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given $|\psi\rangle(t_0) \to |\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$

$\hat{U}$: unitary time evolution operator.

Schrödinger eq-n for $\hat{U}$

$$i\hbar \frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)U(t,t_0)$$

$$\hat{U}(t=t_0) = 1$$

$\hat{H}$: Hamiltonian operator, $\hat{H}^\dagger = \hat{H}$

measures the Energy

when there are no time-dep. external forces

$\hat{H}(t) = \hat{H}$ same $\hat{H}$ $\forall t$

$$\to \hat{U}(t,t_0) = \exp\left(-i\frac{t-t_0}{\hbar}\hat{H}\right).$$

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in the eigenbasis of $\hat{H} = \sum_n |n\rangle E_n \langle n|$

$$\hat{U}(t-t_0) = \sum_n |n\rangle e^{-i\omega_n(t-t_0)}\langle n|$$

$$\omega_n = E_n/\hbar$$

For a state $|\psi\rangle$ of definite energy

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad @\ t_0 = 0.$$

$$|\psi(t>0)\rangle = |\psi(t=0)\rangle \times e^{-iEt/\hbar}$$

same phys. state up to a phase.

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$\forall$ observable A

$\langle A\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle$ is time-independent.

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \left(e^{+iEt/\hbar}\langle\psi(0)|\right)\hat{A}\left(e^{-iEt/\hbar}|\psi(0)\rangle\right)$$

$$= \langle\psi(0)|\hat{A}|\psi(0)\rangle \quad \forall t.$$

states of definite energy are

<u>stationary states</u>

To see motion, need non-stationary state

$t_0 = 0$ $\quad |\psi(0)\rangle = \sum_n c_n |n\rangle$

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

$$|\psi(t)\rangle = \sum_n c_n e^{-i\omega_n t}|n\rangle \qquad \omega_n = E_n/\hbar$$

$$\langle\psi(t)| = \sum_m c_m^* e^{+i\omega_m t}\langle m|.$$

$$\langle\psi|\hat{A}|\psi\rangle(t) = \sum_{n,m} c_m^* c_n \langle m|\hat{A}|n\rangle \times e^{-i(\omega_n-\omega_m)t}.$$

Time evolution: superposition of waves

of frequencies $|\omega_n-\omega_m|$

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Harmonic oscillator

$$E_n = \hbar\Omega(n+\tfrac{1}{2})$$

$$\omega_n = \Omega(n+\tfrac{1}{2})$$

$$\omega_n - \omega_m = \Omega(n-m)$$

$\langle m|\hat{x}|n\rangle = 0$ unless $n-m = \pm 1$

$\langle m|\hat{p}|n\rangle = 0$ " " " "

$\langle\psi|\hat{x}|\psi\rangle$ has terms with $m = n\pm 1$ only

$\rightarrow$ frequency $= |\Omega(n-m)| = |\omega_n - \omega_m|$

$= \Omega$ only.

$\rightarrow$ harmonic oscillator.

Take general $|\psi\rangle(t)$, obeys Schrödinger's

eq-n $\quad i\hbar\frac{\partial}{\partial t}|\psi\rangle(t) = \hat{H}|\psi\rangle(t)$

Take a general observable $A \rightarrow$ operator $\hat{A}$

Assume no inherent time dependence of $\hat{A}$,

only via time evolution of the quantum

states. $\Rightarrow$ time indep $\hat{A}$, same $\forall t$.

Example: in wave-function terms

$\cancel{\hat{p}\psi} = -i\hbar\frac{\partial}{\partial}$ $\hat{p}\psi(x,t) = -i\hbar\frac{\partial}{\partial x}\psi(x,t)$

same action $\forall t$.

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Time dependence of $\langle\psi|\hat{A}|\psi\rangle$.

$$\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \frac{d\langle\psi|}{dt}\cdot\hat{A}|\psi\rangle + \langle\psi|\hat{A}|\frac{d|\psi\rangle}{dt}$$

$$+ \langle\psi|\frac{d\hat{A}}{dt}|\psi\rangle$$

$$\frac{d\hat{A}}{dt} = 0$$

$$\frac{d|\psi\rangle}{dt} = \frac{1}{i\hbar}\hat{H}|\psi\rangle$$

$$\frac{d\langle\psi|}{dt} = \frac{1}{-i\hbar}\langle\psi|\hat{H} \quad \text{bec. } \hat{H}^{\dagger} = \hat{H}$$

$$\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \frac{-1}{i\hbar}\langle\psi|\hat{H}\cdot\hat{A}|\psi\rangle$$

$$+ \frac{1}{i\hbar}\langle\psi|\hat{A}\cdot\hat{H}|\psi\rangle$$

$$+ 0.$$

$$= \frac{1}{i\hbar}\langle\psi|[\hat{A},\hat{H}]|\psi\rangle.$$

Heisenberg-Dirac eq-n

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

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Suppose $\hat{H} = \frac{\vec{\hat{P}}^2}{2m} + \hat{V}$

$$\hat{V} = V(\hat{x}, \hat{y}, \hat{z}).$$

1 particle in a potential.

$\frac{d}{dt}\langle\psi|\vec{\hat{x}}|\psi\rangle$?

$$\Rightarrow \quad i\hbar\frac{d}{dt}\langle\psi|\hat{x}_i|\psi\rangle = \langle\psi|[\hat{x}_i, \hat{H}]|\psi\rangle$$

$$[\hat{x}_i, \hat{V}] = 0$$

$$[\hat{x}_i, \hat{H}] = \frac{1}{2m}[\hat{x}_i, \vec{\hat{P}}^2 = \hat{P}_j\hat{P}_j]$$

$$= \frac{1}{2m}([\hat{x}_i, \hat{P}_j]\hat{P}_j + \hat{P}_j[\hat{x}_i, \hat{P}_j])$$

$$= \frac{1}{2m}(i\hbar\delta_{ij} \times \hat{P}_j + \hat{P}_j \times i\hbar\delta_{ij})$$

$$= \frac{1}{2m}(i\hbar\hat{P}_i \times 2) = \frac{i\hbar}{m}\hat{P}_i$$

$$i\hbar\frac{d}{dt}\langle\psi|\hat{x}_i|\psi\rangle = \frac{i\hbar}{m}\langle\psi|\hat{P}_i|\psi\rangle$$

$$\boxed{\frac{d}{dt}\langle\psi|x_i|\psi\rangle = \frac{1}{m}\langle\psi|\hat{P}_i|\psi\rangle.}$$

$$\frac{d}{dt}\langle\vec{\hat{x}}\rangle = \frac{1}{m}\langle\vec{\hat{P}}\rangle.$$

$$[\hat{p}_i, \frac{\hat{p}_j\hat{p}_j}{2m}] = 0.$$

$$[\hat{p}_i, \hat{H}] = [\hat{p}, V(\hat{x},\hat{y},\hat{z})]$$

$$\Rightarrow -i\hbar(\partial_i V)(\hat{x},\hat{y},\hat{z})$$

$$i\hbar\frac{d}{dt}\langle\psi|\hat{p}_i|\psi\rangle = -i\hbar\langle\psi|\widehat{\partial_i V}|\psi\rangle$$

$$\Rightarrow \boxed{\frac{d}{dt}\langle\vec{p}\rangle = -\langle\widehat{\vec{\nabla}V}\rangle}$$

Ehrenfest eq-n

$$\boxed{m\frac{d^2}{dt^2}\langle\psi|\hat{\vec{x}}|\psi\rangle = -\langle\psi|\vec{\nabla}V(\hat{\vec{x}})|\psi\rangle}$$

3D Harmonic osc.

$$\hat{V} = \frac{1}{2}K_{ij}\hat{x}_i\hat{x}_j \qquad K_{ij} = K_{ji}$$

$$\widehat{\partial_i V} = K_{ij}\hat{x}_j$$

$$m\frac{d^2}{dt^2}\langle\psi|x_i|\psi\rangle = -K_{ij}\langle\psi|x_j|\psi\rangle$$

$\rightarrow$ Harmonic oscillator of

$$\langle\vec{x}\rangle = \langle\psi|\hat{\vec{x}}|\psi\rangle.$$

same as classical

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Non-quadratic $V(\vec{x})$

$\rightarrow$ $\partial_i V$ are non-linear in x_i

$\rightarrow$ ~~$\langle\psi|\partial_i V(\hat{\vec{x}})|\psi\rangle \neq V$~~

$$\langle\psi|\partial_i V(\hat{x},\hat{y},\hat{z})|\psi\rangle \neq V(\langle\psi|x|\psi\rangle, \langle\psi|y|\psi\rangle, \langle\psi|z|\psi\rangle)$$

For a non linear $f(x)$

$$\langle f(x)\rangle \neq f(\langle x\rangle)$$

in 3D $\langle\partial_i V(\hat{\vec{x}})\rangle \neq \partial_i V(\langle\hat{\vec{x}}\rangle)$

$$m\frac{d^2}{dt^2}\langle\hat{\vec{x}}\rangle = -\langle\vec{\nabla}V(\hat{\vec{x}})\rangle$$
$$\neq -\vec{\nabla}V(\langle\vec{x}\rangle)$$

$\rightarrow$ quantum time evolution of $\langle\vec{x}\rangle$ is different from the classical motion of $\vec{x}(t)$.

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Inherently time-dep. observables
for ex time-dep ext. force
$V(x,y,z,t) \to \hat{V}$ time-dep. operator
$\hat{V}(t) = V(\hat{x},\hat{y},\hat{z},t)$.

For such operators, Heisenberg-Dirac eq-n becomes

$$\boxed{\frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\frac{\partial\hat{A}}{\partial t}|\psi\rangle + \frac{1}{i\hbar}\langle\psi|[\hat{A},\hat{H}]|\psi\rangle}$$

Unitary Equivalence

Most General Hilbert space
Most General unitary operator $\hat{W}$, $\hat{W}^{-1} = \hat{W}^{+}$

Map all states & operators acc. to

$$(*)\quad \left.\begin{cases} |\psi\rangle \to |\psi'\rangle = \hat{W}|\psi\rangle \\ \langle\psi| \to \langle\psi'| = \langle\psi|W^{+} \\ \hat{A} \to \hat{A}' = \hat{W}\hat{A}W^{+}. \end{cases}\right\} \text{all for the same } W.$$

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Unitary equivalence (*) preserves:

1> Dirac brackets

$$\langle \psi' | \phi' \rangle = \langle \psi | \underbrace{\hat{W}^\dagger \cdot \hat{W}}_{1} | \phi \rangle = \langle \psi | \phi \rangle.$$

2> Dirac sandwiches

$$\langle \psi' | \hat{A}' | \phi' \rangle = \langle \psi | \underbrace{\hat{W}^\dagger \cdot \hat{W}}_{1} \hat{A} \underbrace{\hat{W}^\dagger \cdot \hat{W}}_{1} | \phi \rangle$$

$$= \langle \psi | \hat{A} | \phi \rangle.$$

3> Operator algebra

$$(\alpha \hat{A} + \beta \hat{B})' = W(\alpha \hat{A} + \beta B) \hat{W}^\dagger$$

$$= \alpha \hat{W} \hat{A} \hat{W}^\dagger + \beta W B W^\dagger = \alpha \hat{A}' + \beta \hat{B}'$$

$$(\hat{A}\hat{B})' = \hat{W} \hat{A} \hat{B} \hat{W}^\dagger = W \hat{A} (1 = W^\dagger W) \hat{B} W$$

$$= \hat{W} \hat{A} \hat{W}^\dagger \cdot \hat{W} \hat{B} \hat{W}^\dagger = \hat{A}' \hat{B}'$$

ditto $(\hat{B}\hat{A})' = \hat{B}' \hat{A}'$

$$([\hat{A}, \hat{B}])' = (AB)' - (BA)' = A'B' - B'A'$$

$$= [A', B'].$$

4> Hermitian conjugation

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

$$= \hat{W} \cdot A^\dagger \hat{W}^\dagger = (\hat{A}^\dagger)'$$

if $H = H^\dagger$ then $H' = H'^\dagger$

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Unitary equivalence maps eigenstates to eigenstates for same eigenvalues

If $\hat{A}|\psi\rangle = a|\psi\rangle$ then

$$\hat{A}'|\psi'\rangle = \hat{W}\hat{A}\underbrace{\hat{W}^{\dagger}\cdot\hat{W}}_{1}|\psi\rangle = \hat{W}(\hat{A}|\psi\rangle)$$

$$= \hat{W}(a|\psi\rangle) = a\,\hat{W}|\psi\rangle = a\,|\psi'\rangle.$$

Bottom line: unitary equivalence preserves the whole mathematical apparatus of Quantum Mechanics

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A time-dependent unitary equiv. $\hat{W}(t)$ changes the pictures of Q.M.

$W(t) = \hat{U}^{-1}(t, t_0)$ changes the Schrödinger picture to the Heisenberg picture.