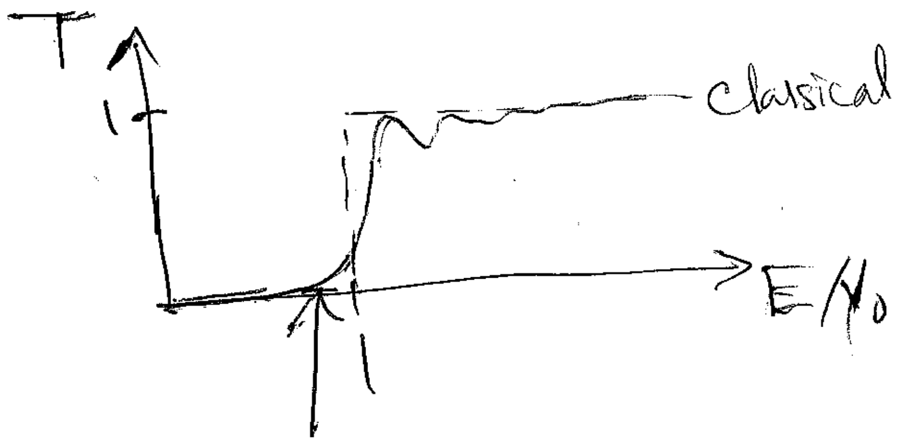
Explicit formulas for $R=|B_I|^2$ and $T=|A_{III}|^2$:

- Nash notes - Wikipedia "finite potential barrier"



$T>0$ for $E<V_0$: QUANTUM TUNNELING

* Example: Alpha decay (α-radiation)

α = 2 prot + 2 neutr. cluster

In heavy nuclei, α-particles are bound by ~~finite~~ potentials. Classically, would stay trapped in nuclei for ever. Due to Quantum Tunneling, They have finite prob^y of being emitted from nucleus: $\;{}^{238}_{92}U \to {}^{234}_{90}Th + \alpha$

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The MOMENTUM OPERATOR

$\hat{p} = -i\hbar \frac{\partial}{\partial x}$ for particle in 1D

$\hat{\vec{p}} = -i\hbar \vec{\nabla}$ for pcle in 3D

Note! $\langle \psi | \hat{p} | \phi \rangle = \int dx\, \psi^*(x)\, \hat{p}\, \phi(x)$

$= -i\hbar \int dx\, \psi^*(x) \frac{\partial \phi(x)}{\partial x}$

Note $\psi^* \hat{p} \phi \neq \hat{p}(\psi^* \phi)$ because $\psi^* \frac{\partial \phi}{\partial x} \neq \frac{\partial}{\partial x}(\psi^* \phi)$

[Unlike position: $\hat{x} = x$

$\psi^* \hat{x} \phi = \psi^* x \phi = x \psi^* \phi$]

E.g., expectation value of $\hat{p}$ in a state $\psi(x)$ is $\int dx\, \psi^*(x)\, \hat{p}\, \psi(x) \neq \int dx\, \hat{p}\left[\psi^*(x)\psi(x)\right]$

* $\hat{p}$ is a hermitian operator:

$\langle \psi | (\hat{p} | \phi \rangle) = \langle (\hat{p}\psi) | \phi \rangle$

Remember: $\langle (\hat{p}\psi) | = \langle \psi | \hat{p}^\dagger$

$|(\hat{p}\phi)\rangle = \hat{p} | \phi \rangle$

Proof: $\alpha = \langle \psi | \hat{p}\phi \rangle = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial \phi}{\partial x}\right) dx$

$\beta = \langle (\hat{p}\psi) | \phi \rangle = \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial \psi}{\partial x}\right)^* \phi \, dx$

$$\alpha - \beta = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \phi}{\partial x} dx - \int_{-\infty}^{\infty} \left(+i\hbar \frac{\partial \psi^*}{\partial x}\right) \phi \, dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \left[\psi^* \frac{\partial \phi}{\partial x} + \frac{\partial \psi^*}{\partial x} \phi\right] dx$$

$$= i\hbar \int_{-\infty}^{\infty} \frac{d}{dx}(\psi^* \phi) \, dx = i\hbar \left[\psi^* \phi\right]_{-\infty}^{\infty}$$

If ψ, ϕ are normalizable, they go to zero for $x \to \pm\infty$. Hence $\alpha - \beta = 0$

$\Rightarrow$ Hermiticity proved for normalizable w.f's.

(Plane waves left out ☹)

* For localized bound states, e.g.

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & x \in [0, L] \\ 0 & \text{elsewhere} \end{cases}$$

or $\psi_n(x) = \text{polynomial} \times e^{-x^2/2\sigma^2}$,

one obtains $\langle \hat{p} \rangle = \int dx\, \psi_n^* \hat{p}\, \psi_n\, dx = 0$

* For plane wave $\psi(x) = A e^{ikx}$:

$$\langle \hat{p} \rangle = \lim_{L\to\infty} \frac{\int_{-L}^{L} dx\, \psi^*(x)\, \hat{p}\, \psi(x)}{\int_{-L}^{L} dx\, \psi^*(x)\, \psi(x)}$$

~~Just~~ $\int_{-\infty}^{\infty} dx\, \psi^* \hat{p}\, \psi$ doesn't work

$$= \lim_{L\to\infty} \frac{|A|^2 \int dx\, e^{-ikx} (-i\hbar)(ik) e^{ikx}}{|A|^2 \int dx\, e^{-ikx} e^{ikx}}$$

$$= \lim_{L\to\infty} \frac{|A|^2\, \hbar k \int_{-L}^{L} dx}{|A|^2 \int_{-L}^{L} dx} = \hbar k$$

Plane wave e^{+ikx} has momentum $\hbar k$

e^{-ikx} has " $-\hbar k$.

* Position & momentum

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$$

Applying on any state $\psi(x)$, one obtains $[\hat{x}, \hat{p}]\psi(x) = i\hbar\,\psi(x)$

$$\boxed{[\hat{x}, \hat{p}] = i\hbar}$$

SHOW!

$$\left[x, \frac{d}{dx}\right] f(x) = x f'(x) - \frac{d}{dx}\left[f(x)\,x\right] = -f(x)$$

* Eigenstates of operator $\hat{p}$: plane waves e^{ikx}

$$\hat{p}\, e^{ikx} = -i\hbar \frac{\partial}{\partial x} e^{ikx} = (\hbar k)\, e^{ikx}$$

* Eigenstates of operator $\hat{x} = x$: Dirac delta function $\delta(x-a)$

$$\hat{x}\, \delta(x-a) = x\,\delta(x-a) = a\,\delta(x-a)$$

because $\delta(x-a)$ is nonzero only at $x = a$.

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* HERMITIAN CONJUGATE (ADJOINT) of OPERATORS

The dual of $\hat{A}|\phi\rangle$ is $\langle\phi|\hat{A}^\dagger$

If $|\chi\rangle = \hat{A}|\phi\rangle$, then $\langle\chi| = \langle\phi|\hat{A}^\dagger$

Informally: $\langle\phi|\hat{A}^\dagger = \underbrace{\langle(\hat{A}\phi)|}_{\text{Dual of } \hat{A}|\phi\rangle}$

* $\hat{A}$ is Hermitian/self-adjoint if $\hat{A} = \hat{A}^\dagger$,

i.e., if $\langle (\hat{A}\phi) | \psi \rangle = \langle \phi | (\hat{A}\psi) \rangle$ for every $|\phi\rangle, |\psi\rangle$

in other words: if $\langle \phi | \hat{A}^\dagger | \psi \rangle = \langle \phi | \hat{A} | \psi \rangle$ for every $|\phi\rangle, |\psi\rangle$

* $(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger$, $(c\hat{A})^\dagger = c^* \hat{A}^\dagger$

* $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$ straightforward to show for matrices:

$(\hat{A}^\dagger)^\dagger = \hat{A}$

$$(AB)^\dagger = \left((AB)^T\right)^* = \left(B^T A^T\right)^* = (B^T)^* (A^T)^* = B^\dagger A^\dagger$$

[I've used $(AB)^T = B^T A^T$]

* If $\hat{Y}$ is hermitian, so is $\hat{Y}^n$:

$$(\hat{Y}^2)^\dagger = (\hat{Y}\hat{Y})^\dagger = \hat{Y}^\dagger \hat{Y}^\dagger = \hat{Y}\hat{Y} = \hat{Y}^2$$

* Ex: Single particle in 1D, $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

$\hat{p}$ is hermitian $\Longrightarrow$ $\frac{\hat{p}^2}{2m}$ is hermitian

also, $V(\hat{x}) = V(x)$ is hermitian

$\hat{x}^\dagger = \hat{x}$

because $\int dx\, [x\phi(x)]^* \psi(x) = \int dx\, [\phi(x)]^* x\psi(x)$

i.e., $\langle (x\phi) | \psi \rangle = \langle \phi | x\psi \rangle$ for any $\phi(x), \psi(x)$

$\Rightarrow V(\hat{x})$ = function of $\hat{x}$ is hermitian.

$\Rightarrow \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ is hermitian.

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* The POSTULATES of QUANTUM MECHANICS

Numbering of postulates not completely standard. "Postulates" summarize rules of QM.

* Postulate 1: Any isolated physical system has a Hilbert space associated with it. Members of the Hilbert space (state vectors/wavefunctions) represents a state of the system.

Comments/extensions:

(1a) If $|\phi_1\rangle$ and $|\phi_2\rangle$ belong to the state space, then so does any combination $\alpha|\phi_1\rangle + \beta|\phi_2\rangle$.

[The superposition principle]

Eg., particle in 1D line: since $\psi_1(x) = e^{-(x-a)^2/2\sigma^2}$

and $\psi_2(x) = e^{-(x+a)^2/2\sigma^2}$ are valid wavefunctions,

so is $\psi_1(x) + \psi_2(x)$ or $\psi_1(x) + i\psi_2(x)$

[particle both at $x=-a$ and $x=+a$]

→ SCHRÖDINGER'S CAT

Ex. 2 spin-$\frac{1}{2}$ object: since

$|\uparrow\rangle = |z,+\rangle$ and $|\downarrow\rangle = |z,-\rangle$ are valid

states, so is $|\uparrow\rangle + |\downarrow\rangle$. (mixture of spin-up & spin-down)

(1b) The overall normalization carries no physical meaning.

Hence we deal with normalized wavefunctions.

Eg. $\Psi(x)$ and $2\Psi(x)$ represent same physical state.

(1c) Components or values of state vectors

represent amplitudes of probabilities,

$$\left|\text{Probability amplitude}\right|^2 = \text{probability}$$

Ex. 1 pcle in 1D: $|\psi(x)|^2 dx$ is the prob^y of finding pcle in region $\left(x - \frac{dx}{2}, x + \frac{dx}{2}\right)$ or $(x, x+dx)$. [dx is infinitesimal]

Ex. 2 Spin-$\frac{1}{2}$: If $|\psi\rangle = c_1|\uparrow\rangle + c_2|\downarrow\rangle$, then $|c_1|^2$ is probability of finding z-component of spin to be up $\left(+\frac{\hbar}{2}\right)$.

(1d) The Hilbert space of a system is spanned by a set of basis vectors. Usually we choose this set to be an orthonormal set.

"Spanned" $\Rightarrow$ any state vector can be expressed as a linear combination of the basis vectors.

Ex. Spin-$\frac{1}{2}$: $\{|\uparrow\rangle = |z;+\rangle, |\downarrow\rangle = |z;-\rangle\}$

But $\{|x;+\rangle, |x;-\rangle\}$ is also a possible basis.

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1e If two physical systems are ~~joined~~ combined, the Hilbert space is the DIRECT PRODUCT of the individual Hilbert spaces.

Ex1: A spin-$\frac{1}{2}$ object: state space is spanned by $\{|\uparrow\rangle, |\downarrow\rangle\}$.

2 spin-$\frac{1}{2}$ objects: state space is spanned by $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$

Ex.2 For a single particle in 1D, state (Hilbert) space is collection of all normalizable functions $\psi_{1p}(x)$. For 2 pcles on a 1D line, Hilbert space is collection of all normalizable functions $\psi_{2p}(x_1, x_2)$:

$$\int dx_1 \int dx_2 \, |\psi_{2p}(x_1, x_2)|^2 = 1$$

Similarly, 2 pcles in 3D: described by wavefunction $\psi_{2p}(\vec{r}_1, \vec{r}_2)$.

Postulate 2 : Each physical observable corresponds to a linear, Hermitian, operator $\hat{A}$.
The eigenvectors/eigenfunctions of an operator form a complete basis (span the Hilbert space).

Comments/Extensions :

(2a) Linear means $\hat{A}\left(c_1|\psi\rangle + c_2|\phi\rangle\right) = c_1 \hat{A}|\psi\rangle + c_2 \hat{A}|\phi\rangle$

(2b') Hermitian : Dual of $\hat{A}|\phi\rangle$ is $\langle\phi|\hat{A}^\dagger$ or $\langle\phi|\hat{A}\psi\rangle = \langle\hat{A}\phi|\psi\rangle$ or $(\phi, \hat{A}\psi) = (\hat{A}\phi, \psi)$
conjug.

(2b) Hermiticity implies that the eigenvalues are real. Proof : If $\hat{A}|\phi\rangle = \alpha|\phi\rangle$, then
$$\langle\phi|\hat{A}|\phi\rangle = \alpha\langle\phi|\phi\rangle = \alpha$$

But $\langle\phi|\hat{A}^\dagger = \langle\phi|\alpha^* \Rightarrow \langle\phi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\phi\rangle\alpha^* = \alpha^*$

Since $\hat{A} = \hat{A}^\dagger$, $\langle\phi|\hat{A}|\phi\rangle = \langle\phi|\hat{A}^\dagger|\phi\rangle \Rightarrow \alpha = \alpha^*$
$\Rightarrow \alpha$ is real.

(2c) Hat notation is not universal $\longrightarrow$ careful!

(2d) Once a basis $\{|\phi_i\rangle\}$ is chosen, and the vector notation $|\phi_1\rangle = \begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}$, $|\phi_2\rangle = \begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix}$, ... is used, operators are represented by a MATRIX, with elements $A_{ij} = \langle\phi_i|\hat{A}|\phi_j\rangle$.

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$\Rightarrow$ See Problem Set 6

* Postulate 3: A measurement of observable Y necessarily yields one of the eigenvalues of the corresponding operator $\hat{Y}$.

If $\hat{Y}|w_n\rangle = y_n|w_n\rangle$, possible measurement outcomes are y_n.

Probability of finding the outcome y_n is

$$P(y_n) = |\langle w_n|\Psi\rangle|^2$$

where $|\Psi\rangle$ is the state of the system.

Comments / implications ~~extensions~~:

(3a) If $|\Psi\rangle$ is expanded in $\{|w_n\rangle\}$:

$|\Psi\rangle = \sum_n c_n|w_n\rangle$, then the probability of outcome y_j is $|\langle w_j|\Psi\rangle|^2 = |c_j|^2$

(3b) Clearly, the expectation value is

$$\langle\hat{Y}\rangle_\Psi = \sum_j y_j\, P(y_j) = \sum_j y_j |\langle w_j|\Psi\rangle|^2$$

This is consistent with $\langle \hat{Y} \rangle_\psi = \langle \psi | \hat{Y} | \psi \rangle$:

$$\langle \psi | \hat{Y} | \psi \rangle = \langle \psi | \left(\sum_j y_j |w_j\rangle\langle w_j| \right) |\psi\rangle$$

$$= \sum_j y_j \langle \psi | w_j \rangle \langle w_j | \psi \rangle = \sum_j y_j |\langle w_j|\psi\rangle|^2$$

Why is $\hat{Y} = \sum_j y_j |w_j\rangle\langle w_j|$?

Because $\hat{A} = \sum_{ij} A_{ij} |w_i\rangle\langle w_j|$ (probl. set 6)

and $Y_{ij} = \langle w_i | \hat{Y} | w_j \rangle = \langle w_i | y_j | w_j \rangle$
$= y_j \delta_{ij}$

Hence $\hat{Y} = \sum_{ij} y_j \delta_{ij} |w_i\rangle\langle w_j| = \sum_j y_j |w_j\rangle\langle w_j|$

<u>Postulate 4</u>: If a measurement of Y yields eigenvalue y_j, then immediately after the measurement, the system is in the eigenstate $|w_j\rangle$ corresponding to the eigenvalue.

Comments:

4a Known as "collapse of the wavefunction" or "Projection postulate". If measurement is instantaneous, the state of the system changes sharply, instantaneously

4b A measurement of Y "projects" state onto one eigenvector of $\hat{Y}$.

If $\hat{P}_n = |w_n\rangle\langle w_n|$, then $\hat{P}_n|\psi\rangle = |w_n\rangle c_n$ where $|\psi\rangle = \sum_j c_j |w_j\rangle$

$$|\psi\rangle \xrightarrow[\text{of } Y \text{ with result } y_n]{\text{after measurement}} \frac{\hat{P}_n|\psi\rangle}{\| \hat{P}_n|\psi\rangle \|}$$

4d Spin $\frac{1}{2}$ example

$\hat{P}_n$ is called a projection operator.

4e Some people find this postulate problematic/disturbing ["Schrodinger's cat"]

Postulate 5: The time evolution of the state vector is determined by the TDSE:

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle$$

Comments/Extensions:

5a If the solution is written as

$$|\Psi(t_f)\rangle = U(t_f, t_i)|\Psi(t_i)\rangle$$

then $U(t_f, t_i)$ is a UNITARY operator

Known as the PROPAGATOR. (Propagates w.f. in time)

5b) For a constant (time-indep.) Hamiltonian,

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle, \quad |\Psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\Psi(0)\rangle$$

and $U(t_f, t_i) = e^{-i\hat{H}(t_f - t_i)/\hbar}$

5c) For a constant Hamiltonian, consider stationary solutions of time-indep. SE:

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$$

If $|\Psi(0)\rangle = |\phi_n\rangle$,

then $|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\phi_n\rangle = e^{-iE_n t/\hbar}|\phi_n\rangle$

[Show: If $\hat{Y}|w_n\rangle = y_n|w_n\rangle$, then

$\hat{Y}^2|w_n\rangle = y_n^2|w_n\rangle$
$\hat{Y}^3|w_n\rangle = y_n^3|w_n\rangle, \ldots$

$e^{\alpha\hat{Y}}|w_n\rangle = e^{\alpha y_n}|w_n\rangle$]

If $|\Psi(0)\rangle$ is expanded: $\boxed{|\Psi(0)\rangle = \sum_n c_n |\phi_n\rangle}$

Then

$$\boxed{|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |\phi_n\rangle}$$

If the eigenvalues/eigenstates of $\hat{H}$ are known, the time evolution of any state can be found in this way, by expanding the initial state in the energy eigenbasis.