Time dependent perturbation theory

Schrodinger Picture

$$|\Psi(t)\rangle = e^{-iHt} |\Psi(0)\rangle$$

$$\langle O(t)\rangle = \langle \Psi(t)| O_s |\Psi(t)\rangle$$

Heisenberg Picture

$$|\Psi_H\rangle = |\Psi(0)\rangle$$

$$O_H(t) = e^{iHt} O_s e^{-iHt}$$

$$\langle O(t)\rangle = \langle \Psi_H | O_H(t) |\Psi_H\rangle$$

Interaction Picture

$$H = H_0 + V(t)$$

$$|\Psi_I(t)\rangle = e^{iH_0 t} |\Psi_S(t)\rangle$$
$$= e^{iH_0 t} e^{-iHt} |\Psi_H\rangle$$

$$O_I(t) = e^{iH_0 t} O_s e^{-iH_0 t}$$

$$\langle O(t)\rangle = \langle \Psi_I(t)| O_I(t) |\Psi_I(t)\rangle$$

All three pictures give the same probabilities, expectation values and ensemble averages

equations of motion

$$\frac{d|\Psi_I(t)\rangle}{dt} = \frac{d}{dt}\left(e^{iH_0t}|\Psi_s(t)\rangle\right)$$

$$= e^{iH_0t}\left(iH_0|\Psi_s(t)\rangle + \frac{d|\Psi_s(t)\rangle}{dt}\right)$$

$$= e^{iH_0t}(iH_0 - iH)|\Psi_s(t)\rangle$$

$$= e^{iH_0t}(-iV)|\Psi_s(t)\rangle =$$

$$= -i\underbrace{e^{iH_0t}Ve^{-iH_0t}}_{V_I(t)}\underbrace{e^{iH_0t}|\Psi_s(t)\rangle}_{|\Psi_I(t)\rangle}$$

$$= -iV_I(t)|\Psi_I(t)\rangle$$

$$\boxed{\begin{aligned} \frac{d|\Psi_I(t)\rangle}{dt} &= -i V_I(t)|\Psi_I(t)\rangle \\ |\Psi_I(0)\rangle &= |\Psi_S(0)\rangle = |\Psi_H\rangle \end{aligned}}$$

The differential equation and initial condition can be replaced by a single integral equation

$$\int_0^t \frac{d|\Psi_I(t')\rangle}{dt'}dt' = -i\int_0^t V_I(t')|\Psi_I(t')\rangle dt'$$

$$\boxed{|\Psi_I(t)\rangle = |\Psi_I(0)\rangle - i\int_0^t V_I(t')|\Psi_I(t')\rangle dt'}$$

* This is useful when $e^{iH_0 t}$ can be calculated explicitly

* This picture has the feature that iteration of the integral equation leads to an expansion in powers of V

* since in general $[H_0, V_s] \neq 0$ this means $[V(t), V(t')] \neq 0$ for $t \neq t'$

* The picture is useful for Hamiltonians with time dependent potentials

The time dependence could be as simple as turning on a time independent perturbation at a given

time in an interaction with
a complex time dependence

Solution by iteration –
this is a generalization
of the method used to
solve differential equations
for small time

$$|\Psi_I(t)\rangle = \lim_{n\to\infty} |\Psi_n(t)\rangle$$

where

$$|\Psi_0(t)\rangle = |\Psi_S(0)\rangle = |\Psi_H\rangle$$

$$|\Psi_n(t)\rangle = |\Psi_I(0)\rangle - i\int_0^t V_I(t')\,|\Psi_{n-1}(t')\rangle\,dt'$$

It is useful to write out
the first few terms in
this series

$$|\Psi_1(t)\rangle = |\Psi_I(0)\rangle - i\int_0^t V_I(t')\,|\Psi_I(0)\rangle\, dt'$$

$$|\Psi_2(t)\rangle = |\Psi_I(0)\rangle$$
$$- i\int_0^t V_I(t')\left[\,|\Psi_I(0)\rangle - i\int_0^{t'} V_I(t'')\,|\Psi_I(0)\rangle\, dt''\right] dt'$$

$$= |\Psi_I(0)\rangle - i\int_0^t dt_1\, V_I(t_1)\,|\Psi_I(0)\rangle\, dt_1$$
$$(-i)^2\int_0^t dt_1\int_0^{t_1} dt_2\, V_I(t_1)\,V_I(t_2)\,|\Psi_I(0)\rangle$$

similarly

$$|\Psi_3(t)\rangle = |\Psi_I(0)\rangle - i\int_0^t dt_1\, V_I(t_1)\,|\Psi_I(0)\rangle$$
$$(-i)^2\int_0^t dt_1\int_0^{t_1} dt_2\, V_I(t_1)\,V_I(t_2)\,|\Psi_I(0)\rangle$$
$$(-i)^3\int_0^t dt_1\int_0^{t_1} dt_2\int_0^{t_2} dt_3\, V_I(t_1)\,V_I(t_2)\,V_I(t_3)$$
$$\times\, |\Psi_I(0)\rangle$$

note that in this expression

$$\boxed{t_1 \geq t_2 \geq t_3} \qquad V_I(t_1)\,V_I(t_2)\,V_I(t_3)$$

One of the complications with this form of the equation is that there are variables in the limits of integratio

for $N=3$ there a $3!$ possible orderings of $t_1 t_2 t_3$ for $0 \leq t_1, t_2, t_3 \leq t$

$t_1 \leq t_2 \leq t_3$ $\quad V_I(t_3) V_I(t_2) V_I(t_1)$

$t_2 \leq t_1 \leq t_3$ $\quad V_I(t_3) V_I(t_1) V_I(t_2)$

$t_3 \leq t_2 \leq t_1$ $\quad V_I(t_1) V_I(t_2) V_I(t_3)$

$t_2 \leq t_3 \leq t_1$ $\quad V_I(t_1) V_I(t_3) V_I(t_2)$

$t_3 \leq t_1 \leq t_2$ $\quad V_I(t_2) V_I(t_1) V_I(t_3)$

$t_1 \leq t_3 \leq t_2$ $\quad V_I(t_1) V_I(t_3) V_I(t_2)$

Integrating of each one of these products of V_I's over the intervals defined by the inequality are identical – they differ by relabeling the t_i

To take advantage of this we define the time ordered product

$$T(V_I(t_1)\cdots V_I(t_N)) =$$

$$\sum_{\text{permutation}} \Theta(\sigma(t_1)-\sigma(t_2))\cdots\Theta(\sigma(t_{N-1})-\sigma(t_N))$$

$$V_I(t_{\sigma(1)})\cdots V_I(t_{\sigma(N)}))$$

For example for $N=2$

$$T(V_I(t_1)V_I(t_2)) =$$

$$\Theta(t_1-t_2)V_I(t_1)V_I(t_2) +$$

$$\Theta(t_2-t_1)V_I(t_2)V_I(t_1)$$

With this notation

$$\Psi_3(t) = |\Psi_I(0)\rangle - i\int_0^t dt_1\, V_I(t_1)\,|\Psi_I(0)\rangle$$

$$\frac{(-i)^2}{2!}\int_0^t dt_1 \int_0^t dt_2\, T\left(V_I(t_1)V_I(t_2)\right)|\Psi_I(0)\rangle$$

$$\frac{(-i)^3}{3!}\int_0^t dt_1 \int_0^t dt_2 \int_0^t dt_3\, T\left(V_I(t_1)V_I(t_2)V_I(t_3)\right)|\Psi_I(0)\rangle$$

The full series can be expressed as

$$\boxed{|\Psi_I(t)\rangle = |\Psi_I(0)\rangle + \sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_0^t dt_1 \cdots \int_0^t dt_n\, T\left(V_I(t_1)\cdots V_I(t_n)\right)}$$

This is called the Dyson series.

It is easy to show that if this series is substituted in the integral equation both sides of the equation are identical

$$\sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int dt_1 \, dt_n \, T(V_I(t_1) \cdots V_I(t_n)) =$$

$$|\Psi_I(0)\rangle - i \int_0^t V_I(t_0) \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int dt_1 \, dt_n \, T(V_I(t_1) \quad V_I(t_n))$$

there are $n+1$ possible places for t_0

$$\int_0^t dt_0 \, dt_n \, V_I(t_0) \, T(V_I(t_1) \quad V_I(t_n)) =$$

$$\frac{1}{n+1} \int dt_0 \quad dt_n \, T(V_I(t_0) \quad V_I(t_n))$$

using this in the equation on the previous page with $n' = n+1$ gives identical expressions on both sides of the equation

$$\boxed{\text{This means if the series converges then it is a solution of the integral equation}}$$

recall

$$\| |\psi\rangle \| = \langle\psi|\psi\rangle^{1/2}$$

$$||| O ||| = \sup_{|\psi\rangle \neq 0} \frac{\| O|\psi\rangle \|}{\| |\psi\rangle \|}$$

From these definition it follows that

$$||| O_2 O_1 ||| \leq ||| O_2 ||| \, ||| O_1 |||$$

$$\| O |\psi\rangle \| \leq ||| O ||| \cdot \| |\psi\rangle \|$$

$$\| |\psi_1\rangle + |\psi_2\rangle \| \leq \| |\psi_1\rangle \| + \| |\psi_2\rangle \|$$

Theorem: Assume $t < \infty$ and $|||V_s(t)||| \leq C < \infty$ for all t then the Dyson series converges

Note the conditions $t < \infty$ and $|||V_s(t)||| < C < \infty$ are important requirements – the series does not necessarily converge when either of these conditions are <u>not</u> satisfied

Proof

First let

$$V_s = \sup_{0 \leq t' \leq t} |||V_s(t')|||$$

next note

$$|||V_I(t')||| \le |||V_s(t')||| \le V_s$$

$$|||V_I(t')||| = |||e^{iH_0t'} V_s(t') e^{-iH_0t'}||| \le$$

$$\underbrace{|||e^{iH_0t'}|||}_{1}\ \underbrace{|||V_s(t')|||}_{\le V_s}\ \underbrace{|||e^{-iH_0t'}|||}_{1}$$

finally note - for any fixed time ordering

$$|||T(V_I(t_1) \quad V_I(t_n))||| =$$

$$|||V_I(t_{\sigma(1)}) \quad V_I(t_{\sigma(n)})||| \le$$

where $t_{\sigma(1)} \ge t_{\sigma(2)} \cdots \ge t_{\sigma(n)}$

$$|||V_I(t_{\sigma(1)})||| \cdot \quad |||V_I(t_{\sigma(n)})||| \le$$

$$V_s^n$$

putting everything together gives

$$\left\| \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \, dt_n \, T\left(V_I(t_1) \cdots V_I(t_n)\right) \times |\Psi_I(0)\rangle \right\|$$

$$\leq \sum_{n=0}^{\infty} \frac{1}{n!} \left\| \int_0^t dt_1 \, dt_n \, T\left(V_I(t_1) \, V_I(t_n)\right) |\Psi_I(0)\rangle \right\|$$

$$\leq \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^t dt_1 \, dt_n \left\| T\left(V_I(t_1) \cdots V_I(t_n)\right) |\Psi_I(0)\rangle \right\|$$

$$\leq \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^t dt_1 \, dt_n \, \left\|\left| T\left(V_I(t_1) \cdots V_I(t_n)\right) \right|\right\| \times \| \Psi_I(0)\rangle \|$$

$$\leq \sum_{n=0}^{\infty} \frac{V_s^n}{n!} \| \Psi_I(0)\rangle \| \int_0^t dt_1 \, dt_n =$$

$$= \sum_{n=0}^{\infty} \frac{t^n V_s^n}{n!} \cdot \| \Psi_I(0)\rangle \|$$

$$= e^{tV} \| \Psi_I(0)\rangle \| < \infty$$

This shows that even though the Dyson series is perturbative, unlike Rayleigh Schrodinger perturbation theory it always converges.

* Solution when

$$H_0 |n\rangle = E_n |n\rangle$$

has been solved.

* expand $|\psi_I(t)\rangle$ in the complete set of eigenstates of H_0

$$\boxed{\begin{aligned} |\psi_I(t)\rangle &= \sum_{n=0}^{\infty} |n\rangle\langle n|\psi_I(t)\rangle \\ &= \sum_{n=0}^{\infty} |n\rangle\, c_n(t) \end{aligned}}$$

in this expansion all of the time dependence of $|\psi_I(t)\rangle$ is in the the coefficients $c_n(t)$

Interpretation of $c_n(t)$

$$|c_n(t)|^2 = |\langle n|\psi_I(t)\rangle|^2 =$$

$$|\langle n|e^{iH_0t}|\psi_s(t)\rangle|^2 =$$

$$|e^{iE_nt}\langle n|\psi_s(t)\rangle|^2 =$$

$$|\langle n|\psi_s(t)\rangle|^2 =$$

probability of finding $|\psi_s(t)\rangle$ in the n^{th} eigenstate of H_0

We can use this expansion in the integral equation to get integral equations of the $c_n(t)$

$$|\Psi_I(t)\rangle = |\Psi_I(0)\rangle - i\int_0^t V_I(t')\,|\Psi_I(t')\rangle\,dt'$$

$$\sum_{n=0}^{\infty} |n\rangle c_n(t) = \sum_{n=0}^{\infty} |n\rangle c_n(0)$$

$$- i\sum_{n=0}^{\infty} \int_0^t V_I(t')\,|n\rangle\, c_n(t')\,dt'$$

multiply both sides of this equation by $\langle m|$

$$\sum_{n=0}^{\infty} \langle m|n\rangle c_n(t) = \sum_{n=0}^{\infty} \langle m|n\rangle c_n(0)$$

$$- i\sum_{n=0}^{\infty} \int_0^t \langle m|V_I(t')|n\rangle\, c_n(t')\,dt$$

which becomes using

$$\langle m|n\rangle = \delta_{mn}$$

$$\langle m|V_I(t)|n\rangle = e^{i(m-n)t}\,\langle m|V_S(t)|n\rangle$$

$$\boxed{c_m(t) = c_m(0) - i\int_0^t e^{i(E_m - E_n)t'} \langle m | V_s(t') | n\rangle c_n(t')\, dt'}$$

This is an infinite set of coupled integral equations for the coefficients $c_m(t)$

The leading approximation for small V is

$$\boxed{c_m(t) \simeq c_m(0) - i\int_0^t e^{i(E_m - E_n)t'} \langle m | V_I(t') | n\rangle c_n(0)}$$

A typical problem is to assume that the system is initially in the n^{th} eigenstate of H_0. Then $c_m(0) = \delta_{mn}$ since $|c_n(0)|^2 = |\langle n|\Psi_s(0)\rangle|^2 = 1$

Then the first order approximation becomes

$$\boxed{c_m(t) = \delta_{mn} - i\int_0^t e^{i(E_m - E_n)t'} \times \langle m|V_s(t')|n\rangle \, dt'}$$

If $V_s(t)$ does not depend on time the integral can be computed analytically

$$C_m(t) \simeq \delta_{mn} + (-i)\frac{1}{i(E_n - E_m)} \times \left(e^{i(E_m-E_n)t} - 1\right)\langle m|V_s|n\rangle$$

$$= \delta_{mn} - \frac{2i}{E_n - E_m} e^{i(E_m-E_n)\frac{t}{2}} \sin\left(\frac{E_m-E_n}{2}t\right) \times \langle m|V|n\rangle$$

for $m \neq n$

$$\boxed{|C_m(t)|^2 = \frac{\sin^2\left(\frac{E_m-E_n}{2}t\right)}{\left((E_n-E_m)/2\right)^2} |\langle m|V|n\rangle|^2}$$

note that although the denominator may vanish — but when it does so does the numerator