Quantum Dynamics Notes

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The time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t) = (\hat{T}+\hat{V})\Psi(x,t)$$

If using atomic unit, $\hbar = 1$, the time-dependent Schrödinger equation becomes:

$$i\frac{\partial\Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t) = (\hat{T}+\hat{V})\Psi(x,t)$$

In Dirac notion, the wave function can be expressed as

$$\langle x|\Psi(t)\rangle = \Psi(x,t)$$
$$\langle \phi_i|\Psi(t)\rangle = c_i$$

Orthogonal Relation:

$$\langle \psi_i|\psi_j\rangle = \delta_{ij}$$
$$\langle x_i|x_j\rangle = \delta(x_i - x_j)$$

Closure Relation:

$$\sum_i |\psi_i\rangle\langle\psi_i| = 1$$
$$\int dx\,|x\rangle\langle x| = 1$$

If $\langle\psi_i|\psi_j\rangle = S_{ij}$, S_{ij} has a specific value, which correspond to the overlap. Using orthogonal and closure relation, it is easy to compute scalar product:

A. In discrete form

$$\begin{aligned}\langle\Psi|\Psi\rangle &= \left\langle \Psi\right|\left[\int dx\,|x\rangle\langle x|\right]\left|\Psi\right\rangle \\ &= \int dx\,\langle\Psi|x\rangle\langle x|\Psi\rangle \\ &= \int dx\Psi^*(x)\Psi(x) = 1\end{aligned}$$

B. In continue form

$$\begin{aligned}\langle\Psi|\Psi\rangle &= \left\langle \Psi\right|\left[\sum_i |\psi_i\rangle\langle\psi_i|\right]\left|\Psi\right\rangle \\ &= \sum_i \langle\Psi|\psi_i\rangle\langle\psi_i|\Psi\rangle \\ &= \sum c_i^* c_i = 1\end{aligned}$$

The effect of operator:

A. Single Operator

$$\begin{aligned}\hat{O}|\Psi\rangle &= \hat{O}\left[\sum_i |\psi_i\rangle\langle\psi_i|\right]|\Psi\rangle \\ &= \sum_i \hat{O}|\psi_i\rangle\langle\psi_i|\Psi\rangle \\ &= \sum_i \hat{O}|\psi_i\rangle c_i \\ \langle\psi_j|\hat{O}|\Psi\rangle &= \sum_i \langle\psi_j|\hat{O}|\psi_i\rangle c_i\end{aligned}$$

B. Many Operator

$$\begin{aligned}\langle\psi_i|\,\hat{A}\hat{B}\hat{C}\,|\psi_i\rangle &= \langle\psi_i|\,\hat{A}\left[\sum_m \left|\psi_m^{'}\right\rangle\left\langle\psi_m^{'}\right|\right]\hat{B}\left[\sum_l \left|\psi_l^{'}\right\rangle\left\langle\psi_l^{'}\right|\right]\hat{C}\,|\psi_i\rangle \\ &= \sum_{ml}\langle\psi_i|\,\hat{A}\left|\psi_m^{'}\right\rangle\left\langle\psi_m^{'}\right|\hat{B}\left|\psi_l^{'}\right\rangle\left\langle\psi_l^{'}|\hat{C}|\psi_i\right\rangle\end{aligned}$$

C. Trace

$$\begin{aligned}Tr\{\hat{A}\hat{B}\hat{C}\hat{\rho}\} &= \sum_i\langle\psi_i|\,\hat{A}\hat{B}\hat{C}\hat{\rho}\,|\psi_i\rangle \\ &= \sum_i\langle\psi_i|\,\hat{A}\left[\sum_j|\psi_j^{'}><\psi_j^{'}|\right]\hat{B}\left[\sum_k|\psi_k^{'}><\psi_k^{'}|\right]\hat{C}\left[\sum_l|\psi_l^{'}><\psi_l^{'}|\right]\hat{\rho}\,|\psi_i\rangle \\ &= \sum_{ijkl}\langle\psi_i|\,\hat{A}|\psi_j^{'}><\psi_j^{'}|\hat{B}|\psi_k^{'}><\psi_k^{'}|\hat{C}|\psi_l^{'}><\psi_l^{'}|\hat{\rho}\,|\psi_i\rangle \\ &= \sum_{ijkl}A_{ij}B_{jk}C_{kl}\rho_{li} \\ &= \sum_{ijkl}\rho_{li}A_{ij}B_{jk}C_{kl} \\ &= Tr\{\hat{\rho}\hat{A}\hat{B}\hat{C}\} = Tr\{\hat{C}\hat{\rho}\hat{A}\hat{B}\} = Tr\{\hat{B}\hat{C}\hat{\rho}\hat{A}\}\end{aligned}$$

D. Commute

$$\begin{aligned}[\hat{x},\hat{p}]\,|\psi_i\rangle &= \hat{x}\hat{p}\,|\psi_i\rangle - \hat{p}\hat{x}\,|\psi_i\rangle \\ &= i\hbar x\frac{\partial}{\partial x}\,|\psi_i\rangle - i\hbar\frac{\partial}{\partial x}(x\,|\psi_i\rangle) \\ &= i\hbar x\frac{\partial}{\partial x}\,|\psi_i\rangle - i\hbar\,|\psi_i\rangle - i\hbar x\frac{\partial}{\partial x}\,|\psi_i\rangle \\ [\hat{x},\hat{p}] &= i\hbar\end{aligned}$$

E. The Function of Operator

$$\begin{aligned}\langle\psi_j|\,f(\hat{A})\,|\Psi\rangle &= \langle\psi_j|\,f(\hat{A})\left[\sum_i|\psi_i><\psi_i|\right]|\Psi\rangle \\ &= \sum_i\langle\psi_j|\,f(\hat{A})\,|\psi_i\rangle\,\langle\psi_i|\Psi\rangle \\ &= \sum_i\langle\psi_j|\left[1+f_1\hat{A}+\frac{1}{2!}f_2\hat{A}^2+\cdots\right]|\psi_i\rangle\,\langle\psi_i|\Psi\rangle\end{aligned}$$

where $f(\hat{A})$ is defined as

$$f(\hat{A}) = \sum_{n=0}^{\infty} f_n\hat{A}^n$$

Solve time-dependent Schrödinger equation:
I) General form

$$\begin{aligned}i\frac{\partial}{\partial t}\,|\Psi(t)\rangle &= \hat{H}\,|\Psi(t)\rangle \\ i\frac{\partial}{\partial t}\,\langle\psi_i|\Psi(t)\rangle &= \langle\psi_i|\,\hat{H}\,|\Psi(t)\rangle \\ i\frac{\partial}{\partial t}\,\langle\psi_i|\Psi(t)\rangle &= \langle\psi_i|\,\hat{H}\left[\sum_j|\psi_j><\psi_j|\right]|\Psi(t)\rangle \\ i\frac{\partial}{\partial t}\,\langle\psi_i|\Psi(t)\rangle &= \sum_j\langle\psi_i|\,\hat{H}\,|\psi_j\rangle\,\langle\psi_j|\Psi(t)\rangle \rightarrow c_j(t) = \langle\psi_j|\Psi(t)\rangle \\ i\frac{\partial}{\partial t}c_i(t) &= \sum_j\langle\psi_i|\,\hat{H}\,|\psi_j\rangle\,c_j(t) \rightarrow H_{ij} = \langle\psi_i|\,\hat{H}\,|\psi_j\rangle \\ i\frac{\partial}{\partial t}c_i(t) &= \sum_j H_{ij}c_j(t)\end{aligned}$$

A. Runge-Kutta Method (4th or 6th)

$$\begin{aligned}
\frac{\partial}{\partial t}y &= f(t,y), \quad y(t_0) = y_0 \\
y_{n+1} &= y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
k_1 &= f(t_n, y_n) \\
k_2 &= f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1) \\
k_3 &= f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2) \\
k_4 &= f(t_n + \frac{h}{2}, y_n + hk_3)
\end{aligned}$$

B. Euler Method

$$\begin{aligned}
\frac{c_i(t+\Delta t) - c_i(t)}{\Delta t} &= -i\sum_j H_{ij}c_j(t) \\
c_i(t+\Delta t) - c_i(t) &= -i\sum_j H_{ij}c_j(t)\Delta t \\
c_i(t+\Delta t) &= c_i(t) - i\sum_j H_{ij}c_j(t)\Delta t
\end{aligned}$$

Problem:
1. $\sum_i |c_i|^2 \neq 1$
2. Need small Δt
II) Eigenstate

$$\begin{aligned}
i\frac{\partial}{\partial t}c_i(t) &= \sum_j \langle\psi_i|\,\hat{H}\,|\psi_j\rangle\, c_j(t) \rightarrow \hat{H}\,|\psi_j\rangle = E_j\,|\psi_j\rangle \\
i\frac{\partial}{\partial t}c_i(t) &= \sum_j E_j\delta_{ij}c_j(t) \\
i\frac{\partial}{\partial t}c_i(t) &= E_i c_i(t) \\
c_i(t) &= e^{-iE_i(t-t_0)}c_i(t_0) \\
|\Psi(t)\rangle &= \sum_j c_j(t)\,|\psi_j(t_0)\rangle \\
&= \sum_j e^{-iE_j(t-t_0)}c_j(t_0)\,|\psi_j(t_0)\rangle \quad Where \quad \sum_j c_j(t_0)\,|\psi_j(t_0)\rangle = |\Psi(t_0)\rangle
\end{aligned}$$

If the matrix of H under an arbitary basis is known, then eigenvalue can be obtained by

$$\begin{aligned}
\hat{H}\,|\psi_j\rangle &= E_j\,|\psi_j\rangle \\
\left\langle\psi'_m\right|\hat{H}\,|\psi_j\rangle &= E_j\left\langle\psi'_m|\psi_j\right\rangle \\
\left\langle\psi'_m\right|\hat{H}\left[\sum_n |\psi'_n><\psi'_n|\right]|\psi_j\rangle &= E_j\left\langle\psi'_m|\psi_j\right\rangle \\
\sum_n \left\langle\psi'_m|\hat{H}|\psi'_n\right\rangle\left\langle\psi'_n|\psi_j\right\rangle &= E_j\left\langle\psi'_m|\psi_j\right\rangle \rightarrow C_{mj} = \left\langle\psi'_m|\psi_j\right\rangle \quad H_{mn} = \left\langle\psi'_m|\hat{H}|\psi'_n\right\rangle \\
HC &= CE
\end{aligned}$$

Or

$$
\begin{aligned}
\left\langle \psi_{j'} | \hat{H} | \Psi \right\rangle &= \left\langle \psi_{j'} | \hat{H} \left[\sum_j |\psi_j >< \psi_j| \right] |\Psi \right\rangle \\
&= \left\langle \psi_{j'} | \hat{H} \left[\sum_j |\psi_j >< \psi_j| \right] \left[\sum_m |\psi_m^{'} >< \psi_m^{'}| \right] |\Psi \right\rangle \\
&= \sum_m E_{j'} \left\langle \psi_{j'} | \psi_m^{'} \right\rangle \left\langle \psi_m^{'} | \Psi \right\rangle \\
&= \sum_m E_{j'} \left\langle \psi_{j'} | \psi_m^{'} \right\rangle \left\langle \psi_m^{'} | \left[\int dx |x >< x| \right] |\Psi \right\rangle \\
&= \sum_m E_{j'} \left\langle \psi_{j'} | \psi_m^{'} \right\rangle \int dx \left\langle \psi_m^{'} | x \right\rangle \langle x | \Psi \rangle
\end{aligned}
$$

From time-dependent Schrödinger equation, it describes the $|\Psi\rangle$ change from t_0 to t, so is there such a time-dependent operator that can directly perform this operation? Introduing time evolution operator:

$$
\begin{aligned}
i\frac{\partial}{\partial t} |\Psi\rangle &= \hat{H} |\Psi\rangle \\
|\Psi(t)\rangle &= e^{-i\hat{H}(t-t_0)} |\Psi(t_0)\rangle \quad \text{time independent} \\
|\Psi(t)\rangle &= e^{-i\int_{t_0}^{t} \hat{H}(t)dt} |\Psi(t_0)\rangle \quad \text{time dependent}
\end{aligned}
$$

The time evolution operator makes time-dependent Schrödinger equation more convience, it can be used to get wavefunction directly, here $|\psi_i\rangle$ is an eigenstate of $\hat{H}$:

$$
\begin{aligned}
\langle x | \Psi(t) \rangle &= \left\langle x | e^{-i\hat{H}t} | \Psi(t_0) \right\rangle \\
&= \left\langle x | \left[\sum_i |\psi_i >< \psi_i| \right] e^{-i\hat{H}(t-t_0)} \left[\sum_j |\psi_j >< \psi_j| \right] |\Psi(t_0) \right\rangle \\
&= \sum_{ij} \langle x | \psi_i \rangle \left\langle \psi_i | e^{-i\hat{H}(t-t_0)} | \psi_j \right\rangle \langle \psi_j | \Psi(t_0) \rangle \\
&= \sum_{ij} \langle x | \psi_i \rangle e^{-iE_j(t-t_0)} \delta_{ij} \langle \psi_j | \Psi(t_0) \rangle \\
&= \sum_{i} \langle x | \psi_i \rangle e^{-iE_i(t-t_0)} \langle \psi_i | \Psi(t_0) \rangle \\
&= \sum_{i} \langle x | \psi_i \rangle e^{-iE_i(t-t_0)} \left\langle \psi_i \left[\int dx^{'} |x^{'} >< x^{'}| \right] \Psi(t_0) \right\rangle \\
&= \sum_{i} \langle x | \psi_i \rangle e^{-iE_i(t-t_0)} \int dx^{'} \left\langle \psi_i | x^{'} \right\rangle \left\langle x^{'} | \Psi(t_0) \right\rangle \\
&= \sum_{i} \left\langle x \left[\sum_m |\psi_m^{'} >< \psi_m^{'}| \right] \psi_i \right\rangle e^{-iE_i(t-t_0)} \int dx^{'} \left\langle \psi_i \left[\sum_n |\psi_n^{'} >< \psi_n^{'}| \right] x^{'} \right\rangle \left\langle x^{'} | \Psi(t_0) \right\rangle
\end{aligned}
$$

If $|\psi_i\rangle$ is an eigenstate of $\hat{H}$, $e^{\hat{A}}$ is defined as

$$
\begin{aligned}
e^{\hat{A}} &= \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!} = 1 + \hat{A} + \frac{1}{2!}\hat{A}^2 + \cdots \\
e^{-i\hat{H}(t-t_0)} &= 1 - i\hat{H}(t-t_0) + \frac{1}{2!}[-i\hat{H}(t-t_0)]^2 + \cdots \\
&= 1 - i(t-t_0)\hat{H} + \frac{1}{2!}[-i(t-t_0)]^2\hat{H}^2 + \cdots
\end{aligned}
$$

thus

$$
\begin{aligned}
\left\langle \psi_i | e^{-i\hat{H}(t-t_0)} | \psi_j \right\rangle &= \left\langle \psi_i | 1 - i(t-t_0)\hat{H} + \frac{1}{2!}[-i(t-t_0)]^2\hat{H}^2 + \cdots | \psi_j \right\rangle \\
&= \langle \psi_i | \psi_j \rangle - i(t-t_0) \left\langle \psi_i | \hat{H} | \psi_j \right\rangle + \frac{1}{2!}[-i(t-t_0)]^2 \left\langle \psi_i | \hat{H}^2 | \psi_j \right\rangle + \cdots \\
&= \delta_{ij} - i(t-t_0)E_j\delta_{ij} + \frac{1}{2!}[-i(t-t_0)]^2 E_j^2 \delta_{ij} + \cdots \\
&= e^{-iE_j(t-t_0)}\delta_{ij}
\end{aligned}
$$

in matrix form:

$$\begin{bmatrix} e^{-iE_1(t-t_0)} & 0 & 0 & \cdots & 0 \\ 0 & e^{-iE_2(t-t_0)} & 0 & \cdots & 0 \\ 0 & 0 & e^{-iE_3(t-t_0)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & e^{-iE_n(t-t_0)} \end{bmatrix}$$

If $\left|\psi_m^{'}\right\rangle$ is not an eigenstate of $\hat{H}$, then

$$\begin{aligned} \left\langle \psi_m^{'}|e^{-i\hat{H}(t-t_0)}|\psi_n^{'} \right\rangle &= \left\langle \psi_m^{'}| \left[\sum_i |\psi_i><\psi_i|\right] e^{-i\hat{H}(t-t_0)} \left[\sum_j |\psi_j><\psi_j|\right] |\psi_n^{'} \right\rangle \\ &= \sum_{ij} \left\langle \psi_m^{'}|\psi_i \right\rangle \left\langle \psi_i|e^{-i\hat{H}(t-t_0)}|\psi_j \right\rangle \left\langle \psi_j|\psi_n^{'} \right\rangle \\ &= \sum_{ij} \left\langle \psi_m^{'}|\psi_i \right\rangle e^{-iE_jt}\delta_{ij} \left\langle \psi_j|\psi_n^{'} \right\rangle \end{aligned}$$

in matrix form:

$$\begin{bmatrix} \left\langle \psi_1^{'}|\psi_1^{'} \right\rangle & \left\langle \psi_2^{'}|\psi_1 \right\rangle & \cdots & \left\langle \psi_n^{'}|\psi_1 \right\rangle \\ \left\langle \psi_1^{'}|\psi_2^{'} \right\rangle & \left\langle \psi_2^{'}|\psi_2 \right\rangle & \cdots & \left\langle \psi_n^{'}|\psi_2 \right\rangle \\ \vdots & \vdots & \cdots & \vdots \\ \left\langle \psi_1^{'}|\psi_n^{'} \right\rangle & \left\langle \psi_2^{'}|\psi_n \right\rangle & \cdots & \left\langle \psi_n^{'}|\psi_n \right\rangle \end{bmatrix} \begin{bmatrix} e^{-iE_1(t-t_0)} & 0 & \cdots & 0 \\ 0 & e^{-iE_2(t-t_0)} & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & e^{-iE_n(t-t_0)} \end{bmatrix} \begin{bmatrix} \left\langle \psi_1|\psi_1^{'} \right\rangle & \left\langle \psi_1|\psi_2^{'} \right\rangle & \cdots & \left\langle \psi_1|\psi_n^{'} \right\rangle \\ \left\langle \psi_2|\psi_1^{'} \right\rangle & \left\langle \psi_2|\psi_2^{'} \right\rangle & \cdots & \left\langle \psi_2|\psi_n^{'} \right\rangle \\ \vdots & \vdots & \cdots & \vdots \\ \left\langle \psi_n|\psi_1^{'} \right\rangle & \left\langle \psi_n|\psi_2^{'} \right\rangle & \cdots & \left\langle \psi_n|\psi_n^{'} \right\rangle \end{bmatrix}$$

$$= \boldsymbol{S}^{+} \left[e^{-iE_it}\right] \boldsymbol{S}$$

thus

$$\begin{bmatrix} c_0(t) \\ c_1(t) \\ \vdots \\ c_n(t) \end{bmatrix} = \boldsymbol{S}^{+} \left[e^{-iE_i(t-t_0)}\right] \boldsymbol{S} \begin{bmatrix} c_0(t_0) \\ c_1(t_0) \\ \vdots \\ c_n(t_0) \end{bmatrix}$$

$$\boldsymbol{c}(t) = \boldsymbol{S}^{+} \left[e^{-iE_i(t-t_0)}\right] \boldsymbol{S}\boldsymbol{c}(t_0)$$

Example: using the Harmonic oscillatoras the basis to get wavefunction

$$\begin{aligned} \langle x|\Psi(x)\rangle &= \left\langle x|e^{-i\hat{H}(t-t_0)}|\Psi(t_0) \right\rangle \\ &= \left\langle x|e^{-i\hat{H}(t-t_0)} \left[\int dx^{'}|x^{'}><x^{'}|\right] \Psi(t_0) \right\rangle \\ &= \int dx^{'} \left\langle x|e^{-i\hat{H}(t-t_0)}|x^{'} \right\rangle \Psi(x^{'},t_0) \\ &= \int dx^{'} \left\langle x \left[\sum_i |\psi_i^{HO}><\psi_i^{HO}|\right] e^{-i\hat{H}(t-t_0)} \left[\sum_j |\psi_j^{HO}><\psi_j^{HO}|\right] x^{'} \right\rangle \Psi(x^{'},t_0) \\ &= \sum_{ij} \int dx^{'} \left\langle x|\psi_i^{HO} \right\rangle \left\langle \psi_i^{HO}|e^{-i\hat{H}(t-t_0)}|\psi_j^{HO} \right\rangle \left\langle \psi_j^{HO}|x^{'} \right\rangle \Psi(x^{'},t_0) \\ &= \sum_{ij} \int dx^{'} \psi_j^{HO}(x) \left\langle \psi_i^{HO}|e^{-i\hat{H}(t-t_0)}|\psi_j^{HO} \right\rangle \psi_j^{*HO}(x^{'})\Psi(x^{'},t_0) \end{aligned}$$

if $\hat{H} = \hat{T} + \frac{1}{2}m\omega^2\hat{x}^2$, then $\left\langle \psi_i^{HO}|e^{-i\hat{H}(t-t_0)}|\psi_j^{HO} \right\rangle$ is a diagnoal matrix.
if $\hat{H} = \hat{T} + \frac{1}{2}m\omega^2\hat{x}^2 + c\hat{x}$, then $\hat{H}$ can be divived into 2 parts, where $H_0 = \hat{T} + \frac{1}{2}m\omega^2\hat{x}^2$, $H_1 = c\hat{x} = \frac{c}{\sqrt{2}}(\hat{a}^{+} + \hat{a}^{-})$, here $\hat{a}^{+}$

and $\hat{a}^-$ are ladder operator, $\hat{a}^+\left|\psi_j^{HO}\right\rangle = \sqrt{j+1}\left|\psi_{j+1}^{HO}\right\rangle$, $\hat{a}^-\left|\psi_j^{HO}\right\rangle = \sqrt{j}\left|\psi_{j-1}^{HO}\right\rangle$.

$$\begin{aligned}
\left\langle \psi_i^{HO}|\hat{H}|\psi_j^{HO}\right\rangle &= \left\langle \psi_i^{HO}|\hat{H}_0+\hat{H}_1|\psi_j^{HO}\right\rangle \\
&= \left\langle \psi_i^{HO}|\hat{H}_0|\psi_j^{HO}\right\rangle + \left\langle \psi_i^{HO}|\hat{H}_1|\psi_j^{HO}\right\rangle \\
&= E_j\delta_{ij} + \left\langle \psi_i^{HO}|\frac{\hat{a}^+ + \hat{a}^-}{\sqrt{2}}|\psi_j^{HO}\right\rangle \\
&= E_j\delta_{ij} + \sqrt{\frac{j+1}{2}}c\left\langle \psi_i^{HO}|\psi_{j+1}^{HO}\right\rangle + \sqrt{\frac{j}{2}}c\left\langle \psi_i^{HO}|\psi_{j-1}^{HO}\right\rangle \\
&= E_j\delta_{ij} + \sqrt{\frac{j+1}{2}}c\delta_{i,j+1} + \sqrt{\frac{j}{2}}c\delta_{i,j-1}
\end{aligned}$$

in matrix form:

$$\begin{bmatrix} E_1 & 0 & 0 & \cdots & 0 \\ 0 & E_2 & 0 & \cdots & 0 \\ 0 & 0 & E_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & E_n \end{bmatrix} + \frac{c}{\sqrt{2}}\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ \sqrt{1} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \sqrt{2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \sqrt{n-1} & 0 \end{bmatrix} + \frac{c}{\sqrt{2}}\begin{bmatrix} 0 & \sqrt{1} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \sqrt{2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \sqrt{n-1} \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} E_1 & c\sqrt{\frac{1}{2}} & 0 & \cdots & 0 & 0 \\ c\sqrt{\frac{1}{2}} & E_2 & c\sqrt{\frac{2}{2}} & \cdots & 0 & 0 \\ 0 & c\sqrt{\frac{2}{2}} & E_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & E_{n-1} & c\sqrt{\frac{n-1}{2}} \\ 0 & 0 & 0 & \cdots & c\sqrt{\frac{n-1}{2}} & E_n \end{bmatrix}$$

$$= \boldsymbol{U}^+\boldsymbol{E}^{\boldsymbol{new}}\boldsymbol{U}$$

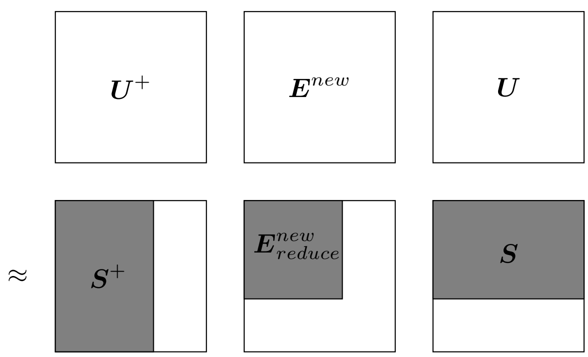
thus the matrix corresponding to $e^{-i\hat{H}(t-t_0)}$ becomes

$$\boldsymbol{U}^+\begin{bmatrix} e^{-iE_1^{new}(t-t_0)} & 0 & 0 & \cdots & 0 \\ 0 & e^{-iE_2^{new}(t-t_0)} & 0 & \cdots & 0 \\ 0 & 0 & e^{-iE_3^{new}(t-t_0)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & e^{-iE_n^{new}(t-t_0)} \end{bmatrix}\boldsymbol{U}$$

Sometimes only part of all generated E_i^{new} is "effective", namely we can use the following form to approximate $\boldsymbol{U}^+\boldsymbol{E}^{\boldsymbol{new}}\boldsymbol{U}$:

$$\left[\left\langle \psi_i^{HO}|\hat{H}|\psi_j^{HO}\right\rangle\right] = \boldsymbol{S}^+\boldsymbol{E}^{\boldsymbol{new}}_{\boldsymbol{reduce}}\boldsymbol{S}$$

where $\boldsymbol{S}$ is only part of $\boldsymbol{U}$, $\boldsymbol{E}^{new}_{reduce}$ is only part of $\boldsymbol{E}^{new}$.



it can be solved by the Lanczos method, which refers to $n\times n \to (n\times l)(l\times l)(l\times n)$.
By spliting $\hat{H}$, if the matrix corresponding to each part of the operator can be calculated, it is easy to get the evolution of wavefunction with time. Normally, $\hat{H}$ is the function of $\hat{x}$ and $\hat{p}$, thus $|x\rangle$ and $|p\rangle$ can be used as the basis:
a. using $|x\rangle$ as the basis:

$$\left\langle x^{'}|f(\hat{x})|x^{"}\right\rangle = f(x^{"})\delta(x^{'}-x^{"})$$

b. using $|p\rangle$ as the basis:

$$\left\langle p^{'}|f(\hat{p})|p^{"}\right\rangle = f(p^{"})\delta(p^{'}-p^{"})$$

e.g

$$\left\langle p^{'}|\frac{\hat{p}^2}{2m}|p^{"}\right\rangle = \frac{p^{"2}}{2m}\delta(p^{'}-p^{"})$$

c. the transform between $|x\rangle$ and $|p\rangle$

$$\langle x|p\rangle = e^{-ipx}$$
$$p(x) = \frac{1}{\sqrt{2}}\cos(px) - \frac{i}{\sqrt{2}}\sin(px) \rightarrow \text{plane wave}$$

proof:

$$\begin{aligned}
\left(1 - i\hat{p}\Delta x^{'}\right)|\alpha\rangle &= \hat{g}(\Delta x^{'})\,|\alpha\rangle \rightarrow \hat{g}(\Delta x^{'})\left|x^{'}\right\rangle = \left|x^{'}+\delta x^{'}\right\rangle \\
&= \int dx^{'}\hat{g}(\Delta x^{'})\left|x^{'}\right\rangle\left\langle x^{'}|\alpha\right\rangle \\
&= \int dx^{'}\left|x^{'}+\Delta x^{'}\right\rangle\left\langle x^{'}|\alpha\right\rangle \\
&= \int dx^{'}\left|x^{'}\right\rangle\left\langle x^{'}-\Delta x^{'}|\alpha\right\rangle \\
&= \int dx^{'}\left|x^{'}\right\rangle\left(\left\langle x^{'}|\alpha\right\rangle - \Delta x^{'}\frac{\partial}{\partial x^{'}}\left\langle x^{'}|\alpha\right\rangle\right) \\
&= |\alpha\rangle - \int dx^{'}\left|x^{'}\right\rangle\left(\Delta x^{'}\frac{\partial}{\partial x^{'}}\left\langle x^{'}|\alpha\right\rangle\right) \\
\hat{p}\,|\alpha\rangle &= \int dx^{'}\left|x^{'}\right\rangle\left(-i\frac{\partial}{\partial x^{'}}\left\langle x^{'}|\alpha\right\rangle\right) \\
\left\langle x^{''}|\hat{p}|\alpha\right\rangle &= -i\frac{\partial}{\partial x^{''}}\left\langle x^{''}|\alpha\right\rangle \\
\left\langle x^{''}|\hat{p}^n|\alpha\right\rangle &= (-i)^n\frac{\partial^n}{\partial x^{''n}}\left\langle x^{''}|\alpha\right\rangle \\
\langle x|\hat{p}|p\rangle &= -i\frac{\partial}{\partial x}\langle x|p\rangle \\
\langle x|p\rangle &= \frac{1}{\sqrt{2\pi}}e^{-ipx}
\end{aligned}$$

e.g

$$\begin{aligned}
\langle p|\Psi\rangle &= \left\langle p\left[\int dx\,|x\rangle\langle x|\right]\Psi\right\rangle \\
&= \int dx\,\langle p|x\rangle\langle x|\Psi\rangle \\
&= \frac{1}{\sqrt{2}}\int dx e^{ipx}\langle x|\Psi\rangle \rightarrow FFT
\end{aligned}$$

Split-Operator Method
if $\hat{H} = \hat{H}_0 + \hat{H}_1$, then

$$e^{-i\hat{H}\Delta t} \approx e^{-i\frac{\hat{H}_0}{2}\Delta t}e^{-i\hat{H}_1\Delta t}e^{-i\frac{\hat{H}_0}{2}\Delta t} \rightarrow \text{small } \Delta t$$

thus

$$\begin{aligned}
\langle\psi_i|\Psi(t+\Delta t)\rangle &= \left\langle\psi_i|e^{-i\hat{H}\Delta t}|\Psi(t)\right\rangle \\
&= \left\langle\psi_i|e^{-i\frac{\hat{H}_0}{2}\Delta t}e^{-i\hat{H}_1\Delta t}e^{-i\frac{\hat{H}_0}{2}\Delta t}|\Psi(t)\right\rangle \\
&= \left\langle\psi_i\left[\sum_a|\psi_a\rangle\langle\psi_a|\right]e^{-i\frac{\hat{H}_0}{2}\Delta t}\left[\sum_b|\psi_b\rangle\langle\psi_b|\right]e^{-i\hat{H}_1\Delta t}\left[\sum_c|\psi_c\rangle\langle\psi_c|\right]e^{-i\frac{\hat{H}_0}{2}\Delta t}\left[\sum_d|\psi_d\rangle\langle\psi_d|\right]\Psi(t)\right\rangle \\
&= \sum_{abcd}\langle\psi_i|\psi_a\rangle\left\langle\psi_a|e^{-i\frac{\hat{H}_0}{2}\Delta t}|\psi_b\right\rangle\left\langle\psi_b|e^{-i\hat{H}_1\Delta t}|\psi_c\right\rangle\left\langle\psi_c|e^{-i\frac{\hat{H}_0}{2}\Delta t}|\psi_d\right\rangle\langle\psi_d|\Psi(t)\rangle \\
&= \sum_{abcd}\langle\psi_i|\psi_a\rangle\,e^{-i\frac{\hat{E}_b^0}{2}\Delta t}\,\langle\psi_a|\psi_b\rangle\,e^{-i\hat{E}_c^1\Delta t}\,\langle\psi_b|\psi_c\rangle\,e^{-i\frac{\hat{E}_d^0}{2}\Delta t}\,\langle\psi_c|\psi_d\rangle\,\langle\psi_d|\Psi(t)\rangle
\end{aligned}$$

e.g: if $\hat{H}=\hat{T}+\frac{1}{2}m\omega^2\hat{x}^2+k\hat{x}=\hat{H}^{HO}+k\hat{x}$, and $\hat{H}^{HO}\left|v\right\rangle=E_v\left|v\right\rangle$, then

$$\begin{aligned}
c_v(t+\Delta t) &= \langle v|\Psi(t+\Delta t)\rangle \\
&= \left\langle v|e^{-i\hat{H}\Delta t}|\Psi(t)\right\rangle \\
&\approx \left\langle v|e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}e^{-ik\hat{x}\Delta t}e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}|\Psi(t)\right\rangle \\
&= \left\langle v|e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}\left[\int dx\left|x\right\rangle\left\langle x\right|\right]e^{-ik\hat{x}\Delta t}\left[\int dx^{'}\left|x^{'}\right\rangle\left\langle x^{'}\right|\right]e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}|\Psi(t)\right\rangle \\
&= \int dx\left\langle v|e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}|x\right\rangle e^{-ikx\Delta t}\left\langle x|e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}|\Psi(t)\right\rangle \\
&= \int dx\left\langle v|e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}\left[\sum_{v^{'}}\left|v^{'}\right\rangle\left\langle v^{'}\right|\right]x\right\rangle e^{-ikx\Delta t}\left\langle x\left[\sum_{u^{'}}\left|u^{'}\right\rangle\left\langle u^{'}\right|\right]e^{-i\frac{\hat{H}^{HO}}{2}\Delta t}\left[\sum_{u"}\left|u"\right\rangle\left\langle u"\right|\right]\Psi(t)\right\rangle \\
&= \sum_{u^{'}}\int dx e^{-i\frac{E_v}{2}\Delta t}\langle v|x\rangle e^{-ikx\Delta t}\left\langle x|u^{'}\right\rangle e^{-i\frac{E_{u^{'}}}{2}\Delta t}\left\langle u^{'}|\Psi(t)\right\rangle
\end{aligned}$$

in matrix form:

$$\left[\boldsymbol{e^{-i\frac{E_v}{2}\Delta t}}\right]_{diag}\left[\langle\boldsymbol{v}|\boldsymbol{x}\rangle\right]\left[\boldsymbol{e^{-ikx\Delta t}}\right]_{diag}\left[\left\langle\boldsymbol{x}|\boldsymbol{u^{'}}\right\rangle\right]\left[\boldsymbol{e^{-i\frac{E_v}{2}\Delta t}}\right]_{diag}\left[\left\langle\boldsymbol{u^{'}}|\boldsymbol{\Psi(t)}\right\rangle\right]$$

Two-dimension situation
e.g: if

$$\hat{H}=\frac{\hat{p}_1^2}{2}+\frac{\hat{p}_2^2}{2}+\frac{1}{2}\hat{x}_1^2+\frac{1}{2}\hat{x}_2^2+\hat{x}_1\hat{x}_2$$

the convolution basis can be used, namely

$$|x_1,x_2\rangle=|x_1\rangle\otimes|x_2\rangle$$

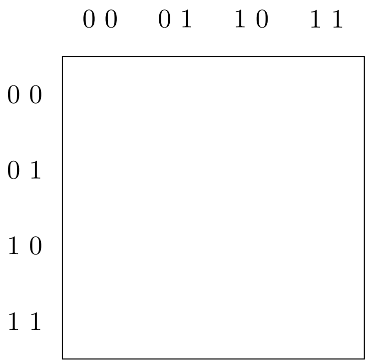
here if $|x_1\rangle$ has 3 different basis, $|x_2\rangle$ has 3 different basis, thus totally 9 basis would be used in the compution.

$$c_{12}(t)=\langle x_1,x_2|\Psi(t)\rangle$$

If $\hat{H}$ are divided into $\hat{T}=\frac{\hat{p}_1^2}{2}+\frac{\hat{p}_2^2}{2}$ and $\hat{V}=\frac{1}{2}\hat{x}_1^2+\frac{1}{2}\hat{x}_2^2+\hat{x}_1\hat{x}_2$.
For $\hat{V}$:

$$\begin{aligned}
\langle x_1,x_2|\,\hat{V}\left|x_1^{'},x_2^{'}\right\rangle &= \langle x_1,x_2|\,\frac{1}{2}\hat{x}_1^2+\frac{1}{2}\hat{x}_2^2+\hat{x}_1\hat{x}_2\left|x_1^{'},x_2^{'}\right\rangle \\
&= \frac{1}{2}x_1^2\delta(x_1-x_1^{'})\delta(x_2-x_2^{'})+\frac{1}{2}x_2^2\delta(x_1-x_1^{'})\delta(x_2-x_2^{'})+\frac{1}{2}x_1x_2\delta(x_1-x_1^{'})\delta(x_2-x_2^{'})
\end{aligned}$$

thus $\langle x_1,x_2|\,\hat{V}\left|x_1^{'},x_2^{'}\right\rangle$ has four index, it can be divived into two groups, where x_1,x_2 belong to group one, $x_1^{'},x_2^{'}$ belong to group two, it can be further transformed into two-dimension matrix by renormalization.



For $\hat{T}$:

$$\begin{aligned}
\langle x_1, x_2| \hat{T} \left|x_1^{'}, x_2^{'}\right\rangle &= \langle x_1, x_2| \frac{1}{2}\hat{p}_1^2 + \frac{1}{2}\hat{p}_2^2 \left|x_1^{'}, x_2^{'}\right\rangle \\
&= \left\langle x_1, x_2 \left[\int dp_1 dp_2 \left|p_1, p_2\right\rangle \left\langle p_1, p_2\right|\right] \frac{1}{2}\hat{p}_1^2 + \frac{1}{2}\hat{p}_2^2 \left[\int dp_1^{'} dp_2^{'} \left|p_1^{'}, p_2^{'}\right\rangle \left\langle p_1^{'}, p_2^{'}\right|\right] x_1^{'}, x_2^{'}\right\rangle \\
&= \int dp_1 dp_2 \left\langle x_1, x_2|p_1, p_2\right\rangle (\frac{1}{2}p_1^2 + \frac{1}{2}p_2^2) \left\langle p_1, p_2|x_1^{'}, x_2^{'}\right\rangle \\
&= \int dp_1 dp_2 \left[\langle x_1| \otimes \langle x_2|\right] \left[|p_1\rangle \otimes |p_2\rangle\right] (\frac{1}{2}p_1^2 + \frac{1}{2}p_2^2) \left[\langle p_1| \otimes \langle p_2|\right] \left[\left|x_1^{'}\right\rangle \otimes \left|x_2^{'}\right\rangle\right] \\
&= \int dp_1 dp_2 \left\langle x_1|p_1\right\rangle \otimes \left\langle x_2|p_2\right\rangle (\frac{1}{2}p_1^2 + \frac{1}{2}p_2^2) \left\langle p_1|x_1^{'}\right\rangle \otimes \left\langle p_2|x_2^{'}\right\rangle
\end{aligned}$$

here the kinetic operator can also be computed in the following:

$$\begin{aligned}
\left\langle x_1, x_2|\frac{\hat{p}_1^2}{2m}|x_1^{'}, x_2^{'}\right\rangle &= \left\langle x_1|\frac{\hat{p}_1^2}{2m}|x_1^{'}\right\rangle \otimes \delta(x_2 - x_2^{'}) \\
&= \int dp_1 \left\langle x_1|p_1\right\rangle \frac{1}{2}p_1^2 \left\langle p_1|x_1^{'}\right\rangle \otimes \delta(x_2 - x_2^{'})
\end{aligned}$$

For the whole:

$$\begin{aligned}
c_{12}(t) &= \langle x_1, x_2|\Psi(t)\rangle \\
&= \left\langle x_1, x_2|e^{-i\hat{H}(t-t_0)}|\Psi(t_0)\right\rangle \\
&= \left\langle x_1, x_2|e^{-i\hat{H}(t-t_0)} \left[\int dx_1^{'} dx_2^{'} \left|x_1^{'}, x_2^{'}\right\rangle \left\langle x_1^{'}, x_2^{'}\right|\right] \Psi(t_0)\right\rangle \\
&= \int dx_1^{'} dx_2^{'} \left\langle x_1, x_2|e^{-i\hat{H}(t-t_0)}|x_1^{'}, x_2^{'}\right\rangle \left\langle x_1^{'}, x_2^{'}|\Psi(t_0)\right\rangle \\
&= \int dx_1^{'} dx_2^{'} \left\langle x_1, x_2|e^{-i\hat{H}(t-t_0)}|x_1^{'}, x_2^{'}\right\rangle \Psi(x_1^{'}, x_2^{'}, t_0)
\end{aligned}$$

If $\hat{H}$ is divived into $\hat{H}_1^{HO} = \frac{\hat{p}_1^2}{2} + \frac{1}{2}\hat{x}_1^2 + k\hat{x}_1$, $\hat{H}_2^{HO} = \frac{\hat{p}_2^2}{2} + \frac{1}{2}\hat{x}_2^2 + k\hat{x}_2$ and $\hat{H}_3 = \hat{x}_1\hat{x}_2$, $\hat{H}_1^{HO}|a\rangle = E_a|a\rangle$ and $\hat{H}_2^{HO}|b\rangle = E_b|b\rangle$, thus $|a, b\rangle$ can be used as the basis:

$$\begin{aligned}
\left\langle a, b|\hat{H}_1^{HO}|a^{'}, b^{'}\right\rangle &= E_a\delta_{aa^{'}}\delta_{bb^{'}} \\
\left\langle a, b|\hat{x}_1\hat{x}_2|a^{'}, b^{'}\right\rangle &= \left\langle a|\hat{x}_1|a^{'}\right\rangle \otimes \left\langle b|\hat{x}_2|b^{'}\right\rangle
\end{aligned}$$