Advanced Quantum Mechanics

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Quantum Dynamics

Lecture #9

Schrodinger and Heisenberg Picture

Time Independent Hamiltonian

Schrodinger Picture: A time evolving state in the Hilbert space with time independent operators

$$i\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \longrightarrow |\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle$$

Eigenbasis of Hamiltonian: $\hat{H}|n\rangle = \epsilon_n|n\rangle \qquad |\psi(t)\rangle = \sum_n c_n(t)|n\rangle \qquad c_n(t) = c_n(0)e^{-i\epsilon_n t}$

Operators and Expectation: $A(t) = \langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(0)|e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}|\psi(0)\rangle = \langle\psi(0)|\hat{A}(t)|\psi(0)\rangle$

Heisenberg Picture: A static initial state and time dependent operators

$$\dot{\hat{A}}(t) = i[\hat{H}, \hat{A}(t)] \longrightarrow \hat{A}(t) = e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}$$

Schrodinger Picture	Heisenberg Picture
$\lvert\psi(0)\rangle \to \lvert\psi(t)\rangle$	$\lvert\psi(0)\rangle \to \lvert\psi(0)\rangle$
$\hat{A} \to \hat{A}$	$\hat{A} \to \hat{A}(t) = e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}$
$i\partial_t\lvert\psi(t)\rangle = \hat{H}\lvert\psi(t)\rangle$	$i\partial_t\hat{A}(t) = [\hat{A}(t), \hat{H}]$

Equivalent description of a quantum system

Time Evolution and Propagator

$$|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(0)\rangle = U(t,0)|\psi(0)\rangle$$

Time Evolution Operator $U(t,0) = e^{-i\hat{H}t}$

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|\hat{U}(t)|\psi(0)\rangle = \int dx^{'} \langle x|\hat{U}(t)|x^{'}\rangle\langle x^{'}|\psi(0)\rangle$$

$$= i\int dx' G(x,x',t)\psi(x',0)$$

Propagator: $G(\alpha,\beta,t) = -i\langle\alpha|\hat{U}(t)|\beta\rangle$

Example : Free Particle $G(k,k',t) = -i\delta_{kk'}e^{-i\frac{k^2}{2m}t}$ $\quad G(x,x',t) = -i\sqrt{\frac{m}{2\pi it}}e^{-i\frac{m}{2t}(x-x')^2}$

The propagator satisfies $(i\partial_t - H)G(x,x',t,t') = \delta(x-x')\delta(t-t')$

and hence is often called the Green's function

Retarded and Advanced Propagator

The following propagators are useful in different contexts

Retarded or Causal Propagator: $G^R(\alpha, t; \beta, t') = -i\Theta(t-t')\langle\alpha|\hat{U}(t-t')|\beta\rangle$

This propagates states forward in time $\psi_\alpha(t) = i\sum_\beta G^R(\alpha, t; \beta, t')\psi_\beta(t')$ for t > t′

Advanced or Anti-Causal Propagator: $G^A(\alpha, t; \beta, t') = i\Theta(t'-t)\langle\alpha|\hat{U}(t-t')|\beta\rangle$

This propagates states backward in time $\psi_\alpha(t) = -i\sum_\beta G^A(\alpha, t; \beta, t')\psi_\beta(t')$ for t < t′

Both the retarded and the advanced propagator satisfies the same diff. eqn., but with different boundary conditions

$$(i\partial_t - H)G^{R(A)}(x, t; x', t) = \delta(x-x')\delta(t-t')$$

$$G^R(t) = 0 \quad for \quad t < 0$$

$$G^A(t) = 0 \quad for \quad t > 0$$

Propagators in Frequency Space

$$G(\alpha,t;\beta,t') = -i\langle\alpha|\hat{U}(t-t')|\beta\rangle = -i\sum_{nn'}\langle\alpha|n\rangle\langle n|e^{-i\hat{H}(t-t')}|n'\rangle\langle n'|\beta\rangle \;= -i\sum_{n}\psi_n^*(\alpha)\psi_n(\beta)e^{-iE_n(t-t')}$$

Energy Eigenbasis |n>

$$G(\alpha,\beta,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G(\alpha,\beta,t) \;= -i\sum_n \psi_n^*(\alpha)\psi_n(\beta)\int_{-\infty}^{\infty} dt e^{i(\omega-E_n)t}$$

The integral is ill defined due to oscillatory nature of the integrand

Integrals for retarded/advanced propagators can be made well defined in the following way:

Retarded Propagator: $G^R(\alpha,t;\beta,t') = -i\Theta(t-t')\sum_n \psi_n^*(\alpha)\psi_n(\beta)e^{-iE_n(t-t')}$

$$G^R(\alpha,\beta,\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G^R(\alpha,\beta,t) = -i\sum_n \psi_n^*(\alpha)\psi_n(\beta)\int_0^{\infty} dt e^{i(\omega-E_n)t}$$

This integral is convergent if we replace $\omega \to \omega + i\eta$, with $\eta \to 0^+$

$$G^R(\alpha,\beta,\omega) = -\sum_n \psi_n^*(\alpha)\psi_n(\beta)\left.\frac{e^{i(\omega+i\eta-E_n)t}}{\omega+i\eta-E_n}\right|_0^{\infty}$$

$$= \sum_n \psi_n^*(\alpha)\psi_n(\beta)\frac{1}{\omega+i\eta-E_n}$$

Positive η provides exponential decay of integrand at large +ve t

Propagators in Frequency Space

Advanced Propagator: $$G^A(\alpha,t;\beta,t') = i\Theta(t'-t)\sum_n \psi_n^*(\alpha)\psi_n(\beta)e^{-iE_n(t-t')}$$

$$G^A(\alpha,\beta,\omega) = \int_{-\infty}^{\infty} dte^{i\omega t}G^A(\alpha,\beta,t) = i\sum_n \psi_n^*(\alpha)\psi_n(\beta)\int_{-\infty}^{0} dte^{i(\omega-E_n)t}$$

This integral is convergent if we replace $\omega \longrightarrow \omega - i\,\eta$, with $\eta \longrightarrow 0^+$

$$G^A(\alpha,\beta,\omega) = \sum_n \psi_n^*(\alpha)\psi_n(\beta)\left.\frac{e^{i(\omega+i\eta-E_n)t}}{\omega - i\eta - E_n}\right|_{-\infty}^{0}$$

$$= \sum_n \psi_n^*(\alpha)\psi_n(\beta)\frac{1}{\omega - i\eta - E_n}$$

Negative η provides exponential decay of integrand at large -ve t

Note that the original integral from -∞ to ∞ cannot be made well defined by either prescription

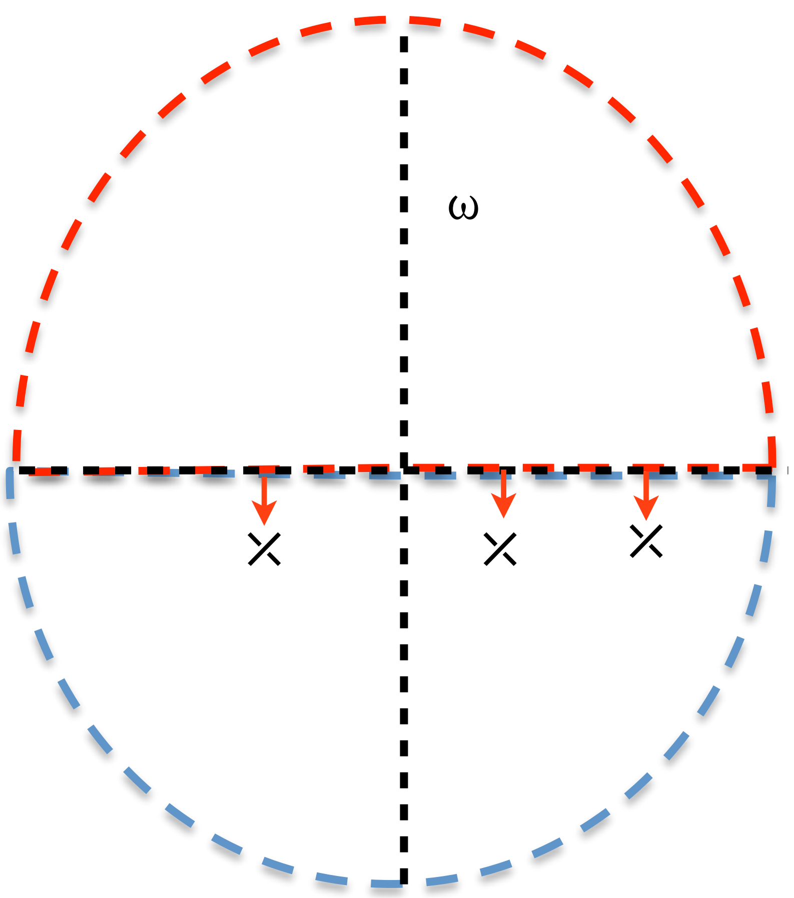
Example: Free Particle $$G^{R(A)}(k,k',\omega) = \delta(k-k')\frac{1}{\omega - \frac{k^2}{2m} \pm i\eta}$$

Example: Harmonic Oscillator $$G^{R(A)}(x,y,\omega)\ e^{-(x^2+y^2)/a_0^2}\sum_n \frac{H_n(x/a_0)H_n(y/a_0)}{\omega - \omega_0(n+\frac{1}{2}) \pm i\eta}$$

Propagators in Fourier Space

Let us make sure that the prescription of adding (subtracting) a small positive imaginary part to the frequency gives back the correct retarded (advanced) propagator on inverse transformation

Retarded Propagator: $$G^R(\alpha,\beta,t) = \sum_n \psi_n^*(\alpha)\psi_n(\beta)\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + i\eta - E_n}$$



- Evaluate the ω integral by contour integration.

  With ω—> ω+ i η, the poles of the integrand are all in lower half-plane.

- For t>0, use the blue contour to do the integration. Note that for t > 0, the integral on the semicircle vanishes.

$$G^R(\alpha,\beta,t>0) = -i\sum_n \psi_n^*(\alpha)\psi_n(\beta)e^{-iE_nt}$$

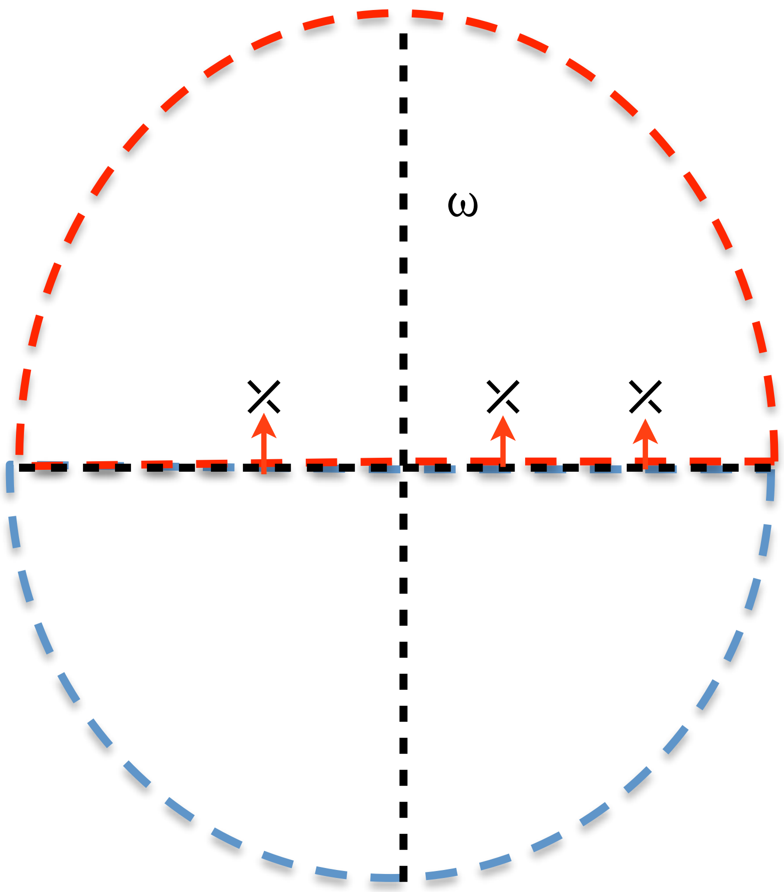
- For t<0, one cannot use the blue contour. For large -ve imaginaryω the integrand blows up. So, instead use the red contour. Since there are no singularities in the upper half-plane, we get 0.

$$G^R(\alpha,\beta,t) = -i\Theta(t)\sum_n \psi_n^*(\alpha)\psi_n(\beta)e^{-iE_nt}$$

Propagators in Fourier Space

Let us make sure that the prescription of adding (subtracting) a small positive imaginary part to the frequency gives back the correct retarded (advanced) propagator on inverse transformation

Advanced Propagator: $$G^A(\alpha,\beta,t) = \sum_n \psi_n^*(\alpha)\psi_n(\beta)\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega - i\eta - E_n}$$



- Evaluate the ω integral by contour integration.

  With $\omega \to \omega - i\eta$, the poles of the integrand are all in upper half-plane.

- For t>0, use the blue contour to do the integration. Since all the singularities are in lower half-plane, we get 0

- For t<0, one cannot use the blue contour. For large -ve imaginary ω the integrand blows up. So, instead use the red contour. Pick up residues from the poles to get

$$G^A(\alpha,\beta,t<0) = i\sum_n \psi_n^*(\alpha)\psi_n(\beta)e^{-iE_nt}$$

So in all $$G^A(\alpha,\beta,t) = i\Theta(-t)\sum_n \psi_n^*(\alpha)\psi_n(\beta)e^{-iE_nt}$$

Time Dependent Hamiltonians

Where do we encounter time dependent Hamiltonians?

✦Experimental probes of systems:

- When we shine light on atoms and measure absorption, we turn on the part of H corresponding to light-matter interaction and switch it off. The absorption is described by a time dependent Hamiltonian

- When we apply voltage and measure current, we are measuring the response of the system to a time dependent Hamiltonian (part corresponding to energy of charges in E field)

- In NMR experiments, we turn on rf pulses, which correspond to a time dependent Hamiltonian

✦Tuning Hamiltonian (Interaction) parameters: In cold atomic systems, the effective interaction between particles can be tuned by changing a magnetic field in a time dependent way. The main difference between this and above is that we do not necessarily turn off the interaction

✦ Coupling to a Bath: If we wish to understand how quantum systems equilibriate, we have to study the problem of a system coupled to a heat bath. Under certain conditions, this problem reduces to a quantum system acted on by a time-dependent random noise.

E.g.: Quantum Brownian Particle, Oscillator kicked by noise from you walking around it, etc.

Propagator for time dependent Hamiltonians

Formal Solution for time-dependent Hamiltonians:

Integral Equation

$$i\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \xrightarrow{\text{Integrate}} |\psi(t)\rangle = |\psi(0)\rangle - i\int_0^t dt'\hat{H}(t')|\psi(t')\rangle$$

Want to get rid of the time dependent |ψ(t') > from the RHS. Do this iteratively. For 1st iteration, replace |ψ(t') > by |ψ(0) >

Use this |ψ(t') > in RHS to get

$$|\psi^{(1)}(t)\rangle = |\psi(0)\rangle - i\int_0^t dt_1\hat{H}(t_1)|\psi(0)\rangle = [1 - i\int_0^t dt_1\hat{H}(t_1)]|\psi(0)\rangle$$

$$|\psi^{(2)}(t)\rangle = |\psi(0)\rangle - i\int_0^t dt_1\hat{H}(t_1)|\psi^{(1)}(t_1)\rangle = [1 - i\int_0^t dt_1\hat{H}(t_1)[1 - i\int_0^{t_1} dt_2\hat{H}(t_2)]]|\psi(0)\rangle$$

$$\vdots$$

$$|\psi^{(n)}(t)\rangle = [1 + \sum_{j=1}^{n}(-i)^j\int_0^t dt_1\int_0^{t_1} dt_2\ldots\int_0^{t_{j-1}} dt_j\hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_j)]|\psi(0)\rangle$$

Note that time argument of H s are decreasing as we go from left to right ⟶ Time ordering

$$|\psi(t)\rangle = [1 + \textstyle\sum_{j=1}^{\infty}(-i)^j\int_0^t dt_1\int_0^{t_1} dt_2\ldots\int_0^{t_{j-1}} dt_j\hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_j)]|\psi(0)\rangle$$

$$= T\left[e^{-i\int_0^t dt'\hat{H}(t')}\right]|\psi(0)\rangle$$

Time Ordering

We have formally written the time evolution operator for a time dependent Hamiltonian as a time-ordered exponential. What does this mean?

$$T[e^{-i\int_0^t dt' \hat{H}(t')}] = 1 + \sum_{j=1}^{\infty}(-i)^j \int_0^t dt_1 \int_0^{t_1} dt_2 .. \int_0^{t_{j-1}} dt_j \hat{H}(t_1)\hat{H}(t_2)...\hat{H}(t_j)$$

In the jth order term above, there are j! possible orderings of $\{t_1,t_2,..t_j\}$. (say $\{t_1 > t_2 > .. t_j\}$, $\{t_2 > t_1 > t_3 > .. t_j\}$ and so on).

The time ordering operator takes any of this j! terms and simply replaces it by the ordering $\{t_1 > t_2 > .. t_j\}$. This results in (a) cancellation of the j! in the expression and (b) change in the limits of integration to reflect this ordering.

$$T[e^{-i\int_0^t dt' \hat{H}(t')}] = 1 + \sum_{j=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 .. \int_0^{t_{j-1}} dt_j \hat{H}(t_1)\hat{H}(t_2)...\hat{H}(t_j)$$

is a correct but almost always useless formula by itself (i.e. without any further approximations).

It is however a good starting point for making various approximations.

Time Dependent Hamiltonians

The main reason that time-dependent Hamiltonians are harder to work with is that the Hamiltonian operator at different times do not commute with each other.

Example: A Harmonic oscillator kicked by a spatially uniform time-dependent external force

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 + f(t)\hat{x} \qquad [\hat{H}(t_1), \hat{H}(t_2)] = \frac{i\hbar(f(t_1)-f(t_2))}{m}\hat{p}$$

Since Hamiltonians at different times do not commute, we cannot diagonalize them simultaneously. There is thus no obvious choice of basis to work with.

We will look at different approximation schemes to deal with time-dependent Hamiltonians, which involve making different choice of basis to expand the problem

- Time Dependent Perturbation Theory: Time dependent part of the Hamiltonian is parametrically small. Expand in eigenbasis of time-independent part of the Hamiltonian.

- Adiabatic Limit: The rate of change of Hamiltonian is parametrically small. Expand in the time dependent basis which diagonalizes the instantaneous Hamiltonian.

- Rotating Wave Approximation: Work with a time-dependent basis and neglect the fast varying part of the Hamiltonian to get an effective time-independent Hamiltonian. Work with eigenbasis of this effective Hamiltonian

Interaction Representation

Consider a Hamiltonian formed of two parts $\hat{H} = \hat{H}_0 + \hat{H}_1$

The breakup can be motivated by different considerations:

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

$\hat{H}_0$	$\hat{H}_1$
A Hamiltonian that can be solved e.g. free particle	Part that cannot be solved e.g. Particle-Particle Interaction

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

$\hat{H}_0$	$\hat{H}_1$
Time indep. part of Hamiltonian	Time dep. part of Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

$\hat{H}_0$	$\hat{H}_1$
Hamiltonian of system	Probe-system Interaction

Interaction Representation: Put the time evolution due to $\hat{H}_0$ on the operators and the rest on the states.

Define $|\psi_I(t)\rangle = e^{i\hat{H}_0 t}|\psi_S(t)\rangle$ $\qquad$ $|\psi_S(t)\rangle = e^{-i\hat{H}_0 t}|\psi_I(t)\rangle$

Schrodinger Eqn.: $$i\partial_t|\psi_S(t)\rangle = (\hat{H}_0 + \hat{H}_1)|\psi_S(t)\rangle$$

$$e^{-i\hat{H}_0 t}(\hat{H}_0 + i\partial_t)|\psi_I(t)\rangle = (\hat{H}_0 + \hat{H}_1)e^{-i\hat{H}_0 t}|\psi_I(t)\rangle$$

$$i\partial_t|\psi_I(t)\rangle = e^{i\hat{H}_0 t}\hat{H}_1 e^{-i\hat{H}_0 t}|\psi_I(t)\rangle$$

Interaction Representation

$$i\partial_t|\psi_I(t)\rangle = \hat{H}_{1I}|\psi_I(t)\rangle \qquad \hat{H}_{1I}(t) = e^{i\hat{H}_0 t}\hat{H}_1(t)e^{-i\hat{H}_0 t}$$

Possible time dependence of parameters of H_1

$$\boxed{\text{Define} \quad \hat{A}_I(t) = e^{i\hat{H}_0 t}\hat{A}e^{-i\hat{H}_0 t}}$$

for any operator A , i.e. operators evolve as in Heisenberg rep, but with H_0

States evolve as in Schrodinger rep., but with the interaction rep. of H_1

We will assume that eigenstates and spectrum of $\hat{H}_0$, or approximations to them, are known

$\hat{H}_0|n\rangle = \epsilon_n|n\rangle$ and expand in this basis

$$|\psi_S(t)\rangle = \sum_n c_n(t)e^{-i\epsilon_n t}|n\rangle \Rightarrow |\psi_I(t)\rangle = \sum_n c_n(t)|n\rangle$$

$$i\partial_t c_n(t) = \sum_m e^{i(\epsilon_n - \epsilon_m)t}\hat{H}_{1mn}(t)$$

Driven Harmonic Oscillator: a special case

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2 = \omega_0(a^\dagger a + 1/2) \qquad H_1 = -f(t)x = -f(t)(a^\dagger + a)$$

Spatially uniform force

Work in the interaction picture : $H_{1I} = e^{iH_0 t} H_1 e^{-iH_0 t} = -f(t) e^{i\omega_0 t a^\dagger a}(a^\dagger + a) e^{-i\omega_0 t a^\dagger a}$

Use $[a^\dagger a, a^\dagger] = a^\dagger \qquad [a^\dagger a, a] = -a$

$$e^{i\omega_0 t a^\dagger a} a^\dagger e^{-i\omega_0 t a^\dagger a} = a^\dagger + \sum_{n=1}^{\infty} (i\omega_0 t)^n / n! [a^\dagger a, [a^\dagger a, \ldots [a^\dagger a, a] \ldots]] = a^\dagger e^{i\omega_0 t}$$

Similarly $e^{i\omega_0 t a^\dagger a} a e^{-i\omega_0 t a^\dagger a} = a e^{-i\omega_0 t}$

Interaction Picture Hamiltonian: $\boxed{H_{1I} = -f(t)(a^\dagger e^{i\omega_0 t} + a e^{-i\omega_0 t})}$

$$[H_{1I}(t), H_{1I}(t')] = f(t)f(t')[(a^\dagger e^{i\omega_0 t} + a e^{-i\omega_0 t}), (a^\dagger e^{i\omega_0 t'} + a e^{-i\omega_0 t'})] = -2if(t)f(t')\sin[\omega_0(t - t')]$$

Constant

Driven Harmonic Oscillator: a special case

$$[H_{1I}(t), [H_{1I}(t'), H_{1I}(t'')]] = 0$$

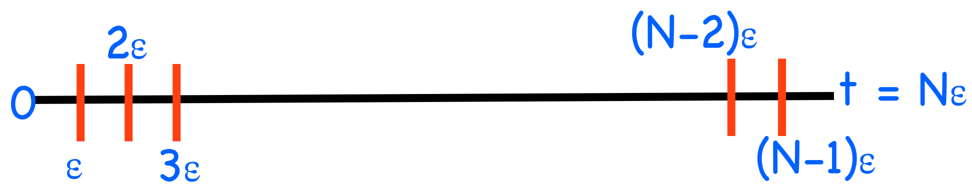
Crucial in making this problem a solvable one

Interaction picture Eqn. of motion:

$$i\partial_t |\psi_I(t)\rangle = \hat{H}_{1I} |\psi_I(t)\rangle$$

Time Evolution Operator:

$$U(t,0) = T[e^{-i\int_0^t H_{1I}(t')dt'}]$$



Total Error ~ N ε² ⟶ 0

when N ⟶∞, ε ⟶ 0,

$N \to \infty \quad \epsilon \to 0 \quad N\epsilon = t$

so that Nε is fixed

$$U(t,0) = Lim_{N\to\infty} \prod_{m=1}^{N} U(m\epsilon, (m-1)\epsilon) = Lim_{N\to\infty} \prod_{m=1}^{\infty} e^{-i\int_{(m-1)\epsilon}^{m\epsilon} H_{1I}(t')dt'}$$

Trotter error due to taking off the time ordering $\sim \epsilon^2$

Driven Harmonic Oscillator

Now $$e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$$ when $$[A,[A,B]]=0$$

So

$$e^{-i\int_{m\epsilon}^{(m+1)\epsilon} H_{1I}(t'')dt''} e^{-i\int_{(m-1)\epsilon}^{m\epsilon} H_{1I}(t')dt'} = e^{-i\int_{(m-1)\epsilon}^{(m+1)\epsilon} H_{1I}(t')dt' - \frac{1}{2}\int_{m\epsilon}^{(m+1)\epsilon} dt'' \int_{(m-1)\epsilon}^{m\epsilon} dt' [H_{1I}(t'),H_{1I}(t'')]}$$

$$U(t,0) = e^{-i\int_0^t H_{1I}(t')dt' - \frac{1}{2}\int_0^t dt' \int_0^{t'} dt'' [H_{1I}(t'),H_{1I}(t'')]}$$

$$= e^{i\beta(t)+\zeta(t)a^\dagger - \zeta^*(t)a} = e^{i\beta(t)}D[\zeta(t)]$$

$$\boxed{\zeta(t) = -i\int_0^t dt' f(t') e^{i\omega_0 t'}}$$

$$\boxed{\beta(t) = \int_0^t dt' \int_0^{t'} dt'' f(t') f(t'') \sin[\omega_0(t'-t'')]}$$

Convert back to Schrodinger picture:

$$U(t) = e^{-iH_0 t} U_I(t) e^{iH_0 t} = e^{i\beta t} D[\zeta(t) e^{-i\omega_0 t}] e^{-iH_0 t}$$

If we start with the ground state, the drive produces coherent states and upto a phase, the dynamics is that of coherent states.