

② General approach to the solution:

Let's first assume that $H(\vec{x}, \vec{p})$ has no explicit time dependence.

Then solve $i\hbar |\dot{\psi}\rangle = \hat{H} |\psi\rangle$

by first solving the eigenvalue problem for \hat{H} :

$$\hat{H} |E\rangle = E |E\rangle$$

Then we expand

$$|\psi(t)\rangle = \sum_E |E\rangle \underbrace{\langle E|\psi(t)\rangle}_{a_E(t)} = \sum_E a_E(t) |E\rangle$$

Insert into S-Eq:

$$\sum_E i\hbar \frac{da_E(t)}{dt} |E\rangle = \sum_E a_E(t) E |E\rangle$$

Project on $\langle E'|$ and use $\langle E|E'\rangle = \delta(E, E')$ (Kronecker δ for discrete E , Dirac- δ for continuous E)

Use $\delta(E, E')$ to kill \sum_E :

$$i\hbar \dot{a}_E(t) = E a_E(t) \Rightarrow \boxed{a_E(t) = a_E(0) e^{-iEt/\hbar}}$$

$(a_E(0) = \langle E|\psi(0)\rangle)$

$$\Rightarrow |\psi(t)\rangle = \sum_E a_E(t) |E\rangle = \sum_E |E\rangle \langle E|\psi(0)\rangle e^{-iEt/\hbar}$$

or

$$\boxed{|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle}$$

with
$$\hat{U}(t) = \sum_E |E\rangle \langle E| e^{-iEt/\hbar}$$

If the eigenstates E are degenerate:

$$\boxed{\hat{U}(t) = \sum_E e^{-iEt/\hbar} \sum_{\alpha=1}^{d_E} |E, \alpha\rangle \langle E, \alpha|}$$

($d_E =$ degeneracy of eigenvalue E)

The normal modes $|E(t)\rangle \equiv |E\rangle e^{-iEt/\hbar}$

are called stationary states: For any time-independent

observable $\hat{\Omega}$, the probability distribution $P(\omega)$ is time-independent in such states:

$$P(\omega, t) = |\langle \omega | E(t) \rangle|^2 = |\langle \omega | E \rangle e^{-iEt/\hbar}|^2 = |\langle \omega | E \rangle|^2 \\ = P(\omega, t=0)$$

We can also write $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ (if \hat{H} does not depend

on time explicitly:

$$e^{-i\hat{H}t/\hbar} = e^{-i\hat{H}t/\hbar} \int_E |E\rangle \langle E| \\ = \int_E \left(e^{-i\hat{H}t/\hbar} |E\rangle \right) \langle E| = \int_E \left(\sum_{n=0}^{\infty} \frac{(-i\hat{H}t/\hbar)^n}{n!} |E\rangle \right) \langle E| \\ = \int_E \left(\underbrace{\sum_{n=0}^{\infty} \frac{(-iEt/\hbar)^n}{n!}}_{e^{-iEt/\hbar}} |E\rangle \right) \langle E| = \int_E |E\rangle \langle E| e^{-iEt/\hbar} \checkmark$$

This expression is very useful. Since $\hat{H} = \hat{H}^\dagger$, $\hat{U}^\dagger(t) = \hat{U}^{-1}(t)$ is unitary \rightarrow "unitary time evolution"

\Rightarrow Time evolution of $|\psi(t)\rangle =$ rotation of $|\psi\rangle$ in Hilbert space.

such that $\langle \psi(t) | \psi(t) \rangle = \langle \psi(0) | \hat{U}^\dagger(t) \hat{U}(t) | \psi(0) \rangle \\ = \langle \psi(0) | \psi(0) \rangle =$ is time-independent.

If instead of the fixed basis $|E\rangle$ with use rotating basis

vectors $|E(t)\rangle = \hat{U}(t)|E\rangle = e^{-iEt/\hbar}|E\rangle$, then

$$|\psi(t)\rangle = \int_E a_E(0) e^{-iEt/\hbar} |E\rangle = \int_E a_E(0) |E(t)\rangle$$

has time independent components, i.e. it appears frozen

Instead, the operators $\hat{\Omega}$ would now become time dependent:

$$\begin{aligned} \langle \varphi(t) | \hat{\Omega} | \psi(t) \rangle &= \langle \varphi(0) | \hat{U}^\dagger(t) \hat{\Omega} \hat{U}(t) | \psi(0) \rangle \\ &= \langle \varphi(0) | \hat{\Omega}(t) | \psi(0) \rangle \end{aligned}$$

Instead of the Schrödinger eq. of motion for $|\psi(t)\rangle$ this view results in a Heisenberg equation of motion for $\hat{\Omega}(t) \rightarrow$ "Heisenberg picture"

The view where $|\psi(t)\rangle$ obeys the S-Eq. is called "Schrödinger picture"

Other pictures are possible, too, and in some cases useful — see chapter 18.

What if $\hat{H} = \hat{H}(t)$ depends explicitly on t ?

Let's look at the evolution $|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle$ over time t , by dividing t into N ($N \rightarrow \infty$) pieces of length $\Delta = \frac{t}{N}$ ($\Delta \rightarrow 0$).

$$\Rightarrow |\psi(\Delta)\rangle = |\psi(0)\rangle + \Delta \left. \frac{d|\psi\rangle}{dt} \right|_{t=0} + O(\Delta^2)$$

As $N \rightarrow \infty, \Delta \rightarrow 0$, we can ignore the terms of $O(\Delta^2)$.

$$\begin{aligned} &= |\psi(0)\rangle - \frac{i}{\hbar} \Delta \hat{H}(0) |\psi(0)\rangle \\ &= \left(1 - \frac{i}{\hbar} \hat{H}(0) \Delta \right) |\psi(0)\rangle \approx e^{-i\hat{H}(0)\Delta/\hbar} |\psi(0)\rangle \end{aligned}$$

where the last approximation is again accurate to $O(\Delta)$ and becomes exact in the limit $\Delta \rightarrow 0$.

Also, if we replace $\hat{H}(0)$ by $\hat{H}(\Delta)$ or $\hat{H}(\frac{\Delta}{2})$, the difference is of order Δ , so in $(1 - \frac{i\Delta}{2}\hat{H})$ the difference is only of order Δ^2 and thus negligible.

Repeating this procedure to get from time Δ to time 2Δ etc.

We get

$$\boxed{|\psi(t)\rangle = \prod_{n=0}^{N-1} e^{-i\Delta \hat{H}(n\Delta)/\hbar} |\psi(0)\rangle}$$

$$\neq e^{-\frac{i}{\hbar} \Delta \sum_{n=0}^{N-1} \hat{H}(n\Delta)} |\psi(0)\rangle$$

$$\left(\begin{array}{l} \Delta \rightarrow 0 \\ \rightarrow \\ N \rightarrow \infty \end{array} e^{-\frac{i}{\hbar} \int_0^t dt' \hat{H}(t')} |\psi(0)\rangle \right)$$

The step labelled by \neq is not allowed since $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$ in general. The correct result is the box. One denotes its limit as $N \rightarrow \infty, \Delta \rightarrow 0$ by the so-called time-ordered integral

$$\hat{T} e^{-\frac{i}{\hbar} \int_0^t dt' \hat{H}(t')} \equiv \lim_{N \rightarrow \infty} \prod_{n=0}^{N-1} e^{-\frac{i}{\hbar} \hat{H}(\frac{n}{N}t) \frac{t}{N}} \equiv \hat{U}(t, 0)$$

On the r.h.s. the factors are ordered by time argument of \hat{H} .

Note that, as a product of unitary operators, $\hat{U}(t)$ is still unitary. It satisfies

$$\hat{U}(t_3, t_2) \hat{U}(t_2, t_1) = \hat{U}(t_3, t_1)$$

$$\hat{U}^\dagger(t_2, t_1) = \hat{U}^{-1}(t_2, t_1) = \hat{U}(t_1, t_2)$$

Basis choice:

To set up the eigenvalue problem, we have to convert the operator \hat{H} into a matrix. So we need a basis in which we can work out the matrix elements. Since $\hat{H} = \hat{H}(\hat{X}, \hat{P})$, the coordinate or momentum eigenkets recommend themselves (either/or!). If we choose the x -basis, we can simply replace

$$|\psi\rangle \longrightarrow \psi(x) = \langle x | \psi \rangle$$

$$\hat{X} \longrightarrow x$$

$$\hat{P} \longrightarrow -i\hbar \frac{d}{dx}$$

$$\hat{H}(\hat{X}, \hat{P}) |E\rangle = E |E\rangle \longrightarrow H(x, -i\hbar \frac{d}{dx}) \psi_E(x) = E \psi_E(x)$$

So the eigenvalue problem for

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{\cosh^2 \hat{X}}$$

becomes in the x -basis

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{\cosh^2 x} \right) \psi_E(x) = E \psi_E(x) \quad (*)$$

In the $|p\rangle$ -basis we would substitute

$$|\psi\rangle \longrightarrow \psi(p) = \langle p | \psi \rangle$$

$$\hat{X} \longrightarrow i\hbar \frac{d}{dp}$$

$$\hat{P} \longrightarrow p$$

$$\hat{H}(\hat{X}, \hat{P}) |E\rangle = E |E\rangle \longrightarrow H(i\hbar \frac{d}{dp}, p) \psi_E(p) = E \psi_E(p)$$

For the above H this gives

$$\left[\frac{p^2}{2m} + \frac{1}{\cosh^2\left(i\hbar \frac{d}{dp}\right)} \right] \psi_E(p) = E \psi_E(p) \quad (**)$$

In both cases the eigenvalue problem has turned into a differential equation. Obviously, $(**)$ is more frightening than $(*)$. This is because the potential $\hat{V}(\hat{X}) = \frac{1}{\cosh^2 \hat{X}}$ is a more complicated function of \hat{X} than the kinetic energy $\hat{T} = \frac{\hat{P}^2}{2m}$ is of \hat{P} . You will probably want to choose a basis that immediately diagonalizes the most complicated part of the Hamiltonian.

As another example, let's look at a particle in a constant force field:

$$H(\hat{X}, \hat{P}) = \frac{\hat{P}^2}{2m} - f \hat{X}$$

In x -basis:
$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_E(x)}{dx^2} - f x \psi_E(x) = E \psi_E(x) \quad (*)$$

In p -basis:
$$\frac{p^2}{2m} \psi_E(p) - i\hbar f \frac{d\psi_E(p)}{dp} = E \psi_E(p)$$

$$\Rightarrow \frac{d\psi_E(p)}{dp} = \frac{i}{\hbar f} \left(E - \frac{p^2}{2m} \right) \psi_E(p)$$

In this case the first order differential equation for $\psi_E(p)$ is easier to solve than the second order differential equation for $\psi_E(x)$. However, if the problem specifies boundary conditions for $\psi_E(x)$, we still must compute $\psi_E(x)$ - by Fourier transformation or by solving $(*)$. The harmonic oscillator is solved equally easily in both the x - and p -bases. But there is a third basis which makes the solution still easier! (See Chapter 7).