* The wave-particle duality

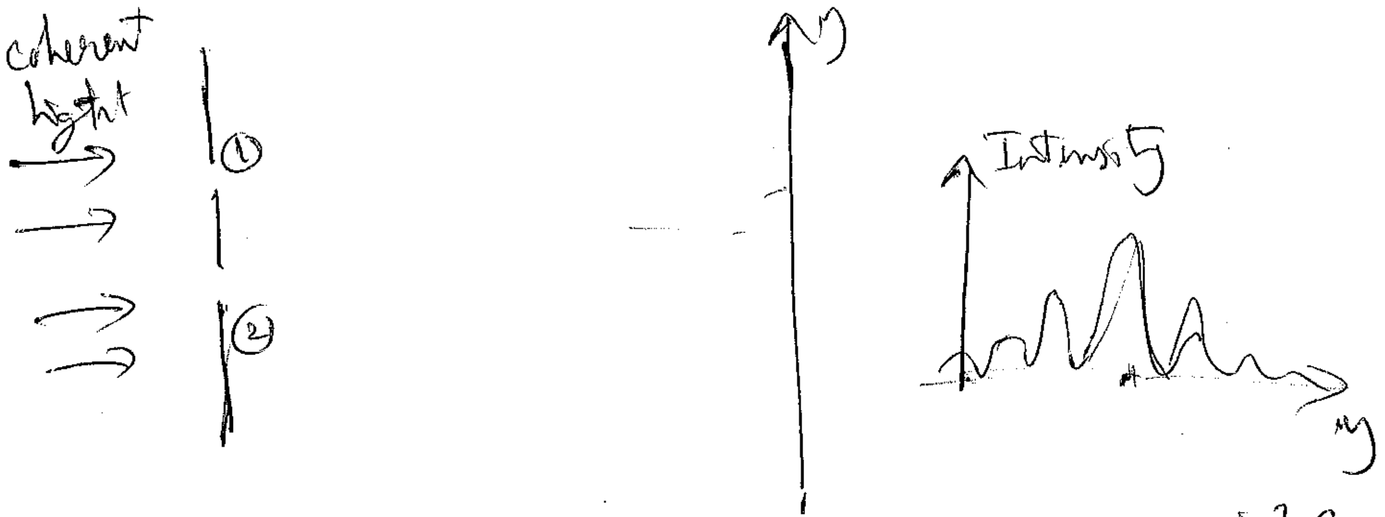
Waves come in particle packets.

Particles have wave natures, are described by a "wave equation".

No strong distinction !

* TWO-SLIT EXPERIMENTS (interference)

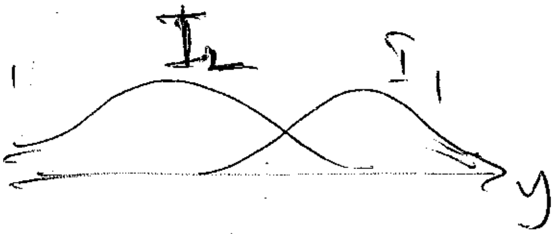
Feynman III, Chapter 1



I Intensity $\propto \frac{\sin^2 Cy}{y^2}$

If only ① is open, I_1

If only ② is open, I_2



$$I \neq I_1 + I_2 \quad (I_1, I_2, I \text{ positive})$$

$$I_1 \propto |E_1|^2 \quad I_2 = |E_2|^2$$

$$I = |E|^2 = |E_1+E_2|^2 = |E_1|^2 + |E_2|^2 + 2E_1E_2$$

INTERLUDE for p. 8

For Euclidean vector, magnitude (norm) is sq. root of a inner product with itself: , $\vec{A}\cdot\vec{A} = A^2 \Rightarrow A = \sqrt{\vec{A}\cdot\vec{A}}$

For wavevector, norm is (~~sq. root of~~) inner product with itself: $\mathcal{N} = \langle\psi|\psi\rangle$

Usually, we deal with wavevectors of unit norm:

$$\langle\psi|\psi\rangle = 1$$

$\rightarrow$ wavefunction is then said to be NORMALIZED

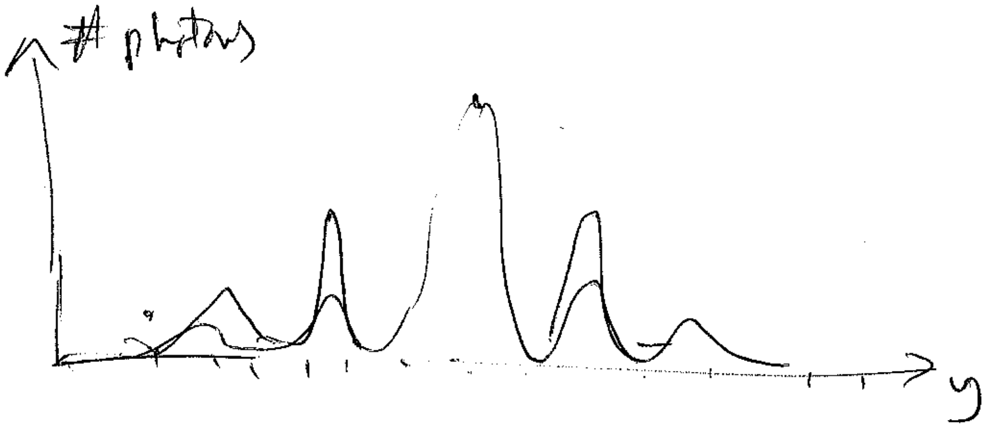
$\neq |E_1|^2 + |E_2|^2$, hence interference.

* Photon picture? Photons thru 1 interfere with photons thru 2? $\rightarrow$ False

Each photon travels thru both; interferes with itself. Very low intensity: photons going thru one by one.

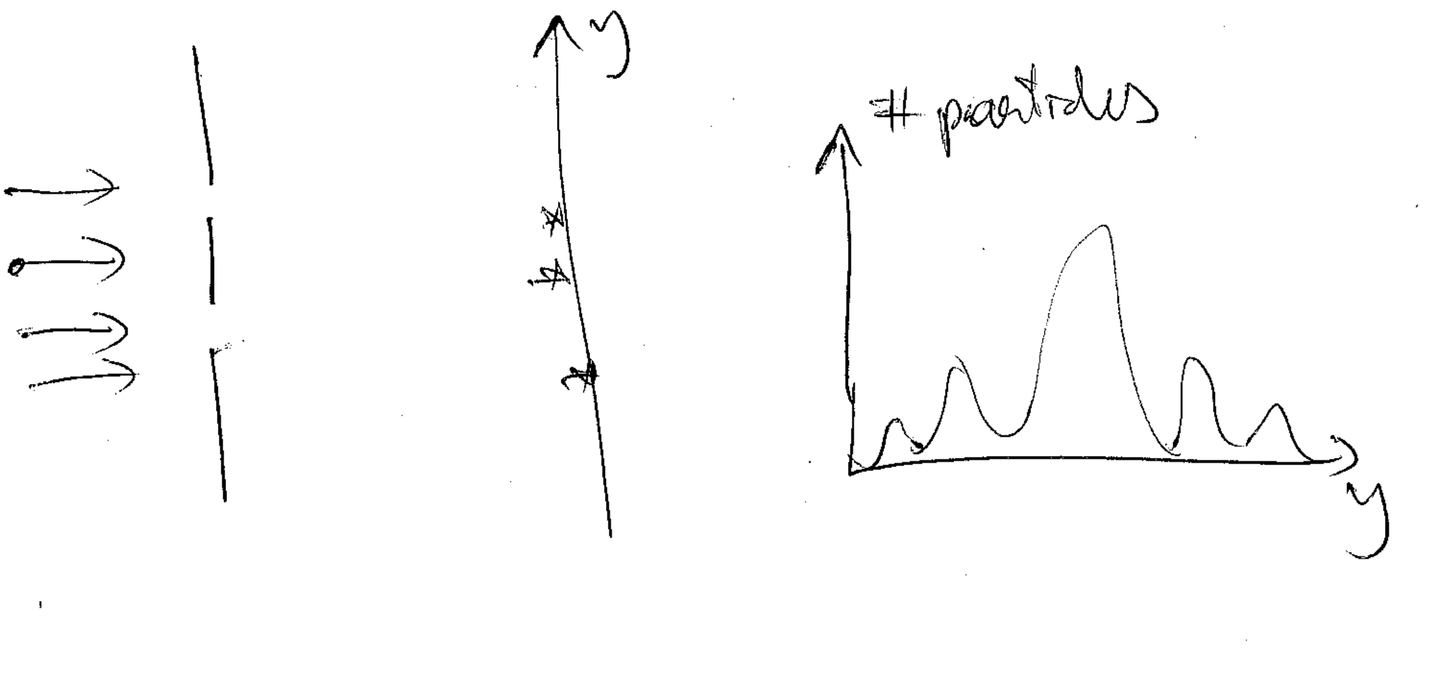
Each photon could be detected on a position on screen. (Detector array)

* Single photon → lands somewhere (probabilistic), After <u>many</u> photons land, their distribution shows interference pattern.



⇒ photons must carry / be guided by / be associated with a probability that behaves like a wave.

* <u>Electrons, helium atoms, and C_{60} molecules</u>



Conclusion: Each atom/electron goes thru both slits!!

What interferes? A The "wavefunction" or the "amplitude" associated with the two slits.

$\Psi(y)$ is complex, so can "interfere"

$$|\Psi_1(y) + \Psi_2(y)|^2 = |\Psi_1|^2 + |\Psi_2|^2 + 2\Psi_1^*\Psi_2$$

* The MEASUREMENT PROCESS

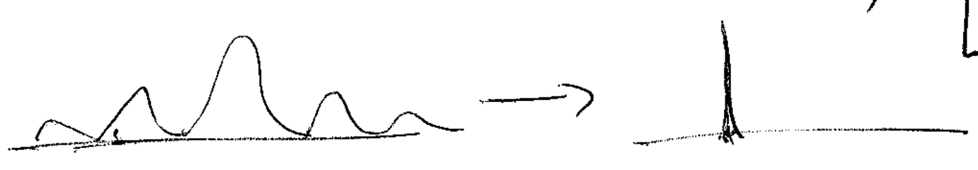
A single particle (on a line) has a probability distribution $|\Psi(x)|^2$, if wavef^n is $\Psi(x)$.

But measurement of position gives sharp value of x.

$\Rightarrow$ After measurement, ~~posit~~ w.f. is

$$\Psi(x) = \delta(x - x_0)$$

[Dirac delta function. $\boxed{\text{Look up!}}$]

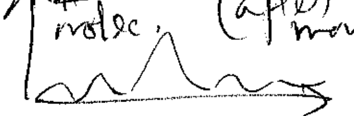


⇒ Measurement changes quantum state sharply. ("Collapse of wavefunction")

⇒ Result of individual measurement not deterministic, but probabilistic.

Ex: Interference with C_{60} molecules:

Impossible to predict exactly where first molecule will be detected. (Probabilities can be predicted)



(after many)

But, the distribution of results of many measurements can be predicted.

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* Observables as OPERATORS

In QM, observables or measureables are represented as operators. An operator acts on a wavefunction/wavevector/state and produces another w.f./state.

(1) Finite Hilbert spaces: operators are finite matrices.

matrix × vector = vector. (operator acting on state gives a state)

Ex. Spin-$\frac{1}{2}$ object.

Choose $\begin{pmatrix}1\\0\end{pmatrix}$ or $|\uparrow\rangle$ to mean spin pointing in +z direction.

$\begin{pmatrix}0\\1\end{pmatrix}$ or $|\downarrow\rangle$ ⟶ spin pointing in −z directⁿ

Then $\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$, $\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$

Each has <u>eigenvalues</u> $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$

* Eigenvalues are the possible values that a measurement can give.

WARNING!! Review Eigenvalues & Eigenvectors !!

② <u>Infinite Hilbert spaces</u>

particle in 1D : position operator $\hat{x} = x$

(Wavefunctions represented as functions of x)

$\hat{x}\Psi(x) = x\Psi(x)$ (a function of x)

Momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$

$\hat{p}\Psi(x) = -i\hbar\frac{\partial\Psi(x)}{\partial x}$ (a function of x)

Kinetic energy operator: $\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$$\hat{T}\,\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2}$$

Hamiltonian operator: $\hat{H} = \hat{T} + V(\hat{x})$

Particle in 3D: position operator $\hat{\vec{r}} = \vec{r}$

Momentum operator: $\hat{\vec{p}} = -i\hbar\vec{\nabla}$

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2 \quad \text{(Laplacian operator)}$$

* If the system is in state $|\psi\rangle$, the expectation value of an observable A (operator $\hat{A}$) is

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle \equiv \langle\psi|(\hat{A}\psi)\rangle$$

* Particle on a line: $\langle A\rangle = \int dx\, \psi^*(x)\hat{A}\psi(x)$

Example: $\langle\hat{p}\rangle$, $\langle\hat{x}\rangle$, $\langle\hat{p}^2\rangle$, $\langle\hat{x}^2\rangle$. [Reminder: $\langle\varphi|\xi\rangle = \int dx\,\varphi^*(x)\xi(x)$]

* Finite Hilbert space: $\langle A\rangle = \left(\psi_1^* \; \psi_2^* \ldots \psi_D^*\right)\begin{pmatrix} A_{11} & \cdots & A_{1D} \\ \vdots & & \vdots \\ A_{D1} & \cdots & A_{DD}\end{pmatrix}\begin{pmatrix}\psi_1 \\ \vdots \\ \psi_D\end{pmatrix}$

(27)

FIRST Do bra's & ket's a. p.33

* The Heisenberg uncertainty principle

Two variables may be impossible to measure (specify) simultaneously precisely.

Example: position & momentum

$$\Delta x \, \Delta p \sim \hbar \quad \left\{ \Delta x = \text{uncertainty in position} \right.$$

[redacted] If operators don't commute, there is an uncertainty relationship. If $\hat{A}\hat{B} \neq \hat{B}\hat{A}$,

Then $$\Delta A \, \Delta B \sim \langle |[\hat{A},\hat{B}]| \rangle \quad \left\{ [\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \right.$$

Example: for spin-$\frac{1}{2}$ system, S_x & S_z, don't [redacted] commute, so can't be measured simultaneously

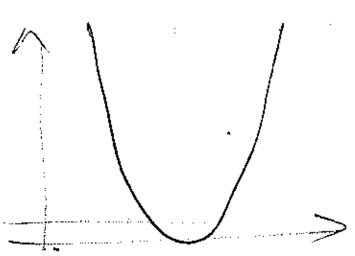
→ Defining ΔA? $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$, $\hat{A}^2 = \langle \psi | \hat{A}^2 | \psi \rangle$

$(\Delta A)^2 = \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \psi \rangle = \langle \psi | \hat{A}^2 | \psi \rangle - \langle \psi | \hat{A} | \psi \rangle^2$

→ Explains "ZERO-POINT ENERGY

[redacted]

EX. Harmonic oscillator.



$V(x) = \frac{1}{2} m \omega^2 (x - x_0)^2$

(centered at $x = x_0$)

Classical particle: lowest-energy state? Sits with zero momentum at $x = x_0$ ⇒ $\boxed{E = 0}$

$\Rightarrow$ Not possible for quantum particle.

$x = x_0$ and $p = 0$, both

can't be sharply defined $\longrightarrow$ violates Heisenberg uncertainty principle.

Quantum solution: lowest-energy state is

$$\Psi(x) \propto e^{-\frac{(x-x_0)^2}{2\sigma^2}} \quad \text{with} \quad \sigma = \sqrt{\frac{\hbar}{m\omega}} \neq 0$$

Finite spread of position, momentum.

$\Rightarrow$ Lowest possible energy is not zero: $E_0 = \frac{1}{2}\hbar\omega$

"ZERO POINT ENERGY"

~~REVIEW~~ READ: Nash, Ch. 2 (2.1–2.4 Urgent)

~~EQUATION~~ KET AND BRA

* p.33

* Hermitian conjugate / adjoint of operator.

+ hermitian operators

$M^\dagger$ is the adjoint operator / matrix of M iff

$$\langle (M^\dagger v) | w \rangle = \langle v | (M w) \rangle \quad \text{for all } |v\rangle \text{ and } |w\rangle$$

where $\langle v | w \rangle$ is the inner product.

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For finite matrices, this means $M^\dagger = (M^T)^*$

because inner product is defined as $\langle v|w\rangle = v_1^* w_1 + v_2^* w_2 + v_3^* w_3 + \ldots$

$\boxed{\rightarrow \text{Notation! } \langle (M^\dagger v)| = \langle v|M, \quad |Mv\rangle = M|v\rangle,}$

$\langle v|M|w\rangle = \langle v|(Mw)\rangle = (\langle v|M^\dagger)|w\rangle$

* Self-adjoint or hermitian matrices !

$$M^\dagger = M \iff M \text{ is hermitian}$$

$$\iff \langle (Mv)|w\rangle = \langle v|(Mw)\rangle \quad \text{for all } |v\rangle, |w\rangle$$

* In QM, observables are represented by hermitian operators.

Hermitian operators have REAL eigenvalues [Show]

(Measurements of observables should give real answers.

~~* Kett vectors $|\phi\rangle$ } think of them as vectors column vectors represent states~~

~~* Corresponding bra vector $\langle\phi|$! think of as row vector, complex-conjugated: if $|\phi\rangle = \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\end{pmatrix}$, then $\langle\phi| = (\phi_1^* \ \phi_2^* \ \phi_3^*)$~~

~~KET & BRA vectors! ϕ, $\ldots$~~

- ~~Strictly operators need to be hermitian~~, define hermitian

* **"Motivation" for single-pcle Schrödinger Equation in continuum space (+ intro plane waves)**

Schrödinger looked for a wave equation describing particles ~~particles~~ i.e. describing de Broglie waves $\lambda = \frac{h}{p}$, $f = \frac{E}{h}$ ~~associated with a particle~~ associated with particles

For "free" particles, natural to assume the waves to be "plane waves"

$$\begin{aligned} \Psi &= A \exp\left[\left(\frac{2\pi}{\lambda} x - 2\pi f t\right) i\right] \\ &= A \exp\left[i(kx - \omega t)\right] \end{aligned}$$

wave variables λ, f k, ω

We want particle variables, use $p = \hbar k$, $E = \hbar\omega$

$$\Psi = A \exp\left[\frac{ipx}{\hbar} - \frac{iEt}{\hbar}\right] = A e^{\frac{i}{\hbar}(px - Et)}$$

We want a wave eq., i.e. differential eq..

Derivative of x (t) gives factor of p (E)

$$\frac{\partial \Psi}{\partial x} = \frac{i}{\hbar} p \Psi, \quad \frac{\partial^2 \Psi}{\partial x^2} = -\frac{1}{\hbar^2} p^2 \Psi$$

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} E \Psi \quad \text{So} \quad E\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

$$\longrightarrow \quad p^2 \Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$$

(31)

A free particle (no force) : $E = \frac{p^2}{2m}$. This suggests $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi$.

Guess : In presence of potential

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

Thus Schrödinger guessed the quantum eq. for a single particle :

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = i\hbar \frac{\partial}{\partial t}\psi \quad \text{1D}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = i\hbar \frac{\partial}{\partial t}\psi \quad \text{3D}$$

Stationary SE obtained by replacing

$i\hbar \frac{\partial}{\partial t}\psi \longrightarrow E\psi$.

For 3D, using $V(\vec{r}) \propto \frac{1}{r}$ (Coulomb potential), one solves the H-atom problem.

Schrödinger found from this solution

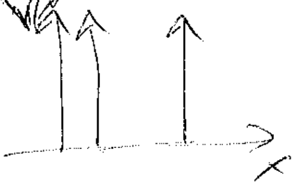
$E_n \propto \frac{1}{n^2}$ possible values of energy

$\rightarrow$ Explains H-spectrum.

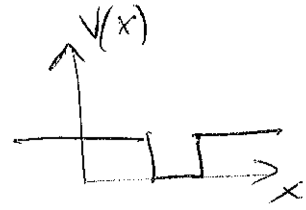
REST of the SEMESTER

* 1 particle in 1D: solution of the stationary SE in various potentials [eigenvalues, eigenstates]:

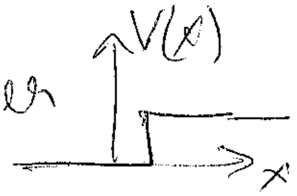
(a) $V(x)=0$ (b) box

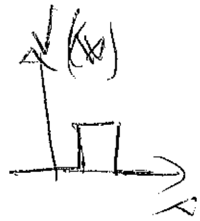


(c) finite potential well



(d) step/barrier





(e) HARMONIC OSCILLATOR

* Aspects of the formalism + list of fundamental principles "postulates"
* Spin-$\frac{1}{2}$ system, (Pauli matrices, etc.) + other finite-D systems
* Time evolution.

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* The FREE PARTICLE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$

Stationary solutions are $\psi = A e^{ipx/\hbar}$ [with $p=\sqrt{\frac{2mE}{\hbar^2}}$]

or $\psi = A\sin(px/\hbar)$ or $A\cos(px/\hbar)$ ← CHECK

or ANY COMBINATION THEREOF, with the same p. (superposition principle)

Eg. $\psi(x) = A\sin\left(\frac{px}{\hbar}\right) + B\cos\left(\frac{px}{\hbar}\right) = C\sin\left(\frac{px}{\hbar}+\delta\right)$

$\boxed{\text{Exercise : find } C, \delta \text{ in terms of } A, B}$

* Any real value of p is allowed. $E = \frac{p^2}{2m}$

$\Rightarrow$ all positive energies E correspond to a plane wave solution of the SE.

$\Rightarrow$ infinite # of eigenvalue, eigenvector pairs, as expected for ∞-dim Hilbert space.

* If particle is not confined in space, the plane-wave solutions CANNOT be normalized.

Interlude for p. 29

* ~~The SUPERPOSITION PRINCIPLE~~ Kets & Bras

* Ket vectors $|\phi\rangle$ represent states } Think of them as column vectors (might not work for ∞-dim Hilbert spaces)

* Corresponding Bra vectors $\langle\phi|$ $\rightarrow$ think as row vector with complex-conj. elements. i.e., if $|\phi\rangle = \begin{pmatrix}\phi_1\\ \phi_2\\ \phi_3\end{pmatrix}$, then $\langle\phi| = (\phi_1^* \; \phi_2^* \; \phi_3^*)$

* $\langle\phi|\psi\rangle = (\phi_1^* \; \phi_2^* \; \phi_3^* \ldots)\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \vdots\end{pmatrix} = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \phi_3^*\psi_3 + \ldots$

[could be finite or infinite sum]

* $|\phi\rangle\langle\psi| = \begin{pmatrix}\phi_1\\ \phi_2\\ \vdots\end{pmatrix}(\psi_1^* \; \psi_2^* \ldots)$ is a MATRIX ! $\leftarrow$ [Review matrix multiplic., convince yourself]

$\longrightarrow$ operators can be represented like this.