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☆ Problems with Time-independent Hamiltonians

Given the initial state $|\psi(t_0)\rangle$, it is possible to give an explicit solution for a later time in terms of the eigenstates & eigenvalues of the Hamiltonians

eigenstate & eigenvalues n (a collective labeling, could include many indices.)

$$H|n\rangle = E_n|n\rangle$$

either discrete, continuous, or even mixed spectrum

$$|\psi(t)\rangle = \sum_n c_n(t)|n\rangle$$

$$\Rightarrow \quad i\hbar \frac{d}{dt} c_n(t) = E_n c_n(t)$$

or $\quad c_n(t) = e^{-i\frac{E_n t}{\hbar}} c_n(0)$

$$\Rightarrow \quad |\psi(t)\rangle = \sum_n e^{-i\frac{E_n t}{\hbar}} c_n(0)|n\rangle, \qquad c_n(0) = \langle n|\psi(0)\rangle$$

One can use it to expand the time evolution operator

$$U(t) = e^{-i\frac{Ht}{\hbar}} = \sum_n |n\rangle e^{-i\frac{E_n t}{\hbar}} \langle n|$$

* usual procedure: ① find the eigenfunctions of the H
② compute $c_n(0)$
③ get the $U(t)$

☆ If the system is known to be in an energy eigenstate at $t=0$

$\Rightarrow$ it stays in this state forever!!

just a time-dependent phase $e^{-i\frac{E_n t}{\hbar}}$

$\Rightarrow$ energy eigenstate is called "stationary state".

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[Particle in a potential]

Hamiltonian is the time evolution generator, but what is it?

particle mass m, in a potential $V(x,t)$

In Newton's mechanics

$$m\vec{a} = -\vec{\nabla} V(x,t)$$

& in CM, $$H = \frac{p^2}{2m} + V(x,t)$$

To go to QM, we promote the $\hat{x}$ and $\hat{p}$ to operators.
can work in the
position eigenkets $|x\rangle$ $\sim$ isomorphic to W.F. $\psi(x)$

$$[\hat{x}_i, \hat{p}_j] = i\hbar\,\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0$$

$QM \xrightarrow{\hbar \to 0} CM$. so we need to guess what $\hat{H}$ is.

* only experiment ~~has~~ the final say. (maybe with the help of CM)
* However, since $QM \supset CM$, there is no logical deduction to obtain QM from CM.

(* N-particle, mass m_i, position x_i, and momentum p_i

$$H_{CM} = \sum_i^N \frac{p_i^2}{2m_i} + V(x_1 \dots x_N) \Big)$$

* Schrödinger Eq. $\psi(x,t) = \langle x|\psi(t)\rangle$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,t) + V(x,t)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

$$\Big(\underline{\langle x|\, i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle} = \langle x|\, \underline{\hat{H}(t)|\psi(t)\rangle} \Big)$$

and $\langle x|p^n|\psi\rangle = (-i\hbar)^n\frac{\partial^n}{\partial x^n}\langle x|\psi\rangle$

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If the $V(x,t) = V(x)$, we often wish to find $\psi_n(x) = \langle x|n\rangle$ the eigenfunction

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\psi_n(x) = E_n\psi_n(x)$$

In the momentum space, if $V(x,t) = V(x)$

just a multiplicative operator

$$\Rightarrow \frac{p^2}{2m}\phi_n(\vec{p}) + \int d^3\vec{p}\,'\ \underbrace{\tilde{V}(\vec{p}-\vec{p}\,')\ \phi_n(\vec{p}\,')}_{} = E_n\phi_n(\vec{p})$$

where $\phi_n(\vec{p}) = \langle\vec{p}|n\rangle$ $\Rightarrow$ becomes an integral operator

and $$\tilde{V}(\vec{p}) = \int\frac{d^3x}{(2\pi\hbar)^3}\, e^{-i\frac{\vec{p}\cdot\vec{x}}{\hbar}}\, V(\vec{x})$$

$\boxed{\text{Probability density \& current}}$

consider a single particle moving in a 3-D potential V.

$\underline{\rho(x,t)} \equiv |\psi(x,t)|^2$ ~~dens~~ probability density finding the particle at $\vec{x}$ and time t

may be time dependent, but

$$\int d^3\vec{x}\,\rho(\vec{x},t) = \int d\vec{x}\,|\psi(x,t)|^2 = \int d^3\vec{x}\,\langle\psi(t)|\vec{x}\rangle\langle\vec{x}|\psi(t)\rangle$$

$= \langle\psi(t)|\psi(t)\rangle = 1$ is always hold.

due to the unitarity of $U(t,t_0)$

Associated with $\rho(x,t)$, is the $\underline{\text{probability current}}$ $\vec{J}(x,t)$ such that

$$\nabla\cdot\vec{J} + \frac{\partial\rho}{\partial t} = 0$$

$\vec{J}$ is usually expressed in terms of the velocity operator

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In the position representation

$$\hat{\vec{V}} = \frac{1}{m}\hat{\vec{P}} = -\frac{i\hbar}{m}\vec{\nabla}$$

$$\Rightarrow \vec{J}(\vec{x},t) = \frac{1}{2}\left[\psi^*(x,t)\,\vec{V}\,\psi(x,t) + \psi(x,t)\,\vec{V}^*\psi^*(x,t)\right]$$

$$\psi^* \times \left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial}{\partial t}\psi\right)$$

$$- \psi \times \left(-\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* = -i\hbar\frac{\partial}{\partial t}\psi^*\right)$$

$$-\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) + \underbrace{\left(\psi^* V\psi - \psi V\psi^*\right)}_{=0} = i\hbar\frac{\partial}{\partial t}(\psi^*\psi)$$

0 because V is real

$$\Rightarrow -\frac{\hbar}{2m}\left(\psi^*\vec{\nabla}_i\vec{\nabla}_i\psi - \psi\vec{\nabla}_i\vec{\nabla}_i\psi^*\right) = i\frac{\partial}{\partial t}(\psi^*\psi)$$

$$\Rightarrow -\frac{\hbar}{2m}\vec{\nabla}_i\left(\psi^*\vec{\nabla}_i\psi - \psi\vec{\nabla}_i\psi^*\right) = i\frac{\partial}{\partial t}(\psi^*\psi)$$

$$\Rightarrow -\frac{\hbar}{2m}\nabla\cdot\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) = i\frac{\partial}{\partial t}(\psi^*\psi)$$

$$\Rightarrow \frac{\partial}{\partial t}(\psi^*\psi) \underbrace{- \frac{i\hbar}{2m}\nabla\cdot\left(\psi^*\vec{\nabla}\psi - \psi(\vec{\nabla}\psi^*)\right)}_{=\, +\frac{1}{2}\nabla\cdot\left(\psi^*\vec{V}\psi - \psi\vec{V}\psi^*\right)} = 0$$

$\star$ Note, if $\psi(x,t)$ is an energy eigenfunction $\psi_n(x)e^{-i\frac{E_n t}{\hbar}}$

$\Rightarrow \vec{J} = 0$, $\rho = |\psi_n(\vec{x})|^2$ is a constant.

$\star$ single particle in 3D, $\vec{J}$ is a 3-vector.

N " " " $3N$-vector

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physical meaning of ρ & $\vec{J}$

ρ is clear based on the postulates of QM.

Note; we should not think that the particle in an individual system has been smeared around in space.

For a charged particle, we never get a fractional charge !!

If we multiply both ρ & $\vec{J}$ by the charge of the particle

$$\rho_c = q\rho, \quad \vec{J}_c = q\vec{J}$$

then $\nabla\cdot\vec{J}_c + \frac{\partial \rho_c}{\partial t} = 0 \Rightarrow$ conservation of charge.

or Statistical interpretation, dipole field of H-atom → Gauss law electric field.

If we write $\psi(x,t) = \sqrt{\rho(x,t)}\, \exp\left(\frac{i S(x,t)}{\hbar}\right)$

then
$$\vec{J} = \frac{1}{2}\left\{ \psi^* \frac{-i\hbar}{m}\vec{\nabla}\left(\sqrt{\rho}\, e^{\frac{iS}{\hbar}}\right) - \psi\left(\frac{-i\hbar}{m}\vec{\nabla}\left(\sqrt{\rho}\, e^{\frac{-iS}{\hbar}}\right)\right)\right\}$$

$$= \frac{-i\hbar}{2m}\left(\sqrt{\rho}\, e^{\frac{-iS}{\hbar}}\left(\cancel{\frac{\vec{\nabla}\rho}{2\sqrt{\rho}}\, e^{\frac{iS}{\hbar}}} + \sqrt{\rho}\, e^{\frac{iS}{\hbar}}\, \frac{i}{\hbar}\vec{\nabla}S\right) - \sqrt{\rho}\, e^{\frac{+iS}{\hbar}}\left(\cancel{\frac{\vec{\nabla}\rho}{2\sqrt{\rho}}\, e^{\frac{-iS}{\hbar}}} + \sqrt{\rho}\, e^{\frac{-iS}{\hbar}}\, \frac{-i}{\hbar}\vec{\nabla}S\right)\right)$$

$$= \frac{\rho}{m}\vec{\nabla}S$$

direction of $\vec{J}$ is <u>normal</u> to the surface of a const phase

& the stronger the phase variation the more intense flux,

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Classical limit

$$-\frac{\hbar^2}{2m}\nabla^2\left(\sqrt{\rho}\,e^{\frac{iS}{\hbar}}\right)+V\sqrt{\rho}\,e^{\frac{iS}{\hbar}} = i\hbar\frac{\partial}{\partial t}\left(\sqrt{\rho}\,e^{\frac{iS}{\hbar}}\right)$$

$$-\frac{\hbar^2}{2m}\nabla\cdot\left(\frac{\vec\nabla\rho}{2\sqrt{\rho}}e^{\frac{iS}{\hbar}}+\frac{i}{\hbar}\sqrt{\rho}\,e^{\frac{iS}{\hbar}}\vec\nabla S\right) \qquad i\hbar\left(\frac{\frac{\partial\rho}{\partial t}}{2\sqrt{\rho}}e^{\frac{iS}{\hbar}}+\frac{i}{\hbar}\sqrt{\rho}\,e^{\frac{iS}{\hbar}}\frac{\partial S}{\partial t}\right)$$

$$=-\frac{\hbar^2}{2m}\left(\frac{\nabla^2\rho}{2\sqrt{\rho}}e^{\frac{iS}{\hbar}}-\frac{(\vec\nabla\rho)^2}{4\rho^{\frac{3}{2}}}e^{\frac{iS}{\hbar}}+\frac{i}{\hbar}\frac{\vec\nabla\rho\cdot\vec\nabla S}{2\sqrt{\rho}}\right.$$

$$\left.+\frac{i}{\hbar}\frac{\vec\nabla\rho\cdot\vec\nabla S}{2\sqrt{\rho}}e^{\frac{iS}{\hbar}}-\frac{1}{\hbar^2}\sqrt{\rho}\,e^{\frac{iS}{\hbar}}(\vec\nabla S)^2+\frac{i}{\hbar}\sqrt{\rho}\,e^{\frac{iS}{\hbar}}\nabla^2 S\right)$$

In the $\hbar\to 0$ limit
We drop everything associated with $\hbar$!

$$\Rightarrow\quad +\frac{\sqrt{\rho}}{2m}e^{\frac{iS}{\hbar}}(\vec\nabla S)^2+V\sqrt{\rho}\,e^{\frac{iS}{\hbar}} = -\sqrt{\rho}\,e^{\frac{iS}{\hbar}}\frac{\partial S}{\partial t}$$

or
$$\boxed{\frac{(\vec\nabla S)^2}{2m}+V+\frac{\partial S}{\partial t}=0}$$

This is exactly the Hamilton - Jacobi equation in CM!!

(recall that, in CM,
$$p_i=\frac{\partial S}{\partial q_i},\qquad E=-\frac{\partial S}{\partial t}$$
)

More about this will be discussed in the WKB section.

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