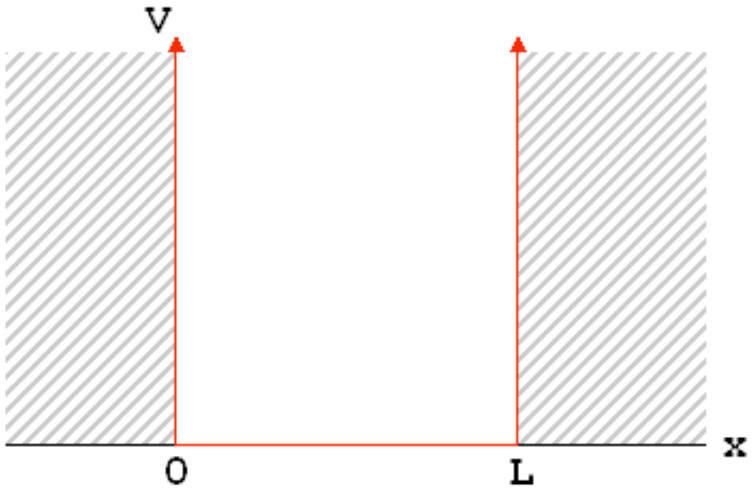
Outline

I. The infinite square well
II. A comment on wavefunctions at boundaries
III. Parity
IV. How to solve the Schroedinger Equation in momentum space

Please read Goswami Chapter 6.

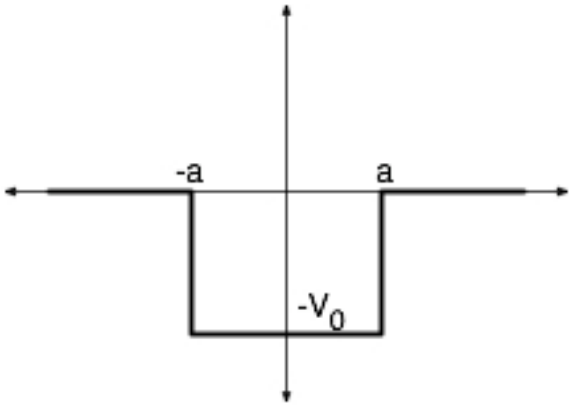
I. The infinite square well



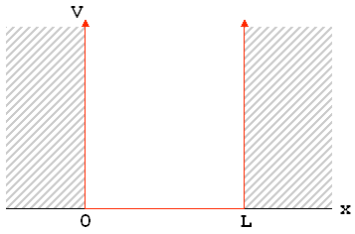
Suppose that the sides of the finite square well are extended to infinity:

It is a simplified case of the finite square well. How they differ:

Finite case



Infinite case



(1) Since V is not infinite in Regions 1 and 3, it is possible to have small damped ψ there.

Since V is infinite in Regions 1 and III, no ψ can exist there. ψ must terminate abruptly at the boundaries.

Finite case

To find the ψ's use the boundary conditions.

Result:

$\psi_2 = B\cos k_1 x$ or $A\sin k_1 x$

(A and B are complicated)

$k_1 = \dfrac{\sqrt{2mE}}{\hbar}$

E is sol'n of a transcendental equation.

Infinite case

The abrupt termination of the wavefunction is nonphysical, but it is called for by this (also nonphysical) well.

Abrupt change: we cannot require dψ/dx to be continuous at boundaries. Instead, replace the boundary conditions with:

Solve for ψ in Region 2 only.
Begin with ψ = Acoskx + Bsinkx
but require ψ = 0 at x = ± a/2. Result:

$\psi_2 = \sqrt{\dfrac{2}{a}}\cos k_n x \quad (n = 1,3,5,...)$ or

$\sqrt{\dfrac{2}{\mathrm{a}}}\sin k_n x \quad (n = 2,4,6,...)$

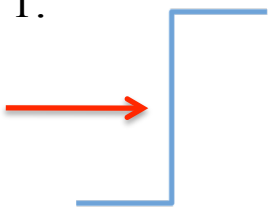
$k_1 = \dfrac{\sqrt{2mE}}{\hbar} = \dfrac{n\pi}{a}$

$E = \dfrac{\pi^2\hbar^2 n^2}{2ma^2} \qquad (n = 1,2,3...)$

II. Comment on wavefunctions at boundaries

Anytime a wave approaches a change in potential, the wave has some probability of reflecting, regardless of whether its E is >V or <V. So consider:

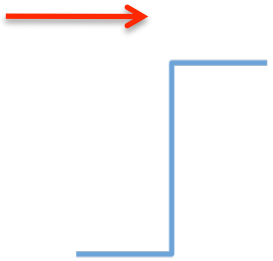
Case 1:



The wave will have some probability to reflect in all 3 cases.

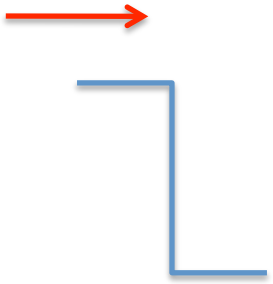
You cannot assume there is no "Be^{-ikx}" in Region 1 of Cases 2 and 3.

Case 2:



The way to see this is to work an example: Put in $Ae^{ikx} + Be^{-ikx}$ for Region 1 and see that the boundary conditions cannot be satisfied unless $B \neq 0$.

Case 3:



We will have a homework about this.

III. Linear combinations of wavefunctions

Suppose that somehow a particle in a well gets into this state:

u(x)=A sin 4πx/L + B sin 6πx/L

Questions: (1) What is its Ψ(x,t)?
(2) Is this a stationary state?

Answers: (1) Recall Ψ=u(x)T(t). Here u=u_1 + u_2, where each u_i goes with a different energy state E_i of the infinite square well:

$$u_1 = u(E_4) \qquad \text{where } E_4 = \frac{\pi^2\hbar^2 4^2}{2ma^2}$$

$$u_2 = u(E_6) \qquad \text{where } E_6 = \frac{\pi^2\hbar^2 6^2}{2ma^2}$$

We have to multiply each u_i by the associated $T_i = e^{-iE_i t/\hbar}$

$$\text{So } \Psi = A\sin\frac{4\pi x}{L} e^{-i\frac{\pi^2\hbar 8t}{ma^2}} + B\sin\frac{6\pi x}{L} e^{-i\frac{\pi^2\hbar 18t}{ma^2}}$$

Answer (2): Recall that if Ψ is a stationary state, then Probability density $=\Psi^*\Psi \neq f(t)$.

Here, Probability density =

$$|A|^2 \sin^2\left(\frac{4\pi x}{L}\right)+|B|^2 \sin^2\left(\frac{6\pi x}{L}\right)+\underbrace{A^* B \sin\left(\frac{4\pi x}{L}\right)\sin\left(\frac{6\pi x}{L}\right)e^{iE_4 t/\hbar}e^{-iE_6 t/\hbar}+AB^* \sin\left(\frac{4\pi x}{L}\right)\sin\left(\frac{6\pi x}{L}\right)e^{-iE_4 t/\hbar}e^{iE_6 t/\hbar}}_{\downarrow}$$

If A and B are real, this term becomes $\quad AB \sin\left(\frac{4\pi x}{L}\right)\sin\left(\frac{6\pi x}{L}\right)\underbrace{\left[e^{i(E_4-E_6)t/\hbar}+e^{-i(E_4-E_6)t/\hbar}\right]}_{\downarrow}$

$$2\cos\left(\frac{E_4-E_6}{\hbar}t\right)$$

Conclude: the probability is a function of time, so a linear combination of stationary states is NOT itself a stationary state.

III. Parity

Parity is a property of a wavefunction.

To understand the definition of parity, consider the result of replacing $\vec{r}$ by $-\vec{r}$ in a ψ.
(That is "reflect ψ through the origin.)

3 results are possible, depending on the detailed form of ψ:

1. ψ could remain unchanged $[\psi(-x) = \psi(x)]$.
Example: if $\psi \propto \cos(\vec{k} \cdot \vec{r})$, it would become $\cos\left(\vec{k} \cdot \{-\vec{r}\}\right) = \cos(\vec{k} \cdot \vec{r})$.
We say this kind of ψ has "even parity."

2. ψ could transform to $-\psi$ $[\psi(-x) = -\psi(x)]$.
Example: If $\psi \propto \sin(\vec{k} \cdot \vec{r})$
We say this kind of ψ has "odd parity."

3. ψ could become something else that is not $\pm \psi_{\text{original}}$.

What determines the parity of ψ ? The form of the potential V.
The ψ's that are eigenfunctions of some Hamiltonian H have definite parity (even or odd) if V(x)=V(-x). Prove this here:

Assumption #1: Consider some ψ that is

1. an eigenfunction of H such that $\underbrace{\frac{-p^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=E\psi}_{\downarrow}$

$$H\psi=E\psi$$

2. non-degenerate in energy, that is, no other eigenfunction of H has the same E

Assumption #2: Consider a V such that $V(x)=V(-x)$ (that is, V is reflection-symmetric).

Suppose we rename $x \rightarrow -x$

Then $H(x)\psi(x)=E\psi(x)$ becomes $H(-x)\psi(-x)=E\psi(-x)$

But $H=\underbrace{\frac{-p^2}{2m}\frac{\partial^2}{\partial x^2}}+\underbrace{V(x)}$ — $V(x)$: unchanged by $x \rightarrow -x$ due to Assumption 2

So $H(x)=H(-x)$ — $\frac{\partial^2}{\partial x^2}$: unchanged by $x \rightarrow -x$ in a second derivative

So $H(x)\psi(-x)=E\psi(-x)$

So if ψ(x) is an eigenfunction of H, then so is ψ(-x).
But we said ψ(x) is non-degenerate, so ψ(-x) cannot be independent of ψ(x).

So $\psi(-x)$ must $= C \cdot \psi(x)$ "Eq. 1"

To find C, rename $x \rightarrow -x$ in Eq. 1.

Eq. 1 becomes

$$\underbrace{\psi(-(-x))}_{\downarrow} = C \cdot \underbrace{\psi(-x)}_{\downarrow}$$

$$\psi(x) = C \cdot \left[C \cdot \psi(x)\right]$$

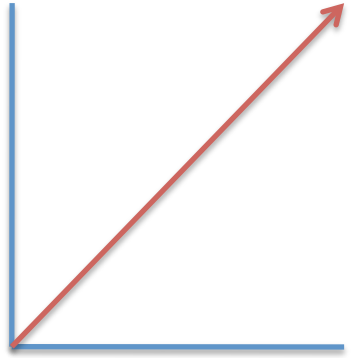
So $C^2 = \pm 1$.

We conclude that there are only 2 possible relationships between ψ(x) and ψ(-x) if Assumptions 1 and 2 hold---given those assumptions, it is impossible for ψ(x) to bear NO relationship to $\psi(-x)$.

IV. How to solve the Schroedinger Equation in momentum space: using p-space wavefunctions.

Message: The Schroedinger Equation, and the states of matter represented by wavefunctions, are so general that theey exist outside of any particular representation (x or p) and can be treated by either.

Example: Consider a potential shaped as



$V(x) = Cx \quad \text{for } x > 0$

$= 0 \quad \text{for } x \leq 0$

Recall the coordinate space Schroedinger Equation: $\left[\frac{p^2}{2m} + V(x)\right]\psi = E\psi$

Plug in this V: $\left[\frac{p^2}{2m} + Cx\right]\psi = E\psi \qquad (x > 0)$

Rewrite as: $\left[\frac{p^2}{2m} + Cx - E\right]\psi = 0$

Convert the equation to p-space:

p^2 remains p^2

$$x \to +i\hbar \frac{\partial}{\partial p}$$

$$\psi(x) \to A(p)$$

So the p-space form of the Schroedinger Equation is:

$\left[\frac{p^2}{2m} + Ci\hbar \frac{\partial}{\partial p} - E \right] A(p) = 0$. To solve it, multiply through by $\frac{i}{C\hbar}$:

$$\frac{i}{C\hbar}\frac{p^2}{2m}A + \frac{i}{C\hbar}Ci\hbar\frac{dA}{dp} - \frac{i}{C\hbar}EA = 0$$

$$\frac{i}{C\hbar}\left(\frac{p^2}{2m} - E\right) = \frac{1}{A}\frac{dA}{dp}$$ Integrate:

$$\frac{i}{C\hbar}\int\left(\frac{p^2}{2m} - E\right)dp = \int\frac{1}{A}dA$$

$$\frac{i}{C\hbar}\left(\frac{p^3}{6m}-Ep\right)=\ln A+K \qquad \text{Exponentiate, and define } K'=e^K$$

$$\exp\left[\frac{i}{C\hbar}\left(\frac{p^3}{6m}-Ep\right)\right]=K'A \qquad \text{Define } K''=1/K'$$

$$A_E=K''\exp\left[\frac{i}{C\hbar}\left(\frac{p^3}{6m}-Ep\right)\right]$$

Index by energy

Normalize the A's AND make them orthogonal (that is, independent): Require

$$\int_{-\infty}^{+\infty} dp A_E^* A_{E'}=\delta(E-E')$$

$$|K''|^2\int\exp\left[\frac{-i}{C\hbar}\frac{p^3}{6m}+\frac{i}{C\hbar}Ep\right]\exp\left[\frac{i}{C\hbar}\frac{p^3}{6m}-\frac{i}{C\hbar}E'p\right]dp=\delta(E-E')$$

$$|K''|^2\int\exp\left[\frac{i}{\hbar}\left(\frac{E}{C}-\frac{E'}{C}\right)p\right]dp=\delta(E-E')$$

Recall $k=\frac{p}{\hbar}$, so $dk=\frac{1}{\hbar}dp$. Then on the lefthand side we have

$$\hbar\left|K''\right|^2\int\exp\left[ik\left(\frac{E-E'}{C}\right)\right]dk$$

Recall $\delta(\text{x-x'})\equiv\frac{1}{2\pi}\int dke^{+ik(x-x')}$

Identify $x=E/C$ and $x'=E'/C$. Then on the lefthand side we have

$2\pi\hbar\left|\text{K}''\right|^2\delta\left(\frac{E-E'}{C}\right)$. Recall $\delta(\alpha\text{x})=\frac{1}{|\alpha|}\delta(x)$. Here $\alpha=\frac{1}{C}$.

$2\pi\hbar\left|\text{K}''\right|^2 C\delta\left(E-E'\right)$. Recall for normalization this must equal the righthand side, $\delta\left(E-E'\right)$

Conclude $2\pi\hbar\left|K''\right|^2=1$

$$K''=\frac{1}{\sqrt{2\pi\hbar C}}$$

$$A(p)=\frac{1}{\sqrt{2\pi\hbar C}}\exp\left[\frac{i}{C\hbar}\left(\frac{p^3}{6m}-Ep\right)\right]$$

How to find the allowed energies in momentum space?

Recall that any potential well produces quantized energies. We find them by applying boundary conditions (BC's). Usually we have the BC's expressed in x-space. So we must either

1. convert BC's to p-space or
2. Convert A(p) to x-space. ← We will do this.

General $\psi(x) = \int_{-\infty}^{+\infty} dk A(k) e^{ikx}$. Convert $k \to \frac{p}{\hbar}$ and put in normalization.

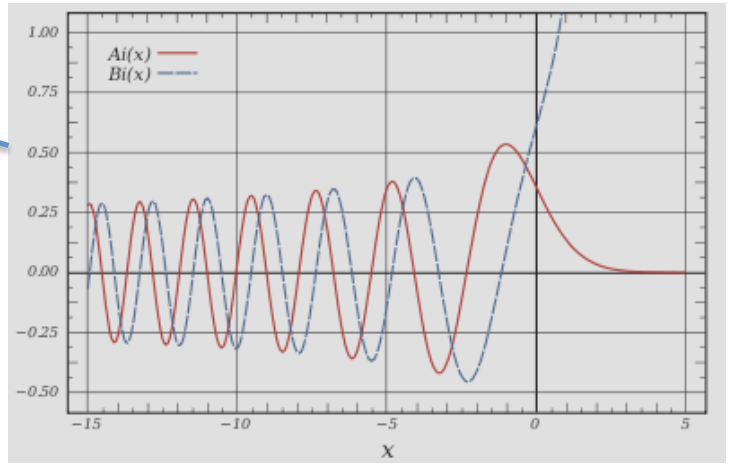
$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dp A(p) e^{ipx/\hbar}.$$ Plug in $A(p)$:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{2\pi\hbar C}} \int dp \exp\left[\frac{i}{C\hbar} \left(\frac{p^3}{6m} - Ep \right) + i \frac{px}{\hbar} \right]$$

Apply the BC that $\psi(0) = 0$:

$$\int dp \exp\left[\frac{i}{C\hbar} \left(\frac{p^3}{6m} - Ep \right) + i \frac{p0}{\hbar} \right] = 0. \qquad \text{Use } e^{i\theta} = \cos\theta + i\sin\theta$$

$$\underbrace{\int \cos\left[\frac{1}{C\hbar}\left(\frac{p^3}{6m} - Ep\right)\right]dp}_{\text{Airy functions } Ai} + i\underbrace{\int \sin\left[\frac{1}{C\hbar}\left(\frac{p^3}{6m} - Ep\right)\right]dp}_{\int \sin(\text{odd power}) = 0}$$



Conclude: $\mathrm{Ai}\left[-\mathrm{E_n}\left(\frac{2m}{C^2\hbar^3}\right)^{1/3}\right] = 0$

Ai_1 occurs when $-\mathrm{E_n}\left(\frac{2m}{C^2\hbar^3}\right)^{1/3} = -2.338$

first zero

Ai_2 occurs when $-\mathrm{E_n}\left(\frac{2m}{C^2\hbar^3}\right)^{1/3} = -4.088$

etc.

Invert these to get $\mathrm{E_1} = 2.338\left(\frac{C^2\hbar^2}{2m}\right)^{1/3}$

$\mathrm{E_2} = 4.088\left(\frac{C^2\hbar^2}{2m}\right)^{1/3}$, *etc*.

Outline

I. What to remember from linear algebra
II. Eigenvalue equations
III. Hamiltonian operators
IV. The connection between physics and math in Quantum Mechanics

Please re-read Goswami Section 3.3.
Please read the Formalism Supplement.

I. What to remember from linear algebra

Consider vectors $|\alpha\rangle$ and scalars a.

(1) A linear combination of vectors has form $a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + ...$

(2) A vector $|\lambda\rangle$ is linearly independent of a set of vectors if it cannot be written as a linear combination of members of the set.

(3) Can represent vector $|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + ... + a_n|e_n\rangle$ by indicating the basis (the $|e_i\rangle$) and the ordered list (ntuple) of components $(a_1, a_2, ..., a_n)$.

(4) Generalize the scalar product to > 3 dimensions. Call it the "inner product." Its symbol: $\langle\beta|\alpha\rangle = a_1^* b_1 + a_2^* b_2 + ... + a_n^* b_n$.

(5) Generalize length to > 3 dimensions. Call it the "norm" $|\alpha| = \sqrt{\langle\alpha|\alpha\rangle}$

(6) Consider the case where the $|e_i\rangle$ are orthonormal.

Then since $|\alpha\rangle = a_1|e_1\rangle + ... + a_n|e_n\rangle$,

any $a_i = \langle e_i|\alpha\rangle = \underbrace{\langle e_i|a_1|e_1\rangle}_{\downarrow\ a\langle e_i|e_1\rangle} + ... + \langle e_i|a_n|e_n\rangle$

$$\begin{cases} = 0 \text{ if } i \neq 1 \\ = 1 \text{ if } i = 1 \end{cases}$$

(7) Consider an operator $\hat{T}$ which transforms all of the basis vectors in a set:

$$\hat{T}|e_1\rangle = T_{11}|e_1\rangle + T_{21}|e_2\rangle + ... + T_{n1}|e_n\rangle$$

$$\hat{T}|e_2\rangle = T_{12}|e_1\rangle + T_{22}|e_2\rangle + ... + T_{n2}|e_n\rangle$$

...

$$\hat{T}|e_n\rangle = T_{1n}|e_1\rangle + T_{2n}|e_2\rangle + ... + T_{nn}|e_n\rangle$$

Rewrite this as

$$\hat{T}|e_j\rangle = \sum_{i=1}^{n} T_{ij}|e_i\rangle$$

Notice if $|\alpha\rangle$ is expressed in the $|e_i\rangle$ basis, then

$$\hat{T}|\alpha\rangle = \hat{T}\sum_j a_j|e_j\rangle$$

$$= \sum_j a_j\left(\hat{T}|e_j\rangle\right)$$

$$= \sum_j a_j \sum_i T_{ij}|e_i\rangle$$

$$= \sum_i \left[\sum_j T_{ij}a_j\right]|e_i\rangle$$

so these are the new components a_i of the vector $|\alpha\rangle$ in the transformed basis

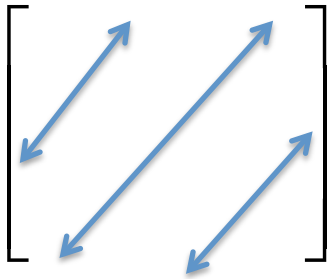
(8) Notice $\left\langle e_i \middle| \hat{T} \middle| e_j \right\rangle = \left\langle e_i \middle| \sum_{i=1}^{n} T_{ij} \middle| e_j \right\rangle = \left\langle e_i \middle| T_{1j} \middle| e_1 \right\rangle + \left\langle e_i \middle| T_{2j} \middle| e_2 \right\rangle + ... + \left\langle e_i \middle| T_{nj} \middle| e_n \right\rangle$

$= T_{1j} \underbrace{\left\langle e_i \middle| e_1 \right\rangle}_{\downarrow} + T_{2j} \left\langle e_i \middle| e_2 \right\rangle + ...$

So $T_{ij} = \left\langle e_i \middle| \hat{T} \middle| e_j \right\rangle$

(9) Consider the matrices

$$T = \begin{bmatrix} T_{11} & T_{12} & ... \\ T_{21} & ... & ... \\ ... & ... & ... \end{bmatrix}$$

transpose: $\tilde{T}=\begin{bmatrix} T_{11} & T_{21} & \cdots \\ T_{12} & \cdots & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix}$ that means: 

A symmetric matrix has $\tilde{T}=T$

A Hermitian matrix has $\tilde{T}^{*}=T$ and is denoted by T^{t}

Since $|\alpha\rangle$ is represented by a 1-column matrix of the coefficients a_{i1}, and $\langle\beta|$ is represented by a 1-column matrix of the coefficients b_{1j}, then

$\langle\alpha|\beta\rangle = a^{\dagger}b$

Inverse T^{-1} is defined such that $T^{-1}T \equiv 1$.

Note $T^{-1} \equiv \dfrac{1}{\det\ T}\tilde{C}$ so T^{-1} does not exist if $\det\ T=0$.

A matrix is called "unitary" if $T^{-1} = T^{\dagger}$

II. (10) Eigenvalue equations

Suppose we have a vector $|a\rangle$ and a transformation T.

If $|a\rangle$ is written in an arbitrary basis, then

$\hat{T}|a\rangle = ...(an\ arbitrary\ result)$

However suppose there is a special choice of basis such that

$\hat{T}|a\rangle_{special\ basis} = \lambda|a\rangle$

eigenvalue, just a number

It is interesting to find this special basis because it allows us to predict the following:

If $|a\rangle$ is a wavefunction (such as ψ) then $\hat{T}$ is an operator (that is, a measurement process, such as p_{op} or x_{op}) then λ is the result we would get by making the measurement.

How to find the special basis:

Given: we want $\hat{T}|a\rangle = \lambda|a\rangle$ (where λ is still unknown in magnitude but definitely just a number.)

Rewrite this as $(\hat{T}\text{-}\lambda\mathbf{1}|a\rangle = 0$

$\mathbf{1}$ is the unit matrix, $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Recall the definition of the inverse matrix,

$M^{-1}M = \mathbf{1}$

Suppose we were able to create $(\hat{T} - \lambda\mathbf{1})^{-1}$ and apply it to both sides of the equation:

$(\hat{T} - \lambda\mathbf{1})^{-1}(\hat{T} - \lambda\mathbf{1})|a\rangle = (\hat{T} - \lambda\mathbf{1})^{-1}0 = 0$

Since we know $T \neq 0$ and $\lambda \neq 0$, then the only way for this to be true would be if $|a\rangle = 0$.

Suppose we want to consider only cases where $|a\rangle \neq 0$.

Then it must be the case that $(\hat{T} - \lambda\mathbf{1})^{-1}$ does not exist.

Recall the definition: $(\hat{T} - \lambda\mathbf{1})^{-1} = \frac{1}{\det(\hat{T} - \lambda\mathbf{1})}\tilde{C}$.

So to find the special basis, we must have this det=0.

Write out $\det(\hat{T} - \lambda\mathbf{1}) = 0$, then solve for the λ's.

Plug the λ's back into $\hat{T}|a\rangle = \lambda|a\rangle$ to get the $|a\rangle$ for each λ.

Notice if we $\underbrace{\text{normalize these eigenvectors } |a\rangle}$ we can use them as a basis:

call them $|a_1\rangle ... |a_n\rangle$

$\hat{T}|a_1\rangle = \lambda_1|a_1\rangle$

...

$\hat{T}|a_n\rangle = \lambda_n|a_n\rangle$

They will look like:

$$|a_1\rangle = \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \end{pmatrix}, \quad |a_2\rangle = \begin{pmatrix} 0 \\ 1 \\ \dots \\ 0 \end{pmatrix}, \dots \quad |a_n\rangle = \begin{pmatrix} 0 \\ 0 \\ \dots \\ 1 \end{pmatrix}$$

Then we can write T in this basis:

$$T = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \dots & \dots \\ 0 & 0 & \dots & \lambda_n \end{bmatrix}$$

We say "T is diagonalized."

III. Hermitian operators

(1) Why do we care about them in physics?

(a) We can always exchange $\langle\alpha|T|\beta\rangle \leftrightarrow \langle T^t\alpha|\beta\rangle$.

(b) Their eigenvalues are real $\rightarrow$ They represent measureable quantities.

(c) Their eigenvalues are orthogonal and (in most cases) span the space in which the operator is defined - - - so we can use them as a new basis.

(d) Their matrices can always be diagonalized $\rightarrow$ we can always find their eigenvalues.

(2) How can we tell if a compound operator is Hermitian if its component operators are?

(For example: p_{op} is Hermitian. Is p_{op}^2 Hermitian?)

Consider $A = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}$ and $B = \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}$

First determine what matrix manipulations are allowed:

For any 2 operators (Hermitian or not), show that $(AB)^\dagger = B^\dagger A^\dagger$:

$$\text{Find } (AB)^\dagger = \left[\begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}\begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}\right]^{*t} = \begin{pmatrix} a_1^* b_1^* + a_2^* b_2^* & a_1^* b_2^* + a_2^* b_4^* \\ a_3^* b_1^* + a_4^* b_3^* & a_3^* b_2^* + a_4^* b_4^* \end{pmatrix}^t$$

$$= \begin{pmatrix} a_1^* b_1^* + a_2^* b_2^* & a_3^* b_1^* + a_4^* b_3^* \\ a_1^* b_2^* + a_2^* b_4^* & a_3^* b_2^* + a_4^* b_4^* \end{pmatrix}$$

$$\text{Now find } B^\dagger A^\dagger = \begin{pmatrix} b_1^* & b_3^* \\ b_2^* & b_4^* \end{pmatrix}\begin{pmatrix} a_1^* & a_3^* \\ a_2^* & a_4^* \end{pmatrix} = \begin{pmatrix} a_1^* b_1^* + a_2^* b_2^* & a_3^* b_1^* + a_4^* b_3^* \\ a_1^* b_2^* + a_2^* b_4^* & a_3^* b_2^* + a_4^* b_4^* \end{pmatrix}$$

SAME

Conclude:

Allowed operation #1: Whenever we have (a product of operators)†, we reverse their order and take "†" (transpose complex conjugate) of each one separately.

Allowed operation #2: $A + B = B + A$ (a usual commutation operation for matrices).

Allowed operation #3: $(A + B)^\dagger = A^\dagger + B^\dagger$

To determine if a compound operator is Hermitian, break it into a product or sum of individually Hermitian operators.

Example: Suppose $\left.\begin{aligned} A^\dagger = A \\ \text{and } B^\dagger = B \end{aligned}\right\}$ that is, "A and B are separately Hermitian."

Does $(AB + BA)^\dagger = (AB + BA)$?

To answer this, deconstruct it:

$(AB)^\dagger + (BA)^\dagger \rightarrow B^\dagger A^\dagger + A^\dagger B^\dagger \rightarrow BA + AB \rightarrow AB + BA.$

The answer is: yes.

III. The connection between ψ's and operators and vectors and transformations

physics math

Notice a formal similarity. Consider:

x, a continuous real variable that can take any one of an infinite number of values on the real axis.

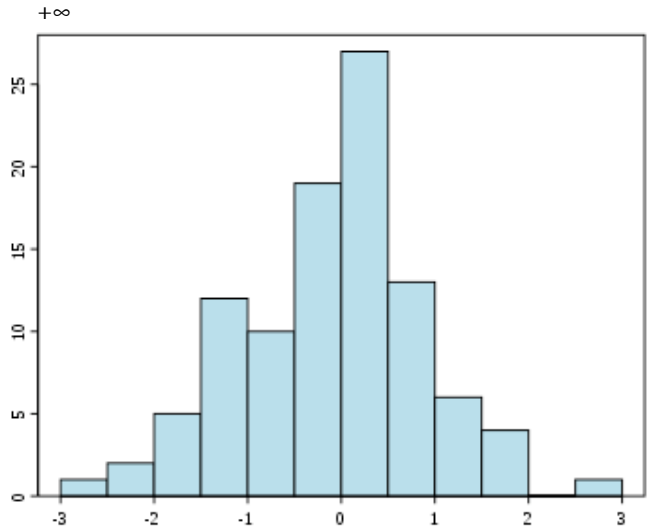
A finite set of basis vectors $|e_i\rangle$

$\psi(x)$, $\psi'(x)$, functions (quantum mechanical wavefunctions) that have value at each x.

Vectors $|\alpha\rangle$ and $|\beta\rangle$ which have "values" (that is, components) associated with each $|e_i\rangle$.

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + ... + a_n|e_n\rangle$$

$$|\beta\rangle = b_1|e_1\rangle + b_2|e_2\rangle + ... + b_n|e_n\rangle$$

Physics	**Math**
The integral	The inner product (dot product) of 2 vectors
	$\alpha^* \cdot \beta = \langle \alpha \mid \beta \rangle = a_1^* b_1 + a_2^* b_2 + ... + a_n^* b_n$
Take the product of the value of ψ and ψ' at each dx (weight by dx), and sum them.	Take the product of the value (component) of each vector for each basis vector, and sum them.

Conclude: The possible values of x .....are like.....basis vectors $\left| e_i \right\rangle$

except:

there is an infinite number of these.	There is (in this example) a finite number of these.

Physics		**Math**
ψ	.....is like.....	$\lvert\alpha\rangle$
$\int \psi(x)\psi(x)dx$	.....is like.....	$\langle\alpha\lvert\beta\rangle$

except:

Here we weight by dx.

Here we cannot "weight" by $\lvert e_i\rangle$.

To make the correspondence more similar, consider vectors $\lvert\alpha\rangle$ that are infinite dimensional.

Notice: all of linear algebra concerns only vectors like $\lvert\alpha\rangle$. We are only allowed to use it for ψ's (that is, for quantum mechanics) because of this formal similarity between $\int \psi(x)\psi(x)dx$ and $\langle\alpha\lvert\beta\rangle$ (when $\lvert\alpha\rangle$, $\lvert\beta\rangle$ are infinite-dimensional).

Outline

I. Hilbert space
II. The linear algebra – Quantum Mechanics connection, continued
III. Dirac Notation

I. Hilbert space

Vocabulary: A Hilbert space is one that

(1) has an inner product $\langle \psi | \psi' \rangle = \int_{-\infty}^{+\infty} \psi \psi' dx$ defined for any pair of its elements.

(2) has a norm defined by $|\psi| = \sqrt{\langle \psi | \psi \rangle}$.

(3) is linear, so that if "a" is a constant and ψ and ψ' are elements in the space, then so are $a\psi$ and $\psi + \psi'$.

(4) is infinite-dimensional (or "complete"); contains all functions that satisfy (1)-(3) for the interval from -∞ to +∞.

The reason why we talk about Hilbert space in quantum mechanics is that the kinds of functions that are defined for it are ones that can represent physical properties of objects (for example length (norm) or superposition $\langle \psi | \psi' \rangle$) which quantum mechanics describes. We were making a table of similarities between ψ's and vectors $|\alpha\rangle$. We continue this now:

Wavefunctions ψ that we use in Quantum Mechanics	Vectors $\lvert\alpha\rangle$ which are the subject of linear algebra
By analogy they are called "orthogonal in Hilbert space" if $\int_{-\infty}^{+\infty} \psi\psi' \, dx = 0.$	Are called orthogonal in 3-dimensional vector space if $\langle\alpha\lvert\beta\rangle = 0.$
By analogy, the eigenfunctions of certain Hamiltonians form a basis that spans Hilbert space. Which eigenfunctions can do this? Ones that are members of an infinite set, for example the eigen-functions of an infinitely high square well. (We call call them the φ_i in analogy to the $\lvert e_i\rangle$.) Notation: because we are treating the eigenfunctions ψ_i like basis vectors, let us extend the analogy and make them unit vectors (that is, norm $\lvert\varphi_i\rvert = \sqrt{\langle\varphi_i\lvert\varphi_i\rangle} = 1$).	The $\lvert e_i\rangle$ span the vector space (for example, these are $\hat{x}$, $\hat{y}$, and $\hat{z}$ in 3-D space.

To represent the fact that different ψ_i are $\left\{\begin{matrix}\text{unit vectors} \\ \\ \text{and orthogonal}\end{matrix}\right\}$:"orthonormal",

we use the symbol δ_{ij} : the Kronecker delta.

$$\langle \varphi_i | \varphi_j \rangle = \delta_{ij} = \left\{\begin{matrix}0 & \text{if } i \neq j \\ \\ 1 & \text{if } i = j\end{matrix}\right\}.$$

Use the Kronecker delta to describe discrete variables (for example i = 1, 2, 3....)

Use the Dirac delta function to describe continuous variables (for example,

k = any real number.)

III. Dirac notation

We will indicate the principal parts of the definition of Dirac notation by *'s.

We have shown that wavefunctions ψ can be described by linear algebra, which is the mathematics of vectors $|\alpha\rangle$.

* To emphasize this, rename ψ as $|\psi\rangle$.

To emphasize the similarity between an infinite set of eigenfunctions φ_i and the basis vectors $|e_i\rangle$,

* Rename φ_i as $|\varphi_i\rangle$.

Since $\int \varphi_i^*(x)\psi(x)dx$ is similar to $\langle\alpha|\beta\rangle$,

* Rename $\int \varphi_i^*(x)\psi(x)dx$ as $\langle\varphi_i|\psi\rangle = c_i$, a scalar constant.

Facts about this inner product $\langle \varphi_i | \psi \rangle$:

(i) The whole item is called a "bracket."

(ii) Its parts are called a "bra" $\langle \varphi_i |$ and a "ket" $| \psi \rangle$. The bra is not exactly a vector. It is a function which, when combined with a vector, produces a scalar.

(iii) Note: this is quantum mechanics terminology, not linear algebra.

(iv) Note $\underbrace{\langle \varphi_i | \psi \rangle}_{\downarrow} \neq \underbrace{\langle \psi | \varphi_i \rangle}_{\downarrow}$: the order in which they appear shows which one is complex-conjugated.

$$\int dx \varphi^* \psi \quad \int dx \psi^* \varphi$$

(v) So $\langle \varphi_i | \psi \rangle = \langle \psi_i | \varphi \rangle^*$.

Facts about bras:

(i) Notice that if $|\psi\rangle$ is a column vector, then $\langle\psi|$ must be a row vector in order for their inner product to be a scalar (c_i):

$$\langle\varphi_i|\psi\rangle = \begin{pmatrix} \varphi_1 & \varphi_2 & \dots \end{pmatrix}^* \begin{pmatrix} \psi_1 \\ \psi_2 \\ \dots \end{pmatrix} = \varphi_{i1}^*\psi_1 + \varphi_{i2}^*\psi_2 + \dots. \qquad \text{(a scalar)}$$

So the bra is the transpose (column → row) and complex conjugate:

the Hermitian conjugate (symbol: †) of the corresponding ket.

(ii) If some operator Q acts on $|\varphi_i\rangle$, then the equivalent operation for $\langle\varphi_i|$ is

$$\langle\varphi_i|Q^t$$

What this means:

if λ is an eigenvalue such that $Q|\varphi_i\rangle = \lambda|\varphi_i\rangle$, then

$$\langle\varphi_i|Q^t = \lambda\ \langle\varphi_i|.$$

Same λ!

*Do not write "Q $\langle\varphi_i|$" or "Q^t $\langle\varphi_i|$": Order is important.

Facts about expectation values in Dirac notation:

For normalized ψ, the expectation value of operator Q is

$$\bar{Q} = \int \psi^* \mathrm{Q} \psi \, \mathrm{dx} \Rightarrow \langle \psi | Q | \psi \rangle .$$

Recall Hermitian operators are defined by $Q^\dagger = Q$.

So in their case $\langle \psi | Q | \psi \rangle = \langle \psi | \lambda | \psi \rangle = \lambda \underbrace{\langle \psi | \psi \rangle}_{\downarrow} = \lambda$

Q acting to the right 1, normalized

and $\langle \psi | Q^\dagger | \psi \rangle = \langle \psi | \lambda | \psi \rangle = \lambda \langle \psi | \psi \rangle = \lambda$

Q acting to the left

Same result λ, so conclude:

If the operator is known to be Hermitian, we can

(1) ignore which direction it operates (that is, on the bra or on the ket)

(2) leave off its "†".

Outline

I. The Projection Operator
II. Position and momentum representations
III. Ways to understand the symbol $\langle\Phi|\psi\rangle$
IV. Commutators and simultaneous measurements

Please read Goswami Chapter 7.

I. The Projection Operator

Facts about expanding ψ in terms of a basis:

Recall we can expand ψ in a basis, which here is any complete set of eigenfunctions.

$\psi(\mathrm{x}) = \mathrm{c}_1\varphi_1(x) + c_2\varphi_2(x) + \ldots$

$\psi(x) = \sum_i c_i\varphi_i(x)$ Convert this to Dirac notation:

$|\psi\rangle = \sum_i \langle\varphi_i|\psi\rangle|\varphi_i\rangle$

This is a vector.
This is a scalar.
So they can appear in any order.
Now reorder them:

$|\psi\rangle = \sum_i |\varphi_i\rangle\langle\varphi_i|\psi\rangle$

Notice that this can be true only if this part = 1.

Conclude: $\sum_i |\varphi_i\rangle\langle\varphi_i| = 1$. Very important! We will use this a lot.

Consider $|\varphi_i\rangle\langle\varphi_i|$ $\left(\text{without the } \sum\right)$. It is called the Projection Operator.

Facts about the Projection Operator :

(i) Because of its structure, it can operate on kets or bras.

Example : apply it to $\langle\beta|$.

We get $\underbrace{\langle\beta|\varphi_i\rangle}\langle\varphi_i| = c_{\beta,\varphi_i}\langle\varphi_i|$

a constant

Apply it to $|\alpha\rangle$.

We get $|\varphi_i\rangle\underbrace{\langle\varphi_i|\alpha\rangle} = c_{\alpha,\varphi_i}|\varphi_i\rangle$

a different constant

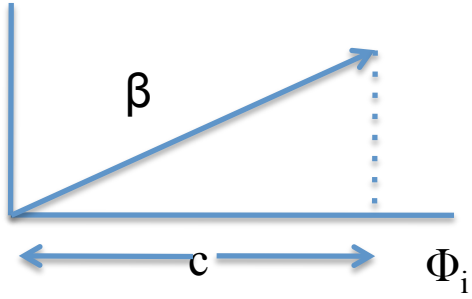
(ii) Notice what the c's are.

Example $c = \langle\beta|\varphi_i\rangle = \int_{-\infty}^{+\infty}\beta(x)\varphi_i(x)dx \Rightarrow$ the amount of overlap between wavefunctions β and φ_i.

–OR –

(If we pretend the β and φ are really vectors)

c is the component of β in the direction of φ_i.



(iii) So applying (for example) $|\varphi_i\rangle\langle\varphi_i|$ to $\langle\beta|$:

$$\langle\beta|\varphi_i\rangle\langle\varphi_i| \rightarrow c_{\beta,\varphi_i}\langle\varphi_i|$$

This transforms the vector $\langle\beta|$ into the direction $\langle\varphi_i|$

and multiplies it by the projection (component) of $\langle\beta|$ along $\langle\varphi_i|$.

Similarly applying $|\varphi_i\rangle\langle\varphi_i|$ to $|\alpha\rangle$:

$$|\varphi_i\rangle\langle\varphi_i|\alpha\rangle \rightarrow c_{\alpha,\varphi_i}|\varphi_i\rangle$$

transforms the vector $|\alpha\rangle$ into the direction $|\varphi_i\rangle$ and multiplies it by the projection of $|\alpha\rangle$ along $|\varphi_i\rangle$.

This is why it is called the Projection Operator.

(iv) Notice that after we project once in a direction, subsequent projections in the same direction have no additional effect:

Example: Begin with $|\varphi_i\rangle\langle\varphi_i|\beta\rangle \rightarrow c_{\beta,\varphi_i}|\varphi_i\rangle$

Subsequent $|\varphi_i\rangle\langle\varphi_i|c_{\beta,\varphi_i}|\varphi_i\rangle = c_{\beta,\varphi_i}|\varphi_i\rangle\underbrace{\langle\varphi_i|\varphi_i\rangle}_{\downarrow} = c_{\beta,\varphi_i}|\varphi_i\rangle$

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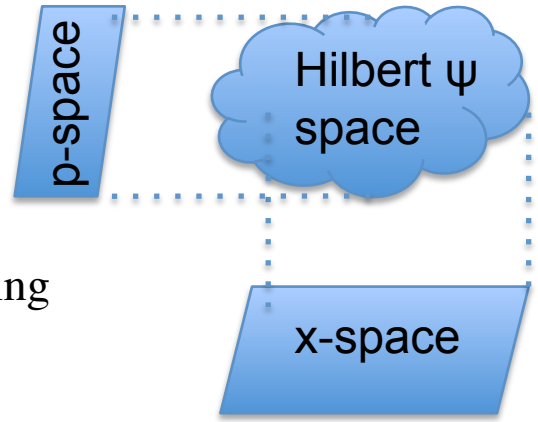
II. Position representation and momentum representation

Recall that the wavefunctions exist in abstract Hilbert space. To calculate with them, we must represent them in coordinate space or momentum space.

The goal of this section: to show that "representing ψ in a space" (for example, position space) means projecting it onto each of the basis vectors of that space.

To do this we will need 2 things:



(1) the eigenfunctions ("eigenkets") of the

position operator. Call them $|x\rangle$. We get these by solving

$$\hat{x}|x\rangle = \lambda_i |x\rangle$$

$|x\rangle$: eigenfunction (not yet determined)

λ_i: eigenvalue (not yet determined)

$\hat{x}$: position operator

It turns out that there are an infinite number of $|x_i\rangle$, so they can serve as a basis for ψ.

(2) The eigenfunctions of the momentum operator. Call them $|p_i\rangle$.

We get them by solving $p|p_i\rangle = \lambda_i |p_i\rangle$. Let's represent them in x-space:

$$-i\hbar \frac{\partial}{\partial x} p_i(x) = \lambda_i p_i(x).$$

This differential equation is solved by

$$p_i(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ikx} \qquad \text{and} \qquad \lambda_i = \hbar k = p$$

(Note these are not the $|p_i\rangle$ that are in Hilbert space- they are the $|p_i\rangle$ after they have been represented in *x*-space.) Notice also that there is an infinite number of them- one for every value that k can take in e^{ikx} ($-\infty < k < +\infty$). So they can act as a basis for ψ.

Now show that ψ(x) is the same as "ψ projected onto the $|x_i\rangle$ basis. To do this, notice there are 2 ways to write $\langle\psi|\psi\rangle$:

Way #1

By definition of the inner product,

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

Way #2

By using the fact that $\sum|\mathrm{x}\rangle\langle x| = 1$ for any basis set (earlier we used the $|\varphi_\mathrm{i}\rangle$ basis):

$$\langle\psi|\psi\rangle = \langle\psi|1|\psi\rangle = \langle\psi|\sum|\mathrm{x}\rangle\langle x||\psi\rangle$$

Because x is a continuous variable, it is reasonable to replace $\sum$ with $\int \mathrm{dx}$.

$\langle\psi|\psi\rangle = \int \mathrm{dx}\langle\psi|\mathrm{x}\rangle\langle x|\psi\rangle$. Now recall $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$:

$$= \int \mathrm{dx}\langle x|\psi\rangle^*\langle x|\psi\rangle$$

----Compare the form of the righthand sides of both equations and conclude:----

$$\psi(\mathrm{x}) = \langle\mathrm{x}|\psi\rangle$$

We saw from the meaning of linear algebra inner products that $\langle\mathrm{x}|\psi\rangle$ is a projection.

So we conclude that $\psi(\mathrm{x})$ must be a projection too. This is "ψ projected into the value x, or basis vector x." Or: "$\psi(\mathrm{x})$ is the position representation of $|\psi\rangle$ at location x."

Now insert into $|\psi\rangle$ the $\sum |p\rangle\langle p| = 1$ instead of the $\sum |x\rangle\langle x| = 1$:

$$|\psi\rangle = \sum |p\rangle\langle p|\psi\rangle.$$

Again because p is continuous we convert $\sum$ to $\int$dp.

$$|\psi\rangle = \int dp\,|p\rangle\langle p|\psi\rangle$$

Now take the inner product of both sides with $\langle x|$:

$$\langle x|\psi\rangle = \int dp\,\langle x|p\rangle\langle p|\psi\rangle$$

This is ψ(x).

This is ψ represented in p-space as "$A(p)$".

These are the set of transformation coefficients from the $|p\rangle$ basis to the $|x\rangle$ basis.

Since they are integrated over dp, we see that there is one for every member of the infinite set of $|p\rangle$'s.

They are the "translation dictionary" between the bases.

Any particular one is the p-space eigenvector, represented in (projected onto) x-space.

We just found out what those are: $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ikx} = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

Plug in everything to see what it looks like in a space (coordinate space) that we are used to:

$$\langle x|p\rangle = \int dp \langle x|p\rangle\langle p|\psi\rangle$$

$$\psi(x) = \int dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} A(p)$$

This is the Fourier transform equation, which we already knew as a translation between bases. We see that the bra-ket notation just expresses it more compactly.

III. Ways to understand the symbol $\langle\varphi|\psi\rangle$

3 equivalent ways:

(1) If $|\varphi\rangle$ is a member of a basis set, then $\langle\varphi|\psi\rangle$ is the representation of the Hilbert space object $|\psi\rangle$ in the basis $|\varphi\rangle$.

(2) If $|\psi\rangle$ and $|\varphi\rangle$ are members of 2 different bases, then $\langle\varphi|\psi\rangle$ is the coefficient of translation between the bases.

What this means physically:

(3) If a system begins in state $|\psi\rangle$, then undergoes a change and ends in state $|\varphi\rangle$, the amplitude for that change to occur is $c_{\varphi\psi} = \langle\varphi|\psi\rangle$, and the probability for it to happen is $|\text{amplitude}|^2 = |\langle\varphi|\psi\rangle|^2$.

IV. More tricks with Dirac notation

(1) Consider $\int dp \langle x|p\rangle\langle p|x'\rangle$. How can we interpret this?

Way #1: We showed earlier that

$$\langle x|p\rangle = p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

Also $\langle p|x'\rangle = \langle x'|p\rangle^* = \left[\frac{1}{\sqrt{2\pi\hbar}} e^{ipx'/\hbar}\right]^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx'/\hbar}$

So $\int dp \langle x|p\rangle\langle p|x'\rangle = \int dp \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx'/\hbar} = \underbrace{\frac{1}{2\pi\hbar} \int dp e^{ip(x-x')/\hbar}}$

We recognize this as δ(x-x')

Way #2:

Rewrite $\int dp \langle x|p\rangle\langle p|x'\rangle = \langle x| \underbrace{\int dp |p\rangle\langle p|}_{=1} |x'\rangle = \langle x|x'\rangle$

But the vector $|x'\rangle$, projected into the $|x\rangle$ basis, has overlap 1 when $|x\rangle$ is the same as $|x'\rangle$, otherwise 0.

So $\langle x|x'\rangle = \delta$(x-x')

(2) How to translate $\langle\psi|$ from Dirac notation to calculus notation:

Since $\langle\psi_1|\psi_2\rangle = \int dx \psi_1^*(x)\psi_2(x)$,

$\langle\psi_1| = \int dx \psi_1^*(x)$

But since x is being integrated over, it could be named anything, so

$\langle\psi_1|$ is also $\int dp \psi^*(p)$ and so forth.

We can write the function ψ in any representation, but we integrate over the full basis for that representation.

(3) Can we similarly rewrite $|\psi\rangle$? No.

$|\psi\rangle \neq \psi(x)$ because $\psi(x) = \langle x|\psi\rangle$.

$|\psi\rangle$ by itself is the Hilbert-space object. We have no other symbol for it.

IV. Commutators and simultaneous measurements

Suppose 2 operators A and B have the same eigenstates but possibly different eigenvalues.

"simultaneous eigenstates"

We can express this as:

$A|\psi\rangle = a|\psi\rangle$

-and-

$B|\psi\rangle = b|\psi\rangle$

Same $|\psi\rangle$

We will see that then $[A,B] = 0$. Show this:

$[A,B] = AB|\psi\rangle - BA|\psi\rangle$

This means measure B first, then measure A second.

This means measure A first, then measure B second.

$= Ab|\psi\rangle - Ba|\psi\rangle$

$= bA|\psi\rangle - aB|\psi\rangle$ Scalars commute.

$= ba|\psi\rangle - ab|\psi\rangle$

$= (ba\text{-}ab)|\psi\rangle = 0$, because these are just numbers.

Conclusion: if we find that 2 operators have the same eigenstates, then the order of these operators' measurements does not matter: one measurement does not disturb the system for the other. Both pieces of information can be known simultaneously.

Example of operators with simultaneous eigenstates: p and $H = p^2/2m + V$.

We can use this information to label a state.

To uniquely label a state, list the eigenvalues of all the operators that have it as their simultaneous eigenstate.

Outline

I. The General Uncertainty Principle
II. The Energy-time Uncertainty Principle
III. The time evolution of a quantum mechanical system

I. The General Uncertainty Principle

We must first prove the Schwarz Inequality from linear algebra:

For 2 vectors ψ_a and ψ_b,

$$\langle \psi_a | \psi_a \rangle \cdot \langle \psi_b | \psi_b \rangle \geq \left| \langle \psi_b | \psi_a \rangle \right|^2$$

Proof:

Construct the linear combination $\psi \equiv \psi_a + c\psi_b$. c is some constant.

Because $\langle \psi | \psi \rangle = |\psi|^2$ (definition of the norm)

$\langle \psi | \psi \rangle \geq 0$ Expand this:

$\langle \psi_a + c\psi_b | \psi_a + c\psi_b \rangle \geq 0$ The elements of the bra are understood to be complex-conjugated:

$$\langle \psi_a | \psi_a \rangle + c^* \langle \psi_b | \psi_a \rangle + c \langle \psi_a | \psi_b \rangle + |c|^2 \langle \psi_b | \psi_b \rangle \geq 0$$

Now find the value of c for which the lefthand side is a minimum.

$$\frac{\partial}{\partial c}\left[\underbrace{\langle \psi_a | \psi_a \rangle}_{\downarrow} + \underbrace{c^* \langle \psi_b | \psi_a \rangle}_{\downarrow} + \underbrace{c \langle \psi_a | \psi_b \rangle}_{\downarrow} + \underbrace{cc^* \langle \psi_b | \psi_b \rangle}_{\downarrow} \right] = 0$$

$$0 \quad + \quad 0 \quad + \langle \psi_a | \psi_b \rangle \; + c^* \langle \psi_b | \psi_b \rangle = 0$$

$$c^* = \frac{-\langle \psi_a | \psi_b \rangle}{\langle \psi_b | \psi_b \rangle}, \qquad \text{so } c = \frac{-\langle \psi_b | \psi_a \rangle}{\langle \psi_b | \psi_b \rangle}$$

Substitute this c, c^* into the original inequality:

$$\langle\psi_a|\psi_a\rangle - \frac{\langle\psi_a|\psi_b\rangle}{\langle\psi_b|\psi_b\rangle}\langle\psi_b|\psi_a\rangle - \frac{\langle\psi_b|\psi_a\rangle}{\langle\psi_b|\psi_b\rangle}\langle\psi_a|\psi_b\rangle + \left|\frac{\langle\psi_b|\psi_a\rangle}{\langle\psi_b|\psi_b\rangle}\right|^2 \langle\psi_b|\psi_b\rangle \geq 0.$$

Multiply both sides by $\langle\psi_b|\psi_b\rangle$:

$$\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle \underbrace{-2\langle\psi_a|\psi_b\rangle\langle\psi_b|\psi_a\rangle}_{\downarrow} + \left|\langle\psi_b|\psi_a\rangle\right|^2 \geq 0.$$

$$\underbrace{-2\langle\psi_b|\psi_a\rangle^*\langle\psi_b|\psi_a\rangle}_{\downarrow}$$

$$-2\left|\langle\psi_b|\psi_a\rangle\right|^2$$

$$\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle - \left|\langle\psi_b|\psi_a\rangle\right|^2 \geq 0$$

$$\langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle \geq \left|\langle\psi_b|\psi_a\rangle\right|^2$$

Now we will use this to derive the Uncertainty Principle:

Consider 2 operators A and B.

Recall that their uncertainties are defined by

$\Delta A \equiv \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$ These are expectation values.

So $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$ and $(\Delta B)^2 = \underbrace{\langle B^2 \rangle - \langle B \rangle^2}$

$$\langle \psi | \mathrm{B}^2 | \psi \rangle - \langle \psi | \mathrm{B} | \psi \rangle^2 .$$

Notice that this can be written as: $\langle \psi | \{ \mathrm{B} - \langle \psi | \mathrm{B} | \psi \rangle \}^2 | \psi \rangle$

(To see this, note $\langle \psi | \{ \mathrm{B} - \langle \psi | \mathrm{B} | \psi \rangle \}^2 | \psi \rangle = \langle \psi | \{ B^2 - 2B \langle \psi | \mathrm{B} | \psi \rangle + \langle \psi | \mathrm{B} | \psi \rangle^2 \} | \psi \rangle$

these are just numbers so they can come out of the inner product.

$$\rightarrow \langle \psi | \mathrm{B}^2 | \psi \rangle - 2 \langle \psi | \mathrm{B} | \psi \rangle \langle \psi | \mathrm{B} | \psi \rangle + \langle \psi | \mathrm{B} | \psi \rangle^2 \underbrace{\langle \psi | \psi \rangle}$$

1

$$\rightarrow \langle \psi | \mathrm{B}^2 | \psi \rangle - \langle \psi | \mathrm{B} | \psi \rangle^2)$$

So $(\Delta B)^2 = \langle\psi|\{B-\langle\psi|B|\psi\rangle\}^2|\psi\rangle$.

Rename: $B-\langle\psi|B|\psi\rangle \Rightarrow B'$

$A-\langle\psi|A|\psi\rangle \Rightarrow A'$

Then $(\Delta A)^2(\Delta B)^2 = \langle\psi|A'^2|\psi\rangle\langle\psi|B'^2|\psi\rangle$

$= \langle\psi|A'\cdot A'|\psi\rangle\langle\psi|B'\cdot B'|\psi\rangle$

directions of operation

Let the operators be Hermitian (that is, representing physically measureable quantities. Recall that means $A'^{\dagger} = A$, $B'^{\dagger} = B$. so the one of the left can operate leftward.

$= \langle A'\psi|A'\psi\rangle\langle B'\psi|B'\psi\rangle$

Now use the Schwarz Inequality: $\langle\psi_a|\psi_a\rangle\cdot\langle\psi_b|\psi_b\rangle \geq |\langle\psi_b|\psi_a\rangle|^2$. Define $A'\psi \equiv \psi_a$ and $B'\psi \equiv \psi_b$.

Then $(\Delta A)^2(\Delta B)^2 = \langle A'\psi|A'\psi\rangle\langle B'\psi|B'\psi\rangle \geq |\langle A'\psi|B'\psi\rangle|^2$

Now use the property of complex numbers that, if Z is complex,

$$|Z|^2 = (\mathrm{Re}\,Z + i\,\mathrm{Im}\,Z)(\mathrm{Re}\,Z - i\,\mathrm{Im}\,Z)$$

$$= (\mathrm{Re}\,Z)^2 + (\mathrm{Im}\,Z)^2$$

$$\geq (\mathrm{Im}\,Z)^2 = \left(\frac{Z - Z^*}{2i}\right)^2 .$$

Replace $Z \to \langle A'\psi | B'\psi \rangle$ and $Z^* \to \langle B'\psi | A'\psi \rangle$. Then we have

$$(\Delta A)^2 (\Delta B)^2 \geq \left|\langle A'\psi | B'\psi \rangle\right|^2 \geq \left(\frac{\langle A'\psi | B'\psi \rangle - \langle B'\psi | A'\psi \rangle}{2i}\right)^2 = \left(\frac{\langle [A', B'] \rangle}{2i}\right)^2$$

Substitute A'=A-$\langle \psi | A | \psi \rangle$ etc.

These cancel in the commutator.

$$= \left(\frac{\langle [A, B] \rangle}{2i}\right)^2$$

So $(\Delta A)^2 (\Delta B)^2 \geq \left(\frac{\langle [A, B] \rangle}{2i}\right)^2$: The generalized uncertainty relation for any 2 operators A and B.

To show an example, suppose $A = x$ and $B = p$.

We can work out that $[A,B] = [x,p] = i\hbar$.

So the generalized Uncertainty Relation becomes

$$(\Delta x)^2 (\Delta p)^2 \geq \left(\frac{i\hbar}{2i} \right)$$

$$So\ \Delta x \Delta p \geq \frac{\hbar}{2}$$

II. The Energy-Time Uncertainty Principle

The goal of this section:

Derive $\Delta E \Delta t \geq \frac{\hbar}{2}$ (ΔE is the uncertainty in the energy of a system)

AND explain what "Δt" means.

Note that a system does not "have a time t".

(In this non-relativistic treatment) so Δt is NOT the "uncertainty in time.")

Consider some observable whose measured value is associated with the operator Q.

We could find the expectation value of Q :

$\langle Q \rangle = \langle \psi | Q\psi \rangle$

It is possible for $\langle Q \rangle$ to be time-dependent, because ψ and Q could be.

Find $\frac{d\langle Q \rangle}{dt} = \left\langle \frac{\partial \psi}{\partial t} \middle| Q\psi \right\rangle + \left\langle \psi \middle| \frac{\partial Q}{\partial t} \psi \right\rangle + \left\langle \psi \middle| Q \frac{\partial \psi}{\partial t} \right\rangle$

Recall the time - dependent Schroedinger Equation :

$$\underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi}=i\hbar\frac{\partial\psi}{\partial t}$$

$$H\psi$$

So we can replace $\left|\frac{\partial\psi}{\partial t}\right\rangle \rightarrow \left|\frac{1}{i\hbar}H\psi.\right\rangle$

We can also use its complex conjugate $\frac{\partial\psi^*}{\partial t}$: $\left\langle\frac{\partial\psi}{\partial t}\right| \rightarrow \frac{-1}{i\hbar}\langle H\psi|$

So $\frac{d\langle Q\rangle}{dt}=\frac{-1}{i\hbar}\langle H\psi|Q\psi\rangle+\underbrace{\left\langle\psi\left|\frac{\partial Q}{\partial t}\psi\right.\right\rangle}+\frac{1}{i\hbar}\langle\psi|QH\psi\rangle$

call this $\left\langle\frac{\partial Q}{\partial t}\right\rangle$

Recall H is Hermitian, so $H^\dagger = H$.

Then for any wavefunction "φ",

$$\langle \mathrm{H}\varphi | \varphi \rangle = \langle \varphi | H\varphi \rangle$$

H has no $\dagger$ because it is in the ket.

H is implicitly $H^\dagger$ because it is in the bra.

In this case "φ" $= Q\psi$.

Rewrite, replacing $\frac{1}{i} \to -i$.

$$\frac{d\langle Q \rangle}{dt} = \frac{i}{\hbar}\langle H\psi | Q\psi \rangle + \left\langle \frac{\partial Q}{\partial t} \right\rangle - \frac{i}{\hbar}\langle \psi | QH\psi \rangle$$

$$= \frac{i}{\hbar}\langle \psi | HQ\psi \rangle - \frac{i}{\hbar}\langle \psi | QH\psi \rangle + \left\langle \frac{\partial Q}{\partial t} \right\rangle$$

$$= \frac{i}{\hbar}\langle \psi [H,Q] \psi \rangle + \left\langle \frac{\partial Q}{\partial t} \right\rangle$$

Message from this: When $Q \neq Q(t)$, so $\frac{\partial Q}{\partial t} = 0$, then $\left\langle \frac{\partial Q}{\partial t} \right\rangle = 0$. This leaves

$\frac{d\langle Q \rangle}{dt} \propto \langle \psi | [H, Q] \psi \rangle$. Thus if Q commutes with H, Q is conserved.

Note we can pick $Q = H$, not a function of time. Then we get

$$\underbrace{\frac{d\langle H \rangle}{dt}} = \frac{i}{\hbar} \langle \psi | \underbrace{[H, H]} \psi \rangle$$

$$\frac{dE}{dt} = 0.$$

*Energy conservation is embedded in quantum mechanics.

Now derive the Energy-Time Uncertainty Principle.

Begin by recalling the generalized Uncertainty Principle:

$$(\Delta A)^2 (\Delta B)^2 \geq \left(\frac{\langle \psi [A,B] \psi \rangle}{2i} \right)^2$$

Let $A = H$ and $B = Q$.

Since $H\psi = E\psi$, $\Delta H = \Delta E$.

$$(\Delta E)^2 (\Delta Q)^2 \geq \left(\frac{\langle \psi [H,Q] \psi \rangle}{2i} \right)^2$$

Suppose $Q \neq Q(t)$, so $\frac{\partial Q}{\partial t} = 0$.

This means we can replace $\frac{i}{\hbar} \langle \psi | [H,Q] \psi \rangle \rightarrow \frac{d\langle Q \rangle}{dt}$.

$$(\Delta E)^2(\Delta Q)^2 \geq \left(\frac{1}{2i}\frac{\hbar}{i}\frac{d\langle Q\rangle}{dt}\right)^2$$

$$(\Delta E)(\Delta Q) \geq \frac{\hbar}{2}\left|\frac{d\langle Q\rangle}{dt}\right|$$

Define $\Delta t \equiv \dfrac{\Delta Q}{\left|\dfrac{d\langle Q\rangle}{dt}\right|}$. Then we get $\Delta E \Delta t \geq \dfrac{\hbar}{2}$

What this means:

We can rewrite it as $\Delta Q = \left|\dfrac{d\langle Q\rangle}{dt}\right| \cdot \Delta t$

This is the usual uncertainty in Q, σ_Q. Conclude that Δt is the amount of time it takes for the expectation value of Q ($\langle Q\rangle$), to change by 1 standard deviation, σ_Q.

III. The time evolution of a quantum mechanical system

Issues: Suppose we know $|\psi(\text{t=0})\rangle$.

$t = 0$ is the "time of the measurement"

How does $|\psi\rangle$ evolve during the time that passes until the next measurement?

The answer:

$|\psi(t)\rangle = \exp\left(\frac{-itH}{\hbar}\right)|\psi(t=0)\rangle$ where this is the specific Hamiltonian (including potential V) that the $|\psi\rangle$ is responding to.

Show this:

Start with the time-dependent Schroedinger Equation:

$$\underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi}_{} = i\hbar\frac{\partial\psi}{\partial t}$$

$$\mathrm{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

So $\frac{\partial\psi}{\partial t} + \frac{i}{\hbar}H\psi = 0.$ We can see that the time development of ψ is controlled by H.

The reason why we cannot simply integrate this to get the exponential function is that H is an operator, not just a number. So we proceed in the formally correct way:

We want to find an operator $U(t,\ t_0)$ that transforms $\psi(t_0)$ into $\psi(t)$, so $\psi(t) = U(t,\ t_0)\psi(t_0)$.
Properties we expect U to have:

(i) $U = U(t)$ U is not a constant: otherwise it could not accommodate different times.

(ii) $U(t_0, t_0) = 1$ That is, no time evolution implies no effect by U.

(iii) $U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$ describes the evolution of ψ during 2 intervals: $t_0 \rightarrow t_1 \rightarrow t_2$

(*iv*) Whatever U is, it must produce results that are consistent with the Schroedinger Equation.

Method: Propose $U = \exp\left[\frac{-i\left(t - t_0\right)H}{\hbar}\right]$, then show that it works. Let $t_0 = 0$ for simplicity.

To show this, consider the operator inverse of U, which is

$$U^{-1} = \exp\left(+\frac{itH}{\hbar}\right)$$

Operate with U^{-1} from left on all terms in the Schroedinger Equation:

$$U^{-1}\left[\frac{\partial\psi}{\partial t} + \frac{i}{\hbar}H\psi\right] = U^{-1}0 = 0$$

$$\exp\left(\frac{itH}{\hbar}\right)\frac{\partial\psi}{\partial t}+\frac{i}{\hbar}\exp\left(\frac{itH}{\hbar}\right)H\psi=0$$

$$\frac{\partial}{\partial t}\left[\exp\left(\frac{itH}{\hbar}\right)\psi\right]=0$$ Integrate over $\int_{t'=0}^{t'=t}$

$$\exp\left(\frac{itH}{\hbar}\right)\psi(t)-\underbrace{\exp\left(\frac{i0H}{\hbar}\right)}_{\downarrow\ 1}\psi(0)=0$$

$$\exp\left(\frac{itH}{\hbar}\right)\psi(t)-\psi(0)=0$$ Multiply on the left with $\exp\left(\frac{-itH}{\hbar}\right)$

$$\underbrace{\exp\left(\frac{-itH}{\hbar}\right)\exp\left(\frac{itH}{\hbar}\right)}_{\downarrow\ 1}\psi(t)-\exp\left(\frac{-itH}{\hbar}\right)\psi(0)=0$$

$$\psi(t)=\exp\left(\frac{-itH}{\hbar}\right)\psi(0)=0$$

Facts about this result:

1. The Hamiltonian causes the system to develop in time.

2. We can expand the exponent to see that this U satisfies the requirements (i)-(iv):

$$\exp\left(\frac{-itH}{\hbar}\right) = 1 - \frac{itH}{\hbar} + \frac{1}{2!}\left(\frac{itH}{\hbar}\right)^2 - \ldots.$$

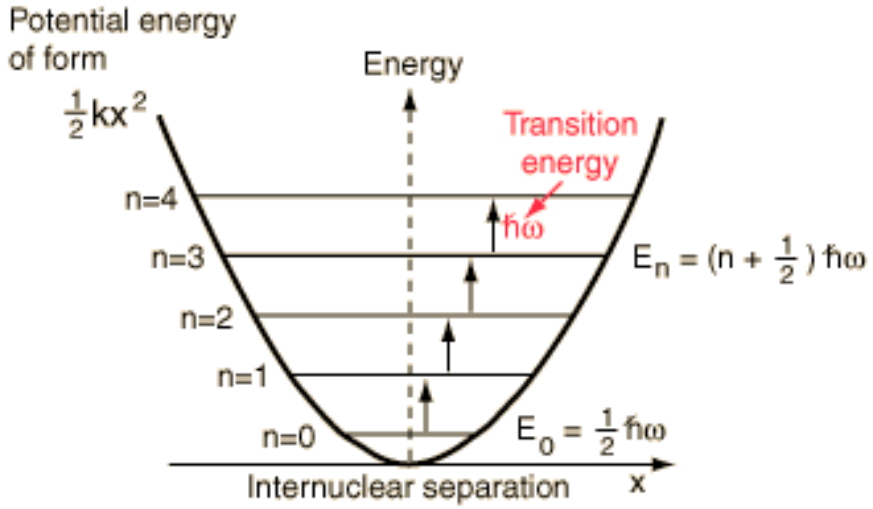
To actually calculate a $\psi(t)$, we have to make this expansion.

Outline

I. The one-dimensional harmonic oscillator
II. Solving the simple harmonic oscillator using power series

I. The one-dimensional harmonic oscillator

Consider a potential of the form $V = kx^2/2$.



Why we care about it:

(1) it describes several real physical systems including excited nuclei, solids, and molecules. It will be generalized in field theory to describe creation and annihilation of particles.

(2) it approximates any potential for small deviations from equilibrium. To see this, Taylor expand an arbitrary $V(x)$ about its equilibrium point x_0:

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

This looks like $\frac{1}{2}kx^2$ if we equate $k = \left(\frac{d^2V}{dx^2}\right)_{x_0}$ and $x_0 = 0$.

$\frac{dV}{dx} = 0$ at $x = x_0$

Since x_0 is the minimum of the parabola, if $V(x_0) \neq 0$, it is just a redefinition of the scale.

II. Solving the simple harmonic oscillator using power series

We want to find $\psi(x,t) = u(x)e^{-iEt/\hbar}$ where $u(x)$ is the solution to the time-independent Schroedinger Equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} + \frac{1}{2}kx^2 u(x) = Eu(x)$$

$$\frac{d^2u(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)u(x) = 0$$

Define:

$$\omega = \sqrt{\frac{k}{m}} \qquad \text{so } \omega^2 = \frac{k}{m}$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \qquad \text{so } x^2 = \frac{\hbar\xi^2}{m\omega}$$

$$\frac{du}{dx} = \frac{du}{d\xi}\frac{d\xi}{dx} = \frac{du}{d\xi}\sqrt{\frac{\mathrm{m}\omega}{\hbar}}$$

$$\frac{d^2u}{dx^2} = \frac{d}{dx}\left[\frac{du}{d\xi}\sqrt{\frac{\mathrm{m}\omega}{\hbar}}\right] = \sqrt{\frac{\mathrm{m}\omega}{\hbar}}\frac{d^2u}{d\xi^2}\frac{d\xi}{dx} = \frac{m\omega}{\hbar}\frac{d^2u}{d\xi^2}$$

Also define: $\varepsilon = \dfrac{2E}{\hbar\omega}$

Plug these into the Schroedinger Equation:

$$\frac{m\omega}{\hbar}\frac{d^2u}{d\xi^2}+\left(\frac{2mE}{\hbar^2}-\frac{2m}{\hbar^2}\frac{1}{2}k\frac{\hbar\xi^2}{m\omega}\right)u=0$$

Multiply through by $\frac{\hbar}{m\omega}$:

$$\frac{d^2u}{d\xi^2}+\left(\frac{\hbar}{m\omega}\frac{2mE}{\hbar^2}-\frac{\hbar}{m\omega}\frac{2m}{\hbar^2}\frac{1}{2}k\frac{\hbar\xi^2}{m\omega}\right)u=0$$

$$\frac{d^2u}{d\xi^2}+\left(\varepsilon-\xi^2\right)u=0$$

To solve this we will make the usual requirements that "ψ" (here u) and $\partial\psi/\partial x$ (here $\partial u/\partial x$) are finite, single-valued, and continuous everywhere.

We need to take special care that ψ remains finite as x $\to\infty$. (It does not happen automatically as in the square well for which $\psi(x\to\infty)\sim e^{-Kx}$.) To develop a u that we are sure is finite as $x\to\infty$, first find $u_\infty\equiv u(x\to\infty)$. Then make sure that the full $u(x<\infty)$ converges to it for large x.

(1) Find $u_\infty\equiv u(x\to\infty)=u(\xi>>0)$

Note that since ξ is a function of x but is dimensionless, and ε is not a function of x but is dimensionless, for u_∞, $\xi>>\varepsilon$.

Begin with $\frac{d^2u}{d\xi^2}+\left(\varepsilon-\xi^2\right)u=0.$ If $\xi >> \varepsilon$, approximate this as:

$$\frac{d^2u_\infty}{d\xi^2}-\xi^2u_\infty=0$$

The solution to this is

$$u_\infty \propto Ae^{-\xi^2/2}+Be^{+\xi^2/2}$$

Small terms are neglected. We can see what they are by taking $\frac{d^2u_\infty}{dx^2}$ on this solution.

To ensure that u_∞ remains finite as $x \to \infty$

$$\xi \to \infty$$

set $B=0$.

(2) Now guess that $u_{\text{finite x}} = u_\infty \cdot h(\xi) = e^{-\xi^2/2} \cdot h(\xi)$

where these are the exact solution to $\frac{d^2u}{d\xi^2}+\left(\varepsilon-\xi^2\right)u=0$

Substitute $u_{\text{finite x}} = u_\infty \cdot h(\xi) = e^{-\xi^2/2} \cdot h(\xi)$ here:

$$\frac{d^2}{d\xi^2}\left[e^{-\xi^2/2}\cdot h(\xi)\right]+\left(\varepsilon-\xi^2\right)e^{-\xi^2/2}\cdot h(\xi)=0$$

$$\frac{d}{d\xi}\left[e^{-\xi^2/2}\frac{\partial h}{\partial\xi}+h\cdot(-2)\frac{\xi}{2}e^{-\xi^2/2}\right]+\left(\varepsilon-\xi^2\right)e^{-\xi^2/2}\cdot h(\xi)=0$$

$$e^{-\xi^2/2}\frac{\partial^2 h}{\partial\xi^2}+(-2)\frac{\xi}{2}e^{-\xi^2/2}\frac{\partial h}{\partial\xi}-\frac{\partial}{\partial\xi}\left[h\xi e^{-\xi^2/2}\right]+\left(\varepsilon-\xi^2\right)e^{-\xi^2/2}\cdot h(\xi)=0$$

$$e^{-\xi^2/2}\frac{\partial^2 h}{\partial\xi^2}-\xi e^{-\xi^2/2}\frac{\partial h}{\partial\xi}-\left[h\xi(-2)\xi e^{-\xi^2/2}+e^{-\xi^2/2}\left(h+\xi\frac{\partial h}{\partial\xi}\right)\right]+\left(\varepsilon-\xi^2\right)e^{-\xi^2/2}\cdot h(\xi)=0$$

Cancel all the exponentials to get :

$$\frac{\partial^2 h}{\partial\xi^2}-\xi\frac{\partial h}{\partial\xi}+h\xi^2-h-\xi\frac{\partial h}{\partial\xi}+\left(\varepsilon-\xi^2\right)h=0$$

$$\frac{\partial^2 h}{\partial\xi^2}-2\xi\frac{\partial h}{\partial\xi}+(\varepsilon-1)h=0 \qquad \text{"Eq 1"}$$

To solve this differential equation, use the most general solution technique possible :

Assume $h(\xi)=\sum_{l=0}^{\infty}a_l\xi^l=a_0+a_1\xi+a_2\xi^2+\ldots$

Take derivatives:

$$\frac{\partial h}{\partial \xi} = \sum_{l=1}^{\infty} l a_l \xi^{l-1} = 1a_1 + 2a_2\xi + 3a_3\xi^2 + ...$$

$$\frac{\partial^2 h}{\partial \xi^2} = \sum_{l=2}^{\infty} l(l-1) a_l \xi^{l-2} = 1 \cdot 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + ...$$

Substitute these into Equation 1:

$$1 \cdot 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + 4 \cdot 5a_5\xi^3 + ...$$

$$-2 \cdot 1a\xi_1 - 2 \cdot 2a_2\xi^2 - 2 \cdot 3a_3\xi^3 - ...$$

$$+(\varepsilon - 1)a_0 + (\varepsilon - 1)a_1\xi + (\varepsilon - 1)a_2\xi^2 + (\varepsilon - 1)a_3\xi^3 + ... = 0$$

This must be true for all values of ξ, which is all values of x, so the coefficients of each power of ξ must individually cancel. Gather the coefficients together and equate them to 0:

Coefficient of

ξ^0 $\quad 1\cdot 2a_2+(\varepsilon-1)a_0=0$

ξ^1 $\quad 2\cdot 3a_3+(\varepsilon-1-2\cdot 1)a_1=0$

ξ^2 $\quad 3\cdot 4a_4+(\varepsilon-1-2\cdot 2)a_2=0$

ξ^3 $\quad 4\cdot 5a_3+(\varepsilon-1-2\cdot 3)a_3=0$

.....

ξ^l $\quad (l+1)(l+2)a_{l+2}+(\varepsilon-1-2\cdot l)a_l=0$

Conclude

$$a_{l+2}=\frac{-(\varepsilon-1-2\cdot l)a_l}{(l+1)(l+2)}$$ The recursion relation for the coefficients

This relates a_2, a_4, a_6, ... to a_0

and a_3, a_5, a_7, ... to a_1

a_0 and a_1 are NOT specified by this, which is reasonable because the original equation ("Eq 1") is second order, so we expect 2 constants of integration requiring 2 initial conditions.

$$h(\xi) = a_0\left(1 + \frac{a_2}{a_0}\xi^2 + \frac{a_4}{a_2}\frac{a_2}{a_0}\xi^4 + \ldots\right) + a_1\left(\xi + \frac{a_3}{a_1}\xi^3 + \frac{a_5}{a_3}\frac{a_3}{a_1}\xi^5 + \ldots\right) \qquad \left(\text{using the form } \frac{a_{l+2}}{a_l}\right)$$

Recall $u(\xi) = u_\infty \cdot h(\xi)$.

We already required that u_∞ remain finite for $x \to \infty$. Now we must guarantee the same about $h(\xi)$.

How does h($\xi \to \infty$) look?

Consider a general function $\exp\left(\mathrm{v}^2\right) = 1 + \frac{v^2}{2!} + \frac{v^4}{3!} + \frac{v^6}{4!} + \ldots.$

Notice this has the same form as the a_0 series or $\frac{a_1}{\xi}$ series of $h(\xi)$.

So $h(\xi \to \infty) \sim \exp\left(\xi^2\right) \Rightarrow \infty$

So $u(x \to \infty) = u_\infty \cdot h(\xi)$

$$= \exp\left(\frac{-\xi^2}{2}\right)\exp\left(\xi^2\right)$$

$$= \exp\left(\frac{+\xi^2}{2}\right) \to \infty \qquad \text{as } x \to \infty$$

So this $h(\xi)$ is not completely acceptable.

Procedure to force $h(\xi)$ to be finite as $x \to \infty$:

Find a way to truncate the series behavior of $h(\xi)$ so that beyond some point "i", all $a_i = 0$.

Then the highest power of the $h(\xi)$ series will be finite (even if it is, for example, as high as $\xi^{1000000}$) which will be dominated by the $e^{-\xi^2/2}$ as $\xi \to \infty$. Procedure:

(1) Set either a_0 or $a_1 = 0$ (but not both).

(2) Then set $\varepsilon = 2n+1$, where $n = 1, 3, 5, \ldots$ if $a_0 = 0$

or $n = 0, 2, 4, \ldots$ if $a_1 = 0$

Notice how this affects the a_i:

Recall in general $a_{l+2} = \dfrac{-(\varepsilon - 1 - 2\cdot l)}{(l+1)(l+2)}\, a_l$.

So when we carry out (1) and (2), then for $l = n$, we get

$$a_{n+2} = \frac{-(2n+1-1-2n)}{(n+1)(n+2)} a_n = 0.$$

So although the a_i (for $i < a_{n+2}$) are non-zero, $a_{n+4}, a_{n+6}, \ldots = 0$

AND the a_i in the other part of the series (based on a_0 versus a_1) are ALL 0.

Our choice of "n" during the truncation process specifies a particular polynomial "H_n" (meaning, "h" truncated so that a_n is the largest non-zero coefficient).

This is a Hermite polynomial of order n.

The H_n have been tabulated for many values of n. The choices made for a_0 and a_1 give

$$H_0(\xi) = 1$$
$$H_1(\xi) = 2\xi$$
$$H_2(\xi) = 4\xi^2 - 2$$
$$H_3(\xi) = 8\xi^3 - 12\xi$$
$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

Then $u_n(\xi) = Ae^{-\xi^2/2} \cdot H_n(\xi)$

Each H (indexed by n) gives a different eigenfunction of the harmonic oscillator. Since the harmonic oscillator restricts the region in which a particle can be (that is, it traps particles), we expect it to produce energy quantization.

The allowed (quantized) energy values are given by

$$\varepsilon = 2n + 1$$

$$\frac{2E}{\hbar\omega} = 2n + 1$$

$$E = \left(n + \frac{1}{2} \right) \hbar\omega \qquad \text{for } n = 0,\ 1,\ 2,\ ....$$

Recall this $\omega = \sqrt{\frac{k}{m}}$

k is determined by the shape of the potential.

m is the mass of the bound particle.

Outline

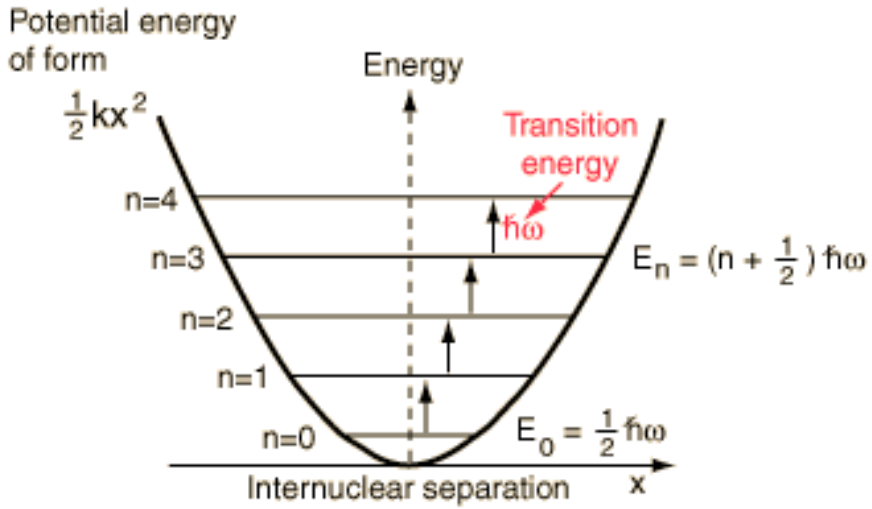
I. Facts about the eigenfunctions and eigenvalues of the simple harmonic oscillator
II. More on the Hermite polynomials
III. Ladder operators

I. Facts about the eigenvalues and eigenfunctions of the harmonic oscillator

(i) They are evenly spaced.

That is, $E_{j+1} - E_j = \left(j+1+\frac{1}{2} \right)\hbar\omega - \left(j+\frac{1}{2} \right)\hbar\omega = \hbar\omega$

This is a constant separation that depends only on $w \propto k$ and m, not on the particular E_j.



This kind of constant separation of levels can actually be observed in spectra from excited molecules. This is why those spectra are inferred to arise from vibration, that is, simple harmonic motion.

(ii) $E_{\text{min}imum} = E_{n=0} = \dfrac{\hbar\omega}{2}$

A particle trapped in a simple harmonic oscillator potential CANNOT have 0 energy.

It can have at minimum $E = \dfrac{\hbar}{2}\sqrt{\dfrac{k}{m}}$, called the "zero-point energy."

This is important because:

(1) It is related to the Uncertainty Principle. Since $E = PE + KE = \dfrac{p^2}{2m} + \dfrac{1}{2}kx^2$,

0 energy could only occur if $x = 0$ and $p = 0$ simultaneously.

(2) It explains why it is experimentally impossible to lower the temperature to absolute zero.

(3) Zero-point energy is a property of ALL potentials (but has a specific formula for each,

for example for the infinite square well of width "a", $E_{\text{min}} = \dfrac{\pi^2\hbar^2}{2ma^2}$

(4) The existence of zero-point energy taking the form $\dfrac{\hbar\omega}{2}$ has been experimentally verified

(Milliken 1924, Nobel 1966)-that is, it is not an unobservable change of scale. It was observed in spectra of vibrating molecules of different isotopes.

(iii) Each eigenfunction has a unique eigenvalue, that is, there is no degeneracy for this potential.

(iv) Notice this is another example of a symmetric potential producing states of definite parity.

States with n odd have odd parity.
States with n even have even parity.

II. More about the Hermite polynomials

(1) They are actually defined by the equation

$$H_n(\xi) = (-1)^n e^{+\xi^2} \frac{\partial^n}{\partial \xi^n}\left(e^{-\xi^2}\right) = e^{+\xi^2/2}\left(\xi - \frac{\partial}{\partial \xi}\right)^n e^{-\xi^2/2}$$

(2) Useful relationships between different orders of them are

(a) $\frac{dH_n(\xi)}{d\xi} = 2nH_{n-1}(\xi)$

(b) $2\xi H_n(\xi) = H_{n+1}(\xi) + 2nH_{n-1}(\xi)$

(3) They are orthogonal: Specifically,

$$\int_{-\infty}^{+\infty} d\xi H_n(\xi) H_m(\xi) e^{-\xi^2} = \sqrt{\pi} 2^n n! \delta_{mn}$$

This leads to the $u(\xi)$ being truly orthonormal:

$$\int d\xi u_n(\xi) u_m(\xi) = \delta_{mn}$$

III. Ladder operators

Recall the time-independent Schroedinger Equation for the harmonic oscillator:

$$\frac{-\hbar^2}{2m}u(x)+\frac{1}{2}kx^2u(x)=Eu(x)$$

Substitute $p_{op}=-i\hbar\frac{\partial}{\partial x}$

$$\underbrace{\frac{p_{op}^2}{2m}u(x)+\frac{1}{2}kx_{op}^2u(x)}_{\downarrow\ Hu(x)}=Eu(x)$$

That is, $H=\frac{p_{op}^2}{2m}+\frac{1}{2}kx_{op}^2$

Recall $\omega=\sqrt{\frac{k}{m}}$

$$H=\frac{p_{op}^2}{2m}+\frac{1}{2}\omega^2mx_{op}^2$$

Define 2 operators:

$$a \equiv \sqrt{\frac{m\omega}{2\hbar}}x_{op} + \frac{ip_{op}}{\sqrt{2m\hbar\omega}} \qquad \text{and } a^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}x_{op} - \frac{ip_{op}}{\sqrt{2m\hbar\omega}}$$

Notice the commutation property of a and $a^\dagger$:

$$\left[a,a^\dagger\right] = \left[\left(\sqrt{\frac{m\omega}{2\hbar}}x_{op} + \frac{ip_{op}}{\sqrt{2m\hbar\omega}}\right),\left(a^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}x_{op} - \frac{ip_{op}}{\sqrt{2m\hbar\omega}}\right)\right]$$

$$= \frac{m\omega}{2\hbar}\underbrace{[x,x]}_{0} + \frac{i}{\sqrt{2m\hbar\omega}}\sqrt{\frac{m\omega}{2\hbar}}\underbrace{[p,x]}_{(-i\hbar)} - i\sqrt{\frac{m\omega}{2\hbar}}\frac{1}{\sqrt{2m\hbar\omega}}\underbrace{[x,p]}_{(+i\hbar)} + \frac{1}{2m\hbar\omega}\underbrace{[p,p]}_{0}$$

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

$$aa^\dagger - a^\dagger a = 1$$

So $aa^\dagger = 1 + a^\dagger a$ and $a^\dagger a = aa^\dagger - 1$

We can invert these to get

$$x_{op} = \frac{a + a^\dagger}{\sqrt{\frac{2m\omega}{\hbar}}} \qquad \text{and} \qquad p_{op} = -i\sqrt{\frac{\hbar m\omega}{2}}\left(a - a^\dagger\right)$$ [Now drop the "*op*" subscripts.]

Notice $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2m} - i\sqrt{\frac{\hbar m\omega}{2}}\left(a - a^\dagger\right)\cdot -i\sqrt{\frac{\hbar m\omega}{2}}\left(a - a^\dagger\right) + \frac{1}{2}m\omega^2 \frac{\left(a + a^\dagger\right)\left(a + a^\dagger\right)}{\frac{2m\omega}{\hbar}}$

$= -\frac{\hbar\omega}{4}\left[a^2 - a^\dagger a - aa^\dagger + a^{\dagger 2}\right] + \frac{\hbar\omega}{4}\left[a^2 + a^\dagger a + aa^\dagger + a^{\dagger 2}\right]$

$= \frac{\hbar\omega}{4}\left[a^\dagger a + aa^\dagger\right]$

Use $aa^\dagger = a^\dagger a + 1$

$= \frac{\hbar\omega}{4}\left[a^\dagger a + a^\dagger a + 1\right]$

$= \frac{\hbar\omega}{2}\left[2a^\dagger a + 1\right]$

$H_{SHO} = \hbar\omega\left[a^\dagger a + \frac{1}{2}\right]$

We can get the eigenvalues and eigenfunctions of H if we can get them for the compound operator $a^\dagger a$.

Our strategy: first understand the separate effects of a and $a^\dagger$, then combine them.

To do this we need 3 things:

(1) $[H,a]=\left[\hbar\omega\left(a^\dagger a+\frac{1}{2}\right),a\right]=\hbar\omega\left[a^\dagger a,a\right]+\frac{\hbar\omega}{2}\underbrace{[1,a]}_{\downarrow\ 0}$

$=\hbar\omega\left(a^\dagger aa-aa^\dagger a\right)$

Use $aa^\dagger=1+a^\dagger a$

$=\hbar\omega\left(a^\dagger aa-\left(1+a^\dagger a\right)a\right)$

$=\hbar\omega\left(a^\dagger aa-a-a^\dagger aa\right)$

$[H,a]=-\hbar\omega a$

(2) Similarly, $\left[H,a^\dagger\right]=+\hbar\omega a^\dagger$

(3) Suppose that we already know the eigenvalues E_i and eigenvectors $|E_i\rangle$ of H. (That is, suppose we go them by applying a series solution to $Hu = Eu$.) Use these to find the behavior of operator a.

Outline

I. The behavior of ladder operator a

II. The behavior of ladder operator $a^{\dagger}$

III. The Number Operator

I. The behavior of ladder operator a

To see what operator a does, begin with:

$[H,a] = -\hbar\omega a$ Expand the commutator:

$Ha - aH = -\hbar\omega a$ Operate on the eigenvectors $|E\rangle$:

$$Ha|E\rangle - a\underbrace{H|E\rangle}_{\downarrow} = -\hbar\omega a|E\rangle$$

$$E|E\rangle$$

$$Ha|E\rangle - aE|E\rangle = -\hbar\omega a|E\rangle$$

$$Ha|E\rangle = (E - \hbar\omega)a|E\rangle$$

What this means: If $|E\rangle$ is an eigenvector of H with eigenvalue E, then "$a|E\rangle$" is ALSO an eigenvector of H, but it has eigenvalue $(E - \hbar\omega)$.

So we discover that the following happens when we apply $Ha|E\rangle$:

First the "a" operates on $|E\rangle$ and lowers its eigenvalue from E to $(E - \hbar\omega)$.

Another way to write this is to say:

$$a|E\rangle = c|E - \hbar\omega\rangle$$

Unspecified normalization

Then the H operates on the result, called "$a|E\rangle$", and extracts the eigenvalue of that new state, $E - \hbar\omega$.

For this reason, a is called $\left\{\begin{array}{l}\text{a lowering operator}\\ \text{a step-down operator}\\ \text{an annihilation operator}\end{array}\right\}$.

Repeated applications of "a" keep lowering the states' energy by $\hbar\omega$ each time, so

$a|E\rangle \sim |E-\hbar\omega\rangle$

$aa|E\rangle \sim |E-2\hbar\omega\rangle$

$aaa|E\rangle \sim |E-3\hbar\omega\rangle$ and so forth.

But eventually $|E\rangle$ reaches $\underbrace{\text{the ground state}}_{\downarrow}$, beyond which its energy cannot be lowered.

call this $|u_0\rangle$

How do we know this?

(1) We know that physically a simple harmonic oscillator has a lowest energy state.

Its energy cannot be decreased to -∞.

(2) Mathematically we see that

$$\langle\psi|H|\psi\rangle=\left\langle\psi\left|\frac{p^2}{2m}+\frac{kx^2}{2}\right|\psi\right\rangle=\frac{1}{2m}\langle\psi|p^2|\psi\rangle+\frac{k}{2}\langle\psi|x^2|\psi\rangle$$

Both of these have the general form:

$\langle\psi|Q^2|\psi\rangle=\langle\psi|QQ|\psi\rangle=\underbrace{\langle Q^\dagger\psi|Q\psi\rangle}_{\downarrow}$. But x, p are both Hermitian:

$\langle Q\psi|Q\psi\rangle\geq 0$ inner product.

So $\langle\psi|H|\psi\rangle=E\geq 0$. E cannot be reduced below 0.

Because mathematically the a is structured so that it could lower E indefinitely,

we must impose a physical constraint:

Demand: there exists a $|u_0\rangle$ (that is, a minimum energy state) whose property is

$a|u_0\rangle=0$.

Find out what is the energy of $|u_0\rangle$:

$$H|u_0\rangle=\left(\hbar\omega a^\dagger a+\frac{\hbar\omega}{2}\right)|u_0\rangle=\hbar\omega a^\dagger\underbrace{a|u_0\rangle}_{\downarrow}+\frac{\hbar\omega}{2}|u_0\rangle$$

$$0$$

So $H|u_0\rangle=\frac{\hbar\omega}{2}|u_0\rangle$. The zero-point energy of the harmonic oscillator is $\frac{\hbar\omega}{2}$.

II. The behavior of operator $a^\dagger$

Recall $\left[H, a^\dagger\right] = \hbar\omega a^\dagger$. Expand:

$$Ha^\dagger - a^\dagger H = \hbar\omega a^\dagger.$$

Operate on $|u_0\rangle$, the minimum energy state:

$$Ha^\dagger|u_0\rangle - a^\dagger \underbrace{H|u_0\rangle}_{\downarrow} = \hbar\omega a^\dagger|u_0\rangle$$

We just showed that this yields $\frac{\hbar\omega}{2}|u_0\rangle$

$$Ha^\dagger|u_0\rangle - a^\dagger \frac{\hbar\omega}{2}|u_0\rangle = \hbar\omega a^\dagger|u_0\rangle.$$

Rewrite:

$$Ha^\dagger|u_0\rangle = \left(\hbar\omega + \frac{\hbar\omega}{2}\right)a^\dagger|u_0\rangle$$

We see that $a^\dagger$ applied to $|u_0\rangle$ converts $|u_0\rangle$ into a new state with (higher) energy $\hbar\omega + \frac{\hbar\omega}{2}$.

We call this new state $|u_1\rangle$, the first excited state of the simple harmonic oscillator.

So $a^\dagger|u_0\rangle = c|u_1\rangle$.

Unspecified normalization

Because of this behavior we call $a^\dagger$ the $\left\{\begin{matrix}\text{raising}\\ \text{step-up}\\ \text{creation}\end{matrix}\right\}$ operator.

Repeated actions of $a^\dagger$ raise the E forever.

So $a^\dagger|u_0\rangle = |u_1\rangle \Rightarrow Ha^\dagger|u_0\rangle = \left(1+\frac{1}{2}\right)\hbar\omega|u_1\rangle$

$a^\dagger a^\dagger|u_0\rangle = \left(a^\dagger\right)^2|u_0\rangle = |u_2\rangle \Rightarrow H\left(a^\dagger\right)^2|u_0\rangle = \left(2+\frac{1}{2}\right)\hbar\omega|u_2\rangle$

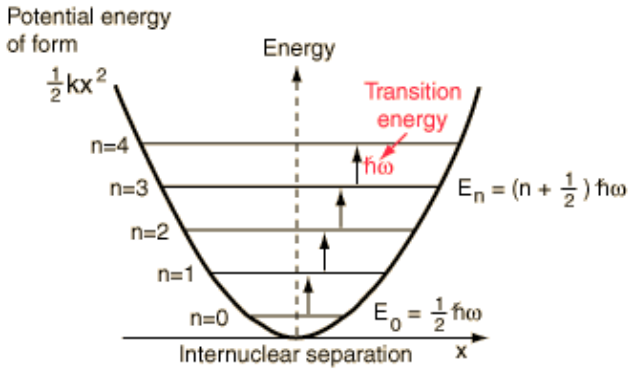
...

$\left(a^\dagger\right)^n|u_0\rangle = |u_n\rangle \Rightarrow H\left(a^\dagger\right)^n|u_0\rangle = \underbrace{\left(n+\frac{1}{2}\right)\hbar\omega}|u_n\rangle$

This is the eigenvalue form we found for E using the series method too.

The a and $a^\dagger$ are together called the "ladder operators" because the energy levels of the simple harmonic oscillator, being evenly spaced, can be represented by a ladder:

and the $a^\dagger$ and a move the system up and down between them.



III. The Number Operator

Recall that $H_{SHO} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$.

The combination "$a^\dagger a$" is called the Number Operator

To see what it does, recall we have found that

$$\underbrace{H}\left(a^\dagger\right)^n|u_0\rangle = \left(n+\frac{1}{2}\right)\hbar\omega|u_n\rangle = \underbrace{\left(n+\frac{1}{2}\right)\hbar\omega}\left(a^\dagger\right)^n|u_0\rangle$$

$$\overbrace{\hbar\omega\left(a^\dagger a+\frac{1}{2}\right)}\left(a^\dagger\right)^n|u_0\rangle = \overbrace{\hbar\omega\left(n+\frac{1}{2}\right)}\left(a^\dagger\right)^n|u_0\rangle$$

These terms are the same except for the "$a^\dagger a$" and the "n".

We see that the operator $a^\dagger a$ is extracting from the state the value n which is the

$$\left\{\begin{array}{l}\text{number of the energy level}\\ -or-\\ \text{number of energy quanta the state possesses}\end{array}\right\}.$$

So we call $a^\dagger a = "N"$ The Number Operator

What N does:

$$\left(a^{\dagger}\right)^{n}\left|u_{0}\right\rangle = c\left|u_{n}\right\rangle$$

Unspecified normalization

$$N\left(a^{\dagger}\right)^{n}\left|u_{0}\right\rangle = nc\left|u_{n}\right\rangle = n\left(a^{\dagger}\right)^{n}\left|u_{0}\right\rangle$$

So $\left|u_{n}\right\rangle$ is the eigenstate that corresponds to the eigenvalue n of the number operator N.

We are now working in "number space."

Normalize the $\left|u_{n}\right\rangle$:

First notice how the $\left|u_{n}\right\rangle$ are related among themselves:

$$\left(a^{\dagger}\right)^{n}\left|u_{0}\right\rangle = c_{n}\left|u_{n}\right\rangle$$

By the form of this equation, $c_0 = 1$.

(That is, $\underbrace{\left(a^{\dagger}\right)^{0}}_{1}\left|u_{0}\right\rangle = c_{0}\left|u_{0}\right\rangle$

Now insist that the $\left|u_{n}\right\rangle$ be normalized. Take the inner product of each side with itself:

$$\left\langle \left(a^{\dagger}\right)^{n} u_{0} \middle| \left(a^{\dagger}\right)^{n} u_{0} \right\rangle = \left|c_{n}\right|^{2} \underbrace{\left\langle u_{n} \middle| u_{n} \right\rangle}$$

Insist that this = 1.

Move the $\left(a^\dagger\right)^n$ from the bra to the ket. In the bra it implicitly has an additional "†" that we must show explicitly in the ket:

$$\left\langle u_0 \left| \left[\left(a^\dagger\right)^n\right]^\dagger \left(a^\dagger\right)^n u_0 \right\rangle \right.$$

But $\left(a^\dagger\right)^\dagger = a.$

$$\left\langle u_0 \left| \underbrace{a^n \left(a^\dagger\right)^n u_0}_{} \right\rangle \right. = \left|c_n\right|^2 \qquad \text{"Eq. 1"}$$

To evaluate this, notice:

$$a\left(a^\dagger\right)^n = aa^\dagger\left(a^\dagger\right)^{n-1} = \left(1 + a^\dagger a\right)\left(a^\dagger\right)^{n-1} = \left(a^\dagger\right)^{n-1} + a^\dagger a\left(a^\dagger\right)^{n-1}$$

By comparing these two terms, we see they differ by n $\rightarrow$ n-1. This is a recursion relation.

$$= \left(a^\dagger\right)^{n-1} + a^\dagger\left[\left(a^\dagger\right)^{n-2} + a^\dagger a\left(a^\dagger\right)^{n-2}\right]$$

$$= 2\left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^2\left[\left(a^\dagger\right)^{n-3} + a^\dagger a\left(a^\dagger\right)^{n-3}\right]$$

$$= 3\left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^3 a\left(a^\dagger\right)^{n-3}$$

So $a\left(a^\dagger\right)^n = n\left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^n a$

Apply all this to $|u_0\rangle$.

$$a\left(a^\dagger\right)^n|u_0\rangle = n\left(a^\dagger\right)^{n-1}|u_0\rangle + \left(a^\dagger\right)^n \underbrace{a|u_0\rangle}_{\downarrow\ 0}$$

So we know that

$$a\left(a^\dagger\right)^n|u_0\rangle = n\left(a^\dagger\right)^{n-1}|u_0\rangle.$$

Develop a recursion relation from this.

$$a^2\left(a^\dagger\right)^n|u_0\rangle = aa\left(a^\dagger\right)^{n-1}|u_0\rangle = an\left(a^\dagger\right)^{n-1}|u_0\rangle = na\left(a^\dagger\right)^{n-1}|u_0\rangle = n(n-1)\left(a^\dagger\right)^{n-2}|u_0\rangle$$

$$a^3\left(a^\dagger\right)^n|u_0\rangle = n(n-1)(n-2)\left(a^\dagger\right)^{n-3}|u_0\rangle$$

...

$$a^n\left(a^\dagger\right)^n|u_0\rangle = n!|u_0\rangle$$

Apply this to Eq. 1, which was $\left\langle u_0\left|a^n\left(a^\dagger\right)^n u_0\right.\right\rangle = |c_n|^2$

$$\left\langle u_0 \left| a^n \left(a^\dagger\right)^n u_0 \right\rangle = \left|c_n\right|^2$$

$$\left\langle u_0 \left| n! \right| u_0 \right\rangle = \left|c_n\right|^2$$

$$n!\left|c_0\right|^2 = \left|c_n\right|^2$$

So $c_n = \sqrt{n!}$

$$c_n \left|u_n\right\rangle = \left(a^\dagger\right)^n \left|u_0\right\rangle$$

So $\left|u_n\right\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n \left|u_0\right\rangle$. These are the normalized eigenstates of the Number Operator.