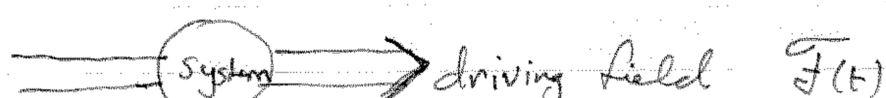
Lecture 24: <u>Introduction to open quantum systems and time dependent perturbation theory</u>

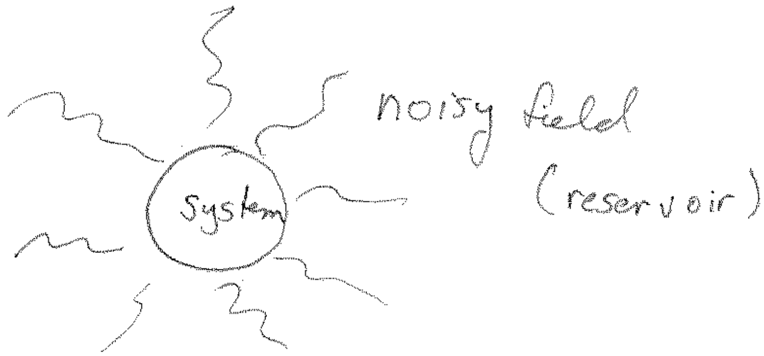
• <u>Overview:</u>

A standard physical paradigm is to take a system of interest and "drive it" with a time dependent force



In some sense this is akin to the scattering problem we have been studying for the last few lectures, except here we treat the incident field <u>classically</u> (e.g. classical E/M wave or $\vec{B}$ field). We can in principle treat such a problem in terms of the quantized field ⇒ scattering of photons (perhaps inelastic and absorption)

When the field has a harmonic time dependence $\mathcal{F}(t) = \mathcal{F}_0 \cos(\omega_0 t + \phi)$, we know that in general there will be <u>resonant</u> behavior if the driving frequency ~~is~~ near to one of the natural ~~resonance~~ oscillation frequencies of the system. Such phenomena will be manifest in the quantum system. This will generally lead to regular time evolution of the system, i.e. <u>coherent evolution</u>.



In addition / alternatively the driving field may not have a regular time dependence but instead be noise; e.g. thermal fluctuation in a bath "reservoir". This can lead to incoherent (irreversible) behavior of the quantum system. Our goal for the next few weeks to ~~better~~ understand these phenomena.

We will generically write the Hamiltonian for such a system as

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_{int}(t)$$

where $\hat{H}_0$ is the unperturbed "free" Hamiltonian

$\hat{H}_{int}(t)$ is the time dependent interaction Hamiltonian arising from the perturbation

Note: in general $\frac{d\hat{A}(t)}{dt} = -\frac{i}{\hbar}[\hat{A}(t), \hat{H}(t)] + \frac{\partial \hat{A}}{\partial t}$

$$\Rightarrow \frac{d\hat{H}(t)}{dt} = \frac{\partial \hat{H}(t)}{\partial t} \neq 0 \Rightarrow$$ Energy is not a constant of the motion

System can absorb or emit energy w.r.t. perturbing field. NO simple stationary states

The Interaction (Dirac) Picture

In dealing with time-dependent problems, it is typically simpler to first remove the time dependence we know from $\hat{H}_0$, and concentrate on the unknown dynamics arising from the perturbation. This amounts to going to Dirac's "Interaction Picture"

Recall: Schrödinger vs. Heisenberg Pictures

- Schrödinger: Evolve states $|\psi(t)\rangle^{(S)} = \hat{U}(t)\,|\psi(0)\rangle^{(S)}$

  Operators $\hat{A}^{(S)}$ are constant (unless explicity classical time dependence)

  Matrix elements: $\langle\psi^{(S)}_{(t)}|\hat{A}^{(S)}|\psi^{(S)}_{(t)}\rangle$

  $= \langle\psi^{(S)}(0)|\hat{U}^{\dagger}_{(t)}\,\hat{A}^{(S)}\,\hat{U}(t)|\psi^{(S)}_{(0)}\rangle$

- Heisenberg: States are constant: $|\psi\rangle^{(H)}$

  Observables evolve: $\hat{A}^{(H)}(t) = \hat{U}^{\dagger}(t)\,\hat{A}^{(H)}\,\hat{U}(t)$

Matrix elements: $\langle\psi^{(H)}|\hat{A}^{(H)}_{(t)}|\psi^{(H)}\rangle = \langle\psi^{(H)}|\hat{U}^{\dagger}_{(t)}\,\hat{A}^{(H)}_{(0)}\hat{U}(t)|\psi^{(H)}\rangle$

$\hat{U}(t)$ is solution to $\dfrac{d\hat{U}(t)}{dt} = -\dfrac{i}{\hbar}\,\hat{H}(t)\,\hat{U}(t)$

↖ Same in S + H picture

Self-consistent ~~if~~ $|\psi^{(H)}\rangle = |\psi^{(S)}(0)\rangle \qquad \hat{A}^{(S)} = \hat{A}^{(H)}(0)$

Schrödinger eqn: $\dfrac{d}{dt}|\psi^{(S)}(t)\rangle = -\dfrac{i}{\hbar}\,\hat{H}(t)\,|\psi^{(S)}(t)\rangle$

Heisenberg eqn: $\dfrac{d}{dt}\hat{A}^{(H)}(t) = -\dfrac{i}{\hbar}\left[\hat{A}^{(H)}_{(t)}, \hat{H}(t)\right] + \dfrac{\partial\hat{A}^{(H)}(t)}{\partial t}$

• <u>Interaction picture:</u> "Half-way" between S + H

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_{int}(t)$$

Evolve operators by $\hat{H}_0$
states by $\hat{H}_{int}$

Define: "Free evolution" operator $\hat{U}_0(t)$

$$\frac{d\hat{U}_0}{dt} = -\frac{i}{\hbar}\hat{H}_0\hat{U}_0 \Rightarrow \hat{U}_0(t) = e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

- Interaction picture operators $\hat{A}^{(I)}(t) = \hat{U}_0^\dagger(t)\,\hat{A}^{(S)}(0)\,\hat{U}_0(t)$

Note at $t=0$ all pictures agree $\hat{A}^{(I)}(0) = \hat{A}^{(S)}$

- Interaction picture states: Remove free evolution

$$|\Psi(t)\rangle^{(I)} = \hat{U}_0^\dagger(t)\,|\Psi(t)\rangle^{(S)}$$

$$= \hat{U}_0^\dagger(t)\,\hat{U}(t)\,|\Psi(0)\rangle^{(S)}$$

$$\Rightarrow \frac{d}{dt}|\Psi(t)\rangle^{(I)} = \left(\frac{d\hat{U}_0^\dagger}{dt}\right)\hat{U}(t)|\Psi(0)\rangle + \hat{U}_0^\dagger\frac{d\hat{U}}{dt}|\Psi(0)\rangle$$

$$= \frac{i}{\hbar}\left(\hat{U}_0^\dagger\hat{H}_0\,\hat{U}(t) - \hat{U}_0^\dagger\hat{H}(t)\,\hat{U}(t)\right)|\Psi(0)\rangle$$

$$= -\frac{i}{\hbar}\left[\hat{U}_0^\dagger(\hat{H}(t) - \hat{H}_0)\,\hat{U}_0\right]\hat{U}_0^\dagger\,\hat{U}(t)\,|\Psi(0)\rangle$$

$$= -\frac{i}{\hbar}\left(\hat{U}_0^\dagger\hat{H}_{int}(t)\,\hat{U}_0\right)\hat{U}_0^\dagger\,\hat{U}(t)\,|\Psi(0)\rangle$$

Now $\hat{U}_0^{+} \hat{H}_{int}(t) \hat{U}_0 = \hat{H}_{int}^{(I)}(t)$ (Interaction Hamiltonian in "Interaction picture")

$$\hat{U}_0^{+} \hat{U}(t) |\Psi(0)\rangle = |\Psi(t)\rangle^{(I)}$$

$$\Rightarrow \boxed{\frac{d}{dt} |\Psi(t)\rangle^{(I)} = -\frac{i}{\hbar} H_{int}^{(I)}(t) \, |\Psi(t)\rangle^{(I)}}$$

Schrodinger Eqn in the Interaction picture

Note: If we define $\hat{U}^{(I)}(t) = \hat{U}_0^{+}(t) \hat{U}(t)$

$$|\Psi(t)\rangle^{(I)} = \hat{U}^{(I)}(t) \, |\Psi(0)\rangle$$

$$\boxed{\frac{d}{dt} \hat{U}^{(I)}(t) = -\frac{i}{\hbar} \hat{H}_{int}^{(I)}(t) \, \hat{U}^{(I)}(t)}$$

Propagator in the interaction picture

Note: Generally $[\hat{H}_{int}^{(I)}(t), \hat{H}_{int}^{(I)}(t')] \neq 0$

$$\Rightarrow \hat{U}^{(I)}(t) \neq e^{-i \int_0^t \hat{H}_{int}(t') dt'}$$

<u>Dyson - series</u>

A formal solution for the propagator is

$$\hat{U}^{(I)}(t) = \hat{\mathbb{1}} - \frac{i}{\hbar} \int_0^t \hat{H}_{int}^{(I)}(t') \, \hat{U}^{(I)}(t') \, dt'$$

having used $\hat{U}^{(I)}(0) = \hat{\mathbb{1}}$

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We can now write an infinite series solution by iteration:

$$\hat{U}^{(I)}(t) = \hat{\mathbb{1}} - \frac{i}{\hbar}\int_0^t \hat{H}^{(I)}_{int}(t')\left(\hat{\mathbb{1}} - \frac{i}{\hbar}\int_0^{t'} \hat{H}^{(I)}_{int}(t'')\, \hat{U}^{(I)}_{int}(t'')\right)$$

$$= \hat{\mathbb{1}} - \frac{i}{\hbar}\int_0^t \hat{H}^{(I)}_{int}(t')\,dt' + \left(\frac{-i}{\hbar}\right)^2 \int_0^t \hat{H}^{(I)}_{int}(t') \int_0^{t''} \hat{H}^{(I)}_{int}(t'')\, \hat{U}^{(I)}_{int}(t'')$$

$$= \hat{\mathbb{1}} - \frac{i}{\hbar}\int_0^t dt'\, \hat{H}^{(I)}_{int}(t') + \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt''\, \hat{H}^{(I)}_{int}(t')\, \hat{H}^{(I)}_{int}(t'')$$

$$+ \left(\frac{-i}{\hbar}\right)^3 \int_0^t dt' \int_0^{t'} dt'' \int_0^{t''} dt'''\, \hat{H}^{(I)}_{int}(t')\, \hat{H}^{(I)}_{int}(t'')\, \hat{H}^{(I)}_{int}(t''')$$

$$+ \cdots$$

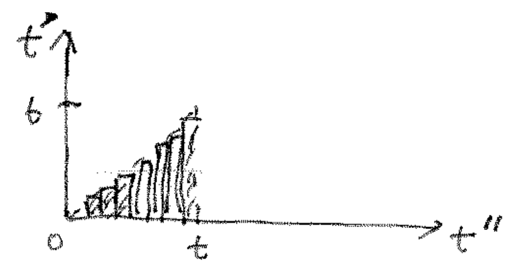
"Dyson series" (Analogous to time-independent Green's function we studied in scattering)

Note: In a given term there is a "time-ordering"

e.g. 2nd order term $\int_0^t dt' \int_0^{t'} dt''\, \hat{H}^{(I)}_{int}(t')\, \hat{H}^{(I)}_{int}(t'')$

$t'' < t'$ always

Integration region:



If $\left[\hat{H}^{(I)}_{int}(t'), \hat{H}^{(I)}_{int}(t'')\right] = 0$

$$\Rightarrow \int_0^t dt' \int_0^{t'} dt''\, \hat{H}^{(I)}_{int}(t')\, \hat{H}^{(I)}_{int}(t'') = \frac{1}{2}\left[\int_0^t dt'\, \hat{H}_{int}(t')\right]^2$$

Similarly third order term $= \frac{1}{3!}\left[\int_0^t dt'\, \hat{H}_{int}(t')\right]^3$

Thus, if $[\hat{H}^{(I)}_{int}(t_1), \hat{H}^{(I)}_{int}(t_2)] = 0 \quad \forall t_1, t_2$

$$\Rightarrow \hat{U}^{(I)}_{int}(t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar} \int_0^t dt' \, \hat{H}^{(I)}_{int}(t') \right)^n = e^{-\frac{i}{\hbar} \int_0^t \hat{H}^{(I)}_{int}(t') dt'}$$

as expected

However, in most cases $\hat{H}^{(I)}_{int}(t)$ <u>does not</u> commute at different times.

$$\Rightarrow \int_0^t dt' \int_0^{t'} dt'' \, \hat{H}^{(I)}_{int}(t') \, \hat{H}^{(I)}_{int}(t'') = \frac{1}{2} T \left\{ \int_0^t dt' \, \hat{H}_{int}(t')^2 \right\}$$

where I have used the "time-ordering" operator

$$T\{ \hat{A}(t_1) \hat{B}(t_2) \} = \begin{cases} \hat{A}(t_1) \hat{B}(t_2) & t_1 < t_2 \\ \hat{B}(t_2) \hat{A}(t_1) & t_2 < t_1 \end{cases}$$

In the general case:

$$\hat{U}^{(I)}_{int}(t) = \sum_{n=0}^{\infty} \frac{1}{n!} T \left\{ \left(\frac{-i}{\hbar} \int_0^t dt' \, \hat{H}_{int}(t') \right)^n \right\}$$

$$\Rightarrow \boxed{\hat{U}^{(I)}_{int}(t) = T \left\{ \exp\left[\frac{-i}{\hbar} \int_0^t dt' \, \hat{H}_{int}(t') \right] \right\}}$$

"Time ordered exponential"

This is a very useful expression in relativistic quantum field theory

Transition Probability and Perturbation theory

Suppose the system is initially prepared in state of $\hat{H}_0$

$$|\psi(0)\rangle = |u_i\rangle \qquad \hat{H}_0 |u_i\rangle = E_i$$

When the external forcing field is applied the system will generally not remain in $|u_i\rangle$ but evolve in time. If the field is sufficiently "weak" it can be thought of as a "perturbation" which does not change (drastically) the basic energy level structure. It can however induce transitions between these levels. The basic goal of Time dependent perturbation theory is to determine the transition rate.

In the interaction picture the time-evolved state is

$$|\psi(t)\rangle^{(I)} = \hat{U}^{(I)}(t)\, |\psi(0)\rangle = \hat{U}^{(I)}(t)\, |u_i\rangle$$

$\Rightarrow$ Probability to find state $|u_f\rangle$ at time t given state $|u_i\rangle$ at $t=0$

$$P_{f\leftarrow i}(t) = \left|\langle u_f | \psi(t)\rangle^{(I)}\right|^2 = |\langle u_f|\, \hat{U}^{(I)}(t)\, |u_i\rangle|^2$$

$$= \left|\langle u_f|\, T\left\{ e^{-\frac{i}{\hbar}\int_0^t dt'\, \hat{H}^{(I)}_{int}(t')} \right\} |u_i\rangle\right|^2$$

$$= \left|\langle u_f| \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n T\left\{\left(-\frac{i}{\hbar}\int_0^t dt'\, \hat{H}^{(I)}_{int}(t')\right)^n\right\} |u_i\rangle\right|^2$$

Now we make the approximation that the interaction is <u>weak</u> so that we only take into account finite powers of the interaction Hamiltonian.

$$\Rightarrow \hat{U}^{(I)}(t) = \underbrace{\hat{\mathbb{1}}}_{\text{zero}^{\text{th}}\text{ order}} \underbrace{- \frac{i}{\hbar}\int_0^t dt' \, \hat{H}^{(I)}_{int}(t')}_{\text{first order}} \underbrace{+ \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int^{t'} dt'' \, \hat{H}_{int}(t') \, \hat{H}_{int}(t'')}_{\text{second order}}$$

$$\Rightarrow P_{f \leftarrow i}(t) = \left| c^{(0)}_{fi} + c^{(1)}_{fi} + c^{(2)}_{fi} + \dots \right|^2$$

$$c^{(0)}_{fi} = \langle u_f | \hat{\mathbb{1}} | u_i \rangle = \delta_{fi}$$

$$c^{(1)}_{fi} = -\frac{i}{\hbar} \int_0^t dt' \, \langle u_f | \hat{H}^{(I)}_{int}(t') | u_i \rangle$$

$$c^{(2)}_{fi} = \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \, \langle u_f | \hat{H}^{(I)}_{int}(t') \, \hat{H}^{(I)}_{int}(t'') | u_i \rangle$$

etc.

The transcition rate $w_{f \leftarrow i} = \dfrac{dP_{f \leftarrow i}}{dt}$

<u>Note</u>: This is a very "classical" picture. It conjures this image of the system actually "being" in state $|u_i\rangle$ and the "jumping" to state $|u_f\rangle$. One of our goals is to better understand when this is a good picture.