

Schrödinger Equation

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Exam 1 average 72 >	HW #4 Due by Oct. 11
Solutions posted	Full Break Oct. 6

We now start Chapt. 2: Quantum Dynamics.
How does the state change in time?

$$t_0 \longrightarrow t > t_0$$

$$|\alpha\rangle = |\alpha, t_0\rangle \longrightarrow \underbrace{|\alpha, t_0; t\rangle}_{\text{book}} \equiv |\alpha, t\rangle$$

Time is just a parameter, not an operator
~~Time operator~~, \exists Position operator

Time Evolution Operator

$$\underbrace{|\alpha, t\rangle} = U(t, t_0) \underbrace{|\alpha, t_0\rangle}$$

$$\begin{aligned} |\alpha, t\rangle &= \sum_{a'} C_{a'}(t) |a'\rangle & |\alpha, t_0\rangle &= \sum_{a'} |a'\rangle \underbrace{\langle a' | \alpha, t_0 \rangle}_{C_{a'}(t_0)} \\ & & &= \sum_{a'} C_{a'}(t_0) |a'\rangle \end{aligned}$$

$$|C_{a'}(t)| \neq |C_{a'}(t_0)|$$

$$\text{However, } \sum_{a'} |C_{a'}(t)|^2 = \sum_{a'} |C_{a'}(t_0)|^2 = 1$$

$$\text{because } \langle \alpha, t_0 | \alpha, t_0 \rangle = \langle \alpha, t | \alpha, t \rangle = 1.$$

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This requires

$$U^\dagger(t, t_0) U(t, t_0) = I,$$

since

$$\begin{aligned} \langle \alpha, t | \alpha, t \rangle &= \langle \alpha, t_0 | \underbrace{U^\dagger(t, t_0) U(t, t_0)}_I | \alpha, t_0 \rangle \\ &= \langle \alpha, t_0 | \alpha, t_0 \rangle \end{aligned}$$

Unitarity of the time-evolution operator is intimately related to the conservation of the probability sum.

Reminder of the space translation operator

$$T_L = e^{-\frac{i p L}{\hbar}}, \quad T_L^\dagger = e^{\frac{i p L}{\hbar}}$$

$$T_L^\dagger T_L = I$$

Note also $T_{L_2} T_{L_1} = T_{L_1 + L_2}$

Similarly in time-evolution operator,

$$U(t_2, t_1) U(t_1, t_0) = U(t_2, t_0)$$

with the time sequence $t_2 > t_1 > t_0$.

As $T_{\delta x} = I - \frac{i p \delta x}{\hbar}$,
 indep. of displacement

where p (momentum) is the generator of space translation and $p = p\hat{x}$,

$U(t+\delta t, t) = I - \frac{i H \delta t}{\hbar}$,
 indep. of t

where H (Hamiltonian or energy) is the generator of time translation and $H = H\hat{t}$.

From $U(t_2, t_1)U(t_1, t_0) = U(t_2, t_0)$,
 take $t_2 = t + \delta t$ and $t_1 = t$.

Then, $U(t+\delta t, t)U(t, t_0) = U(t+\delta t, t_0)$
 $I - \frac{i H \delta t}{\hbar}$

and thus we get

$$U(t+\delta t, t_0) - U(t, t_0) = -\frac{i H \delta t}{\hbar} U(t, t_0)$$

$$\text{or } \frac{U(t+\delta t, t_0) - U(t, t_0)}{\delta t} = -\frac{i H}{\hbar} U(t, t_0)$$

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

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

Eg. (2.1.25) p. 69.

We obtained the operator equation for time-evolution. ④

$$\left[-i\hbar \frac{\partial U(t, t_0)}{\partial t} = H U(t, t_0) \right] \quad \left\{ \begin{array}{l} \text{Schrödinger Eq.} \\ \text{for the time-evolution} \\ \text{operator.} \end{array} \right.$$

Applying this to the state $|\alpha\rangle = |\alpha, t_0\rangle$,
we get

$$-i\hbar \frac{\partial U(t, t_0)}{\partial t} \underbrace{|\alpha, t_0\rangle}_{|\alpha, t\rangle} = H \underbrace{U(t, t_0) |\alpha, t_0\rangle}_{|\alpha, t\rangle}$$

$$\text{or } \left[-i\hbar \frac{\partial}{\partial t} |\alpha, t\rangle = H |\alpha, t\rangle \right] \quad \left\{ \begin{array}{l} \text{Eq. (2.1.27)} \\ \text{Schrödinger Eq.} \\ \text{for the state } |\alpha, t\rangle \end{array} \right.$$

In case H is indep. of time, then

$$U(t, t_0) = e^{-\frac{iH(t-t_0)}{\hbar}}$$

since it satisfies the Schrödinger equation for the time-evolution operator

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

and is unitary $U(t, t_0)^\dagger U(t, t_0) = I$

as well as $U(t_0, t_0) = I$ from the initial condition.

Time-Dependent Wave Equation

$$\langle \vec{x}' | \alpha, t \rangle = \psi(\vec{x}', t)$$

From $i\hbar \frac{\partial}{\partial t} |\alpha, t\rangle = H |\alpha, t\rangle$,

we get

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x}' | \alpha, t \rangle = \langle \vec{x}' | H | \alpha, t \rangle.$$

Taking $H = \frac{\vec{p}^2}{2m} + V(\vec{x})$,

we have

$$\langle \vec{x}' | \frac{\vec{p}^2}{2m} | \alpha, t \rangle = -\frac{\hbar^2}{2m} \nabla'^2 \langle \vec{x}' | \alpha, t \rangle$$

Note $\langle \vec{x}' | \vec{p} | \alpha, t \rangle = \frac{\hbar}{i} \nabla' \langle \vec{x}' | \alpha, t \rangle$

and $\langle \vec{x}' | \vec{p}^2 | \alpha, t \rangle = -\hbar^2 \nabla'^2 \langle \vec{x}' | \alpha, t \rangle$

and

$$\underbrace{\langle \vec{x}' | V(\vec{x}) | \alpha, t \rangle}_{V(\vec{x}') \langle \vec{x}' | \alpha, t \rangle} = V(\vec{x}') \langle \vec{x}' | \alpha, t \rangle$$

With $\langle \vec{x}' | \alpha, t \rangle = \psi(\vec{x}', t)$, we get

$$\boxed{i\hbar \frac{\partial}{\partial t} \psi(\vec{x}', t) = -\frac{\hbar^2}{2m} \nabla'^2 \psi(\vec{x}', t) + V(\vec{x}') \psi(\vec{x}', t)}$$

Time-Dependent Schrödinger Equation.

Wave-Mechanics: $|\psi(\vec{x}', t)|^2 = \rho(\vec{x}', t)$ probability density

$$\int d^3\vec{x}' \rho(\vec{x}', t) = \int d^3\vec{x}' |\psi(\vec{x}', t)|^2 = \int d^3\vec{x}' \langle \alpha, t | \vec{x}' \rangle \langle \vec{x}' | \alpha, t \rangle = \langle \alpha, t | \alpha, t \rangle = 1$$