PHYS 621 Lecture Notes 13

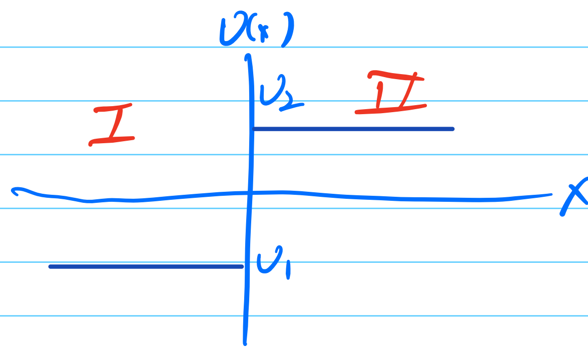
Probability Current and Scattering

Continuity Equation in 1D:

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

$$J(x,t) = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

Consider scattering off a potential step:



We have found solutions to the Schrödinger equation of the form:

$$\psi_I(x,t) = e^{-iEt/\hbar}\left(e^{ik_1x} + Re^{-ik_1x}\right), \quad x<0$$

$$\psi_{II}(x,t) = e^{-iEt/\hbar}\left(Se^{ik_2x}\right), \quad x>0$$

Region I: $J(x,t) = \frac{\hbar i k_1}{2mi}\left[\left(e^{-ik_1x} + R^* e^{ik_1x}\right)\left(e^{ik_1x} - Re^{-ik_1x}\right) + c.c.\right]$

complex conjugate of other term in bracket.

$$\text{I}: \quad J(x,t) = \frac{\hbar k_1}{2m}\Big[\big(1 + R^* e^{2ik_1x} - R e^{-2ik_1x} - |R|^2\big) + \big(1 + R e^{-2ik_1x} - R^* e^{2ik_1x} - |R|^2\big)\Big]$$

$$= \frac{\hbar k_1}{m}\left[1 - |R|^2\right]$$

$$\equiv J_{inc} + J_{refl}$$

incident reflected

where $J_{inc} \equiv \frac{\hbar k_1}{m}$

$J_{refl} \equiv -\frac{\hbar k_1}{m}|R|^2$

Region II: $J_{trans}(x,t) = \frac{\hbar i k_2}{2mi}\left[|S|^2 + |S|^2\right]$

transmitted $= \frac{\hbar k_2}{m}|S|^2$

Conservation of probability:

$$(J_{inc} + J_{refl})\big|_{x=0} = J_{trans}\big|_{x=0}$$

$$\rightarrow 1 - |R|^2 = \underbrace{\frac{k_2}{k_1}|S|^2}$$

$|R|^2$ = prob of reflection

$T = \frac{k_2}{k_1}|S|^2$ = prob. of transmission

N 8.1

The Harmonic Oscillator (1D)

$$F = -Kx \quad , \quad V = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2x^2$$

K: spring constant

$$(K = m\omega^2)$$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \qquad \text{Hamiltonian operator}$$

N8.2

We introduce the operators

$$\hat{a} \equiv \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} + \frac{i}{\sqrt{m\omega\hbar}}\,\hat{p}\right)$$

$$\hat{a}^+ \equiv \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} - \frac{i}{\sqrt{m\omega\hbar}}\,\hat{p}\right)$$

The commutator of $\hat{a}$ and $\hat{a}^+$ is:

$$[\hat{a}, \hat{a}^+] = \frac{1}{2}\left[\left(\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} + \frac{i}{\sqrt{m\omega\hbar}}\,\hat{p}\right), \left(\sqrt{\frac{m\omega}{\hbar}}\,\hat{x} - \frac{i}{\sqrt{m\omega\hbar}}\,\hat{p}\right)\right]$$

$$= -\frac{i}{2\hbar}\left([\hat{x},\hat{p}] - [\hat{p},\hat{x}]\right)$$

$$= \frac{-i}{2\hbar}\cdot 2i\hbar\hat{\mathbb{1}} = \hat{\mathbb{1}}$$

$$\Rightarrow \quad \boxed{[\hat{a}, \hat{a}^+] = \hat{\mathbb{1}}}$$

Solving for $\hat{x}$, $\hat{p}$ in terms of $\hat{a}, \hat{a}^+$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^+)$$

$$\hat{p} = \sqrt{\frac{m\omega\hbar}{2}}\,i\,(\hat{a}^+ - \hat{a})$$

The Hamiltonian can now be written in terms of $\hat{a}, \hat{a}^{+}$:

$$\hat{H} = \frac{1}{2m}\left(-\frac{m\omega\hbar}{2}\right)(\hat{a}^{+}-\hat{a})^2 + \frac{1}{2}m\omega^2 \cdot \frac{\hbar}{2m\omega}(\hat{a}+\hat{a}^{+})^2$$

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

$$= \frac{1}{2}\hbar\omega\left(2\hat{a}^{+}\hat{a} + [\hat{a},\hat{a}^{+}]\right)$$

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

Define $\hat{N} \equiv \hat{a}^{+}\hat{a} = \hat{N}^{+}$ (Hermitian)

$\hat{N}$ is a positive semidefinite operator, i.e. its eigenvalues are ≥ 0:

Suppose $|n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue n:

$$\hat{N}|n\rangle = n|n\rangle.$$

Then $\langle n|\hat{N}|n\rangle = \langle n|a^{+}a|n\rangle = \| \hat{a}|n\rangle \|^2 \geq 0$

$$= n\langle n|n\rangle$$

$\rightarrow$ $n \geq 0$ as claimed.

Smallest eigenvalue $n=0$ $\longleftrightarrow$ $\boxed{\hat{a}|0\rangle = 0}$

Since $\hat{H} = \hbar\omega(\hat{N}+\frac{1}{2})$, the states $|n\rangle$ are eigenstates of $\hat{H}$ with eigenvalues

$$\boxed{E_n = \hbar\omega(n + 1/2)}$$

Ground state: $n=0$ $\rightarrow$ $\boxed{E_0 = \frac{1}{2}\hbar\omega}$ Ground state energy.

Calculate $[\hat{N}, \hat{a}] = [\hat{a}^+ \hat{a}, \hat{a}] = \hat{a}^+ \cancel{[\hat{a}, \hat{a}]} = [\hat{a}^+, \hat{a}]\hat{a}$ 0

$$\boxed{[\hat{N}, \hat{a}] = -\hat{a}}$$

Similarly, $[\hat{N}, \hat{a}^+] = [\hat{a}^+\hat{a}, \hat{a}^+] = \hat{a}^+[\hat{a}, \hat{a}^+] + \cancel{[\hat{a}^+, \hat{a}^+]}\hat{a}$ 0

$$\boxed{[\hat{N}, \hat{a}^+] = \hat{a}^+}$$

Consider the state $\hat{a}^+|0\rangle$.

$$\hat{H}(\hat{a}^+|0\rangle) = \hbar\omega\left(\hat{a}^+\hat{a} + \tfrac{1}{2}\right)(\hat{a}^+|0\rangle)$$

$$= \hbar\omega\Big(\underbrace{\cancel{\hat{a}^+\hat{a}^+\hat{a}}^{\hat{a}|0\rangle = 0} + \hat{a}^+[\hat{a}, \hat{a}^+]}_{\hat{a}^+\hat{a}} + \tfrac{1}{2}\hat{a}^+\Big)|0\rangle$$

$$= \hbar\omega\left(1 + \tfrac{1}{2}\right)(\hat{a}^+|0\rangle)$$

Hence, $\hat{a}^+|0\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue

$$\boxed{E_1 = \tfrac{3}{2}\hbar\omega}$$

More generally:

$$\hat{H}(\hat{a}^+|n\rangle) = \hbar\omega\left(\hat{a}^+\hat{a} + \tfrac{1}{2}\right)(\hat{a}^+|n\rangle)$$

$$= \hbar\omega\left(\hat{a}^+\hat{a}^+\hat{a} + \hat{a}^+[\hat{a}, \hat{a}^+] + \tfrac{1}{2}\hat{a}^+\right)|n\rangle$$

$$= \hbar\omega\left(\hat{a}^+\hat{N} + \hat{a}^+ + \tfrac{1}{2}\hat{a}^+\right)|n\rangle$$

$$= \hbar\omega\left(n + 1 + \tfrac{1}{2}\right)(\hat{a}^+|n\rangle)$$

$\Rightarrow$ $\hat{a}^+|n\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue

$$\boxed{E_{n+1} = \hbar\omega\left(n + 1 + \tfrac{1}{2}\right)}$$

Normalization: $\| \hat{a}^\dagger |n\rangle \|^2 = \langle n | \hat{a}\hat{a}^\dagger | n\rangle$

$$= \langle n | \left(\hat{a}^\dagger \hat{a} + [\hat{a}, \hat{a}^\dagger] \right) | n\rangle$$

$$= \langle n | (\hat{N} + \hat{1}) | n\rangle$$

$$= (n+1) \langle n | n\rangle$$

$\Rightarrow$ Normalize states $|n+1\rangle = \frac{1}{\sqrt{n+1}} a^\dagger |n\rangle$

Then $\langle n+1 | n+1\rangle = \frac{1}{n+1} \| \hat{a}^\dagger |n\rangle \|^2$

$$= \langle n | n\rangle$$

If the ground state is normalized such that $\langle 0|0\rangle = 1$, then the normalized state $|n\rangle$ is

$$\boxed{|n\rangle = \prod_{j=1}^{n} \frac{1}{\sqrt{j}} (\hat{a}^\dagger)^n |0\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle}$$

$$\boxed{E_n = (n + 1/2)\hbar\omega} \quad , \; n = 0, 1, 2, \ldots$$

Matrix elements: $\langle m | \hat{a} | n\rangle = \sqrt{n}\, \delta_{m,n-1}$

$$\langle m | \hat{a}^\dagger | n\rangle = \sqrt{n+1}\, \delta_{m,n+1}$$

As matrices,

$$\underline{a} = \begin{pmatrix} 0 & \sqrt{1} & & & \\ 0 & 0 & \sqrt{2} & & \\ 0 & 0 & 0 & \sqrt{3} & \\ & & & \ddots & \ddots \end{pmatrix} \qquad a^\dagger = \begin{pmatrix} 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \ddots \\ 0 & 0 & \sqrt{3} & \ddots \end{pmatrix}$$

N 8.6

Position basis $\{|x\rangle\}$

Ground state wavefunction:

$\psi_0(x) = \langle x|0\rangle$

$\hat{a}|0\rangle = 0 \rightarrow \int dx' \langle x|\hat{a}|x'\rangle\langle x'|0\rangle$

$= \int dx' \langle x|\hat{a}|x'\rangle \psi_0(x') = 0$

$\langle x|\hat{a}|x'\rangle = \langle x|\left(\sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}\right)|x'\rangle$

$= \delta(x-x')\left(\sqrt{\frac{m\omega x'}{2\hbar}} + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx'}\right)$

$\int dx' \, \delta(x-x')\left(\sqrt{\frac{m\omega x'}{2\hbar}}\psi_0(x') + \sqrt{\frac{\hbar}{2m\omega}}\frac{d\psi_0(x')}{dx'}\right) = 0$

$$\boxed{\sqrt{\frac{m\omega x}{2\hbar}}\psi_0(x) + \sqrt{\frac{\hbar}{2m\omega}}\frac{d\psi_0(x)}{dx} = 0}$$

$\frac{d\psi_0}{dx} + \sqrt{\frac{m\omega}{\hbar}}\, x\, \psi_0(x) = 0$

Solution: $\boxed{\psi_0(x) = A_0 e^{-\frac{m\omega x^2}{2\hbar}}}$

Normalization constant

$$\int dx\, |\psi_0(x)|^2 = |A_0|^2 \int_{-\infty}^{\infty} dx\; e^{-\frac{m\omega x^2}{\hbar}}$$

$$= |A_0|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

$$\rightarrow |A_0| = \sqrt{\frac{m\omega}{\pi\hbar}}$$

Finally, $$\boxed{\psi_0(x) = \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\frac{m\omega x^2}{2\hbar}}}$$ Normalized ground state wavefunction

$$\int dx\, |\psi_0(x)|^2 = 1.$$

Excited states: $|n\rangle = \frac{1}{\sqrt{n!}} (a^{+})^n |0\rangle$

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x| (a^{+})^n |0\rangle$$

$$= \frac{1}{\sqrt{n!}} \langle x| \left(\sqrt{\frac{m\omega}{2\hbar}}\, \hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\, \hat{p} \right)^n |0\rangle$$

$$\psi_n(x) = \frac{1}{\sqrt{n!}} \left(\sqrt{\frac{m\omega}{2\hbar}}\, x - \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} \right)^n \psi_0(x)$$

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{n!}} \sqrt{\frac{m\omega}{\pi\hbar}} \left(\sqrt{\frac{m\omega}{2\hbar}}\, x - \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} \right)^n e^{-\frac{m\omega x^2}{2\hbar}}}$$

$$= \left[\frac{m\omega}{\pi\hbar\, 2^{2n} (n!)^2} \right]^{1/4} e^{-m\omega x^2/2\hbar}\; H_n\!\left(\sqrt{\frac{m\omega}{\hbar}}\, x \right)$$

Hermite polynomials

$H_n(y)$ satisfies $H_n''(y) - 2y H_n'(y) + 2n H(y) = 0$