$[H, a^\dagger] \equiv Ha^\dagger - a^\dagger H \quad \text{and} \quad Ha^\dagger = a^\dagger H + [H, a^\dagger] = a^\dagger H + (\hbar\omega)a^\dagger\,.$$

The operator $(a^\dagger)$ acting on a state raises its energy by one unit of $\hbar\omega$. Therefore, $a^\dagger$ is known as the raising operator.