Lecture 4

Perturbation theory with path integrals.

Before we embark on this topic, let us reconsider the propagator

$$K(x'',t'';x',a') = \langle x'', t'' \mid x', t' \rangle$$
$$= \langle x'' \mid e^{-\frac{i}{\hbar} H (t''-t')} \mid x' \rangle$$

So far we have only defined K for $t'' > t'$. We can also define it as above for $t'' < t'$ but it will not have the most convenient physical interpretation.

Instead we define the causal propagator:

$$\bar{K}(x'',t'';x',t') = \langle x'', t'' \mid x', t' \rangle \text{ if } t'' > t'$$
$$= 0 \quad \text{if } t'' < t'.$$

This object has a discontinuous derivative at $t'' = t'$. Therefore it no longer satisfies the Schrödinger eqn when ~~[illegible]~~ $t'' \to t'$.

In fact, as $t'' \to t'$ we have

$$\overline{K}(x'', t'+\epsilon; x', t') \to \delta(x''-x') \quad \text{as } \epsilon \to 0+$$
$$= 0 \qquad \text{as } \epsilon \to 0-$$

Thus it contains a step function:

$$\overline{K}(x'', t''; x', t') \to \delta(x''-x')\,\theta(t''-t') + \cdots$$

for t'' near t'.

It follows that

$$\frac{\partial}{\partial t''}\overline{K}(x'', t''; x', t') = \delta(x''-x')\,\delta(t''-t')$$

Hence the Schrödinger eqn satisfied by K is replaced by:

$$-i\hbar\frac{\partial}{\partial t''}\overline{K}(x'', t''; x', t') + H\left(-i\hbar\frac{\partial}{\partial x''}, x''\right)\overline{K}(\cdots)$$
$$= -i\hbar\,\delta(x''-x')\,\delta(t''-t')$$

Thus $\overline{K}$ is a <u>Green's function</u> for the Schrodinger equation.

Now let us consider a Hamiltonian of the form

$$H = H_0 + \lambda V$$

where H_0 is a solvable part (e.g. free particle or harmonic oscillator) and V is a perturbation.

Examples:

i) $H_0 = \frac{\hat{p}^2}{2m}$, $V = \frac{\lambda}{4!}\hat{x}^4$

ii) $H_0 = \frac{\hat{p}^2}{2m} - \frac{1}{2}m\omega^2\hat{x}^2$, $V = \frac{\lambda}{4!}\hat{x}^4$ (or $\hat{x}^6$ or $\sin k\hat{x}$ --)

As far as possible we will avoid specifying H_0 and V in what follows. However we assume λ is a suitably small number so that one can expand the answer

$$K_V(x'', t''; x', t'; \lambda) = K_V(x'', t''; x', t'; 0) + \lambda \frac{\partial}{\partial \lambda} K_V(x'', t''; x', t'; \lambda)\Big|_{\lambda=0} + \frac{1}{2}\lambda^2 \frac{\partial^2}{\partial \lambda^2} K_V(\; --- \; ;\lambda)\Big|_{\lambda=0} + \cdots$$

Clearly $K_V(x'', t''; x', t'; \lambda=0)$ is the same as $K_0(x'', t''; x', t')$ namely the kernel for the solvable Hamiltonian H_0. Our task is to find expressions for the remaining terms in the series in λ.

For this, we simply write:

$$K_V = \int [dx]\, e^{+\frac{i}{\hbar}\int_{t'}^{t''} (L_0 - V)\, dt}$$

where $L_0 - V$ is the Lagrangian corresponding to the Hamiltonian $H = H_0 + V$ (strictly this is true only for velocity-independent forces).

Now

$$e^{\frac{i}{\hbar}\int (L_0 - V)\, dt} = e^{\frac{i}{\hbar}\int L_0\, dt}\; e^{-\frac{i}{\hbar}\int V\, dt}$$

and the second factor can be expanded:

$$e^{-\frac{i}{\hbar}\int V(x(t))\, dt} = 1 - \frac{i}{\hbar}\int_{t'}^{t''} V(x(t))\, dt$$

$$+ \frac{1}{2!}\left(\frac{-i}{\hbar}\right)^2 \int_{t'}^{t''} dt_1 \int_{t'}^{t''} dt_2\; V(x(t_1))\, V(x(t_2))\, dt_1\, dt_2$$

$$+ \cdots$$

Thus if we write

$$K_V(x'', t''; x', t'; \lambda)$$

$$= K_0(x'', t''; x', t')$$

$$+ \sum_{n=1}^{\infty} \lambda^n K_n(x'', t''; x', t')$$

then we can compare terms and find:

$$K_1 = -\frac{i}{\hbar} \int [dx]\, e^{\frac{i}{\hbar} S_0} \int_{t'}^{t''} V(x(t))\, dt$$

$$K_2 = \frac{1}{2!} \left(-\frac{i}{\hbar}\right)^2 \int [dx]\, e^{\frac{i}{\hbar} S_0} \int_{t'}^{t''}\!\!\int_{t'}^{t''} V(x(t_1)) V(x(t_2))\, dt_1\, dt_2$$

etc.

The problem reduces to finding the average values of integrals of V in time, averaged over paths.

Consider K_1. Here we have to evaluate:

$$-\frac{i}{\hbar} \int_{t'}^{t''} dt \int [dx]\, e^{\frac{i}{\hbar} S_0}\, V(x(t))$$

We have already seen how to compute such "insertions" for quantities like $x(t)$ or $x(t_1)\, x(t_2)$. Here we have instead a quantity like $x(t)^4$ <u>and</u> we need to integrate over t.

The principle is the same as was used in lectures 1–2 to calculate the insertion of, say, $x(t)$. Namely, consider all paths from x' to x'' that pass through a fixed point x at time t. Before that we get the (free) propagator $K_0(x,t;x',t')$ and after that we have again a free propagator $K_0(x'',t'';x,t)$. Only when integrating the intermediate variable x, we need to keep track of the insertion $V(x(t))$.

Thus,

$$K_1 = -\frac{i}{\hbar}\int_{-\infty}^{+\infty} dx \int_{t'}^{t''} dt \; K_0(x'',t'';x,t)\, V(x) \times K_0(x,t;x',t')$$

This is now a well-defined calculation given, say, $V(x) = \frac{1}{4!}x^4$ and K_0 to be the free-particle propagator.

In the next order we encounter a subtlety. Consider

$$\int [dx]\, e^{\frac{i}{\hbar} S_0}\, V(x_1, t_1)\, V(x_2, t_2)$$

(which is to be eventually integrated over t_1, t_2). We find different answers in terms of free propagators, depending on whether $t_1 > t_2$ or $t_2 > t_1$

~~B.~~ For $t_1 > t_2$ the above becomes:

$$\text{I} \quad K(x'', t''; x_1, t_1) V(x_1) K_0(x_1, t_1; x_2, t_2) V(x_2)\, K_0(x_2, t_2; x', t')$$

while for $t_2 > t_1$ it becomes instead:

$$\text{II} \quad K(x'', t''; x_2, t_2)\, V(x_2)\, K_0(x_2, t_2; x_1, t_1)\, V(x_1) K_0(x_1, t_1; x', t')$$

Now ~~to~~ in our problem both orderings occur:

$$\int_{t'}^{t''} dt_1 \int_{t'}^{t''} dt_2 = \underbrace{\int_{t'}^{t''} dt_1 \int_{t'}^{t_1} dt_2}_{t_1 > t_2} + \underbrace{\int_{t'}^{t''} dt_2 \int_{t'}^{t_2} dt_1}_{t_2 > t_1}$$

~~Consider the~~ Thus,

$$K_2 = \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 \left[\int_{t'}^{t''} dt_1 \int_{t'}^{t_1} dt_2 \ \text{I} \ + \int_{t'}^{t''} dt_2 \int_{t'}^{t_2} dt_1 \ \text{II} \right]$$

~~Now we use the fact that~~

In I and II we encounter K_0 with the time ordering always correct, i.e. right to left. So each K_0 can be replaced by $\overline{K_0}$ (which is defined for both time orderings, but vanishes for the "wrong" one).

Now $\int_{t'}^{t''} dt_1 \int_{t'}^{t_1} dt_2 \; \overline{\text{I}} = \int_{t'}^{t''} dt_1 \int_{t'}^{t''} dt_2 \; \overline{\text{I}}$

and $\int_{t'}^{t''} dt_2 \int_{t'}^{t_2} dt_1 \; \overline{\text{II}} = \int_{t'}^{t''} dt_1 \int_{t'}^{t''} dt_2 \; \overline{\text{II}}$

where $\overline{\text{I}}$ and $\overline{\text{II}}$ are written in terms of $\overline{K_0}$ which vanishes on the "wrong" time ordering. Now the time integrals are independent and unrestricted. Then we easily see that $\int_{t'}^{t''} dt_1 \int_{t'}^{t''} dt_2 \left[\overline{\text{I}} + \overline{\text{II}}\right]$

However by interchanging $\begin{bmatrix} x_1 \leftrightarrow x_2 \\ t_1 \leftrightarrow t_2 \end{bmatrix}$ in $\overline{\text{II}}$ we can convert it to $\overline{\text{I}}$. Hence,

$$\overline{K_2} = \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 \int_{t'}^{t''} dt_1 \int_{t'}^{t''} dt_2$$

$$\overline{K_0}(x'', t''; x_2, t_2)\, \overline{K_0}(x_2, t_2; x_1, t_1)\, \overline{K_0}(x_1, t_1; x', t')$$

$$V(x_1)\, V(x_2)$$

In the same way,

$$\bar{K}_n = \left(\frac{-i}{\hbar}\right)^n \int_{-\infty}^{+\infty} dx_1 \cdots dx_n \int_{t'}^{t''} dt_1 \cdots dt_n$$

$$\bar{K}_0(x'',t'';x_n,t_n)\,\bar{K}_0(x_n,t_n;x_{n-1},t_{n-1}) \cdots \bar{K}_0(x_1,t_1;x',t')$$

$$\times\; V(x_1) \cdots V(x_n) \,.$$

(The potential factor of $\frac{1}{n!}$ gets cancelled by combining $n!$ terms).

We see the usefulness of the causal propagator $\bar{K}_0$ in giving us a simple formula (and the final answers $\bar{K}_1$, $\bar{K}_2$ etc are also causal)

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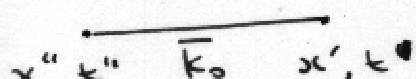
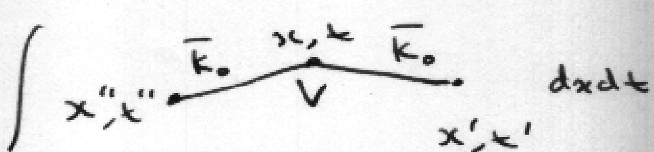
Physical interpretation of perturbation series.

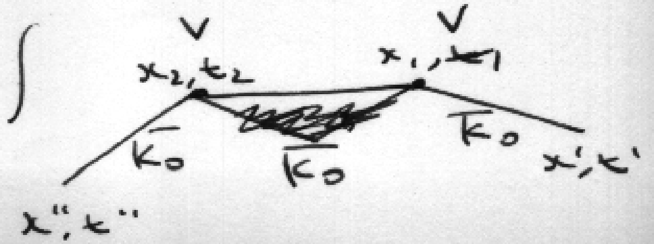
K_0: free propagation:



K_1: propagation with one "scattering" on V



K_2: propagation with two "scatterings"



etc.

Integral equation

Suppressing position labels and integrations for notational simplicity, we can write:

$$\overline{K}_V(t'', t'; \lambda) = \overline{K}_0(t'', t')$$

$$- \frac{i\lambda}{\hbar}\int \overline{K}_0(t'', t) V \overline{K}_0(t, t') \, dt$$

$$+ \left(-\frac{i\lambda}{\hbar}\right)^2 \int \overline{K}_0 V \overline{K}_0 V \overline{K}_0 \, dt_1 dt_2$$

$$+ \cdots$$

$$= \overline{K}_0(t'', t') - \frac{i\lambda}{\hbar}\int dt_1 \overline{K}_0(t'', t_1) V(t_1) \Big[\overline{K}_0(t_1, t')$$

$$- \frac{i\lambda}{\hbar}\int \overline{K}_0(t_1, t_2) V(t_2) \overline{K}_0(t_2, t') \, dt_2$$

$$+ \cdots \Big]$$

Now the expression in brackets is again K_V! Thus,

$$\overline{K}_V(x'', t''; x', t'; \lambda) = \overline{K}_0(x'', t''; x', t')$$

$$- \frac{i\lambda}{\hbar}\int \overline{K}_0(x'', t''; x, t) V(x) \overline{K}_V(x, t; x', t') \, dt \, dx$$

which is an integral equation that self-consistently determines K_V.

Now suppose K_0 is the free particle kernel.
Given that $\overline{K}_0(x'', t''; x', t')$ satisfies

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x''^2} - i\hbar \frac{\partial}{\partial t''} \right) \overline{K}_0 = -i\hbar\, \delta(x''-x')\, \delta(t''-t')$$

we can show that $\overline{K}_V$ satisfies the full Schrödinger eqn:

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x''^2} + \lambda V(x'') - i\hbar \frac{\partial}{\partial t''} \right) \overline{K}_V$$

$$= -i\hbar\, \delta(x''-x')\, \delta(t''-t')$$

Proof:

$$\overline{K}_V = \overline{K}_0 - \frac{i\lambda}{\hbar} \int \overline{K}_0 V \overline{K}_V$$

Then $\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x''^2} + \lambda V(x'') - i\hbar \frac{\partial}{\partial t''} \right) \overline{K}_V(x'', t''; x', t')$

$$= \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x''^2} - i\hbar \frac{\partial}{\partial t''} \right) \overline{K}_0(x'', t''; x', t')$$

$$+ \lambda V(x'')\, \overline{K}_0(x'', t''; x', t')$$

$$- \frac{i\lambda}{\hbar} \int \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x''^2} - i\hbar \frac{\partial}{\partial t''} \right] \overline{K}_0(x'', t''; x, t)$$

$$\times \lambda V(x)\, \overline{K}_0(x, t; x', t') \quad dx\, dt$$

$$- \frac{i\lambda^2}{\hbar} V(x'') \int \overline{K}_0(x'', t''; x, t)\, V(x)\, \overline{K}_V(x, t; x', t') \quad dx\, dt$$

$$= \quad -i\hbar\,\delta(x''-x')\,\delta(t''-t')$$

$$+\lambda V(x'')\,\bar{K}_0(x'',t'';x',t')$$

$$-\frac{i\lambda}{\hbar}\int(-i\hbar)\,\delta(x''-x)\,\delta(t''-t)\,V(x)\,\bar{K}_V(x,t;x',t')\,dx\,dt$$

$$-\frac{i\lambda^2}{\hbar}V(x'')\int\bar{K}_0(x'',t'';x,t)\,V(x)\,\bar{K}_V(x,t;x',t')\,dx\,dt$$

~~= V(x'') t~~

Third line =

$$-\lambda V(x'')\,\bar{K}_V(x'',t'';x',t')$$

Combining $\rightarrow \quad -i\hbar\,\delta(x''-x')\,\delta(t''-t')$

$$+\lambda V(x'')\bar{K}_0(x'',t'';x',t') - \lambda V(x'')\,\bar{K}_V(x'',t'';x',t')$$

$$-\frac{i\lambda^2}{\hbar}V(x'')\int\bar{K}_0 V\bar{K}_V$$

$$= -i\hbar\,\delta(x''-x')\,\delta(t''-t')$$

$$+\lambda\underbrace{\left\{ V(x'')\left(\bar{K}_0-\frac{i\lambda}{\hbar}\int\bar{K}_0 V K_V\right) - V(x'')\bar{K}_V\right\}}_{\rightarrow 0 \text{ by integral eqn}}$$

$$= -i\hbar\,\delta(x''-x')\,\delta(t''-t').$$

Shift of energy to lowest order.

A familiar formula in QM is that (in the absence of degeneracies) each energy eigenvalue $E_n^{(0)}$ receives a correction:

$$\delta E_n = \lambda \langle n | V | n \rangle = \lambda V_{nn},$$

to lowest order in λ. Let's try to recover this in the path-integral approach. To lowest order, we have:

$$K_V(x'',t'';x',t') = K_0(x'',t'';x',t') - \frac{i\lambda}{\hbar}\int K_0(x'',t'';x,t)\, K_0(x,t;x',t')\, V(x)\, dx\, dt$$

Now use: $K_0(x'',t'';x',t') =$

$$\sum_n e^{-i\frac{E_n^{(0)}}{\hbar}(t''-t')}\, \psi_n^{(0)}(x'')\, \psi_n^{*(0)}(x')$$

The second term is:

$$-\frac{i\lambda}{\hbar}\int dx \int_{t'}^{t''} dt \sum_{n_1,n_2} e^{-i\frac{E_{n_1}^{(0)}}{\hbar}(t''-t)}\, e^{-i\frac{E_{n_2}^{(0)}}{\hbar}(t-t')}$$

$$\times\ \psi_{n_1}^{0}(x'')\, \psi_{n_1}^{*0}(x)\, \psi_{n_2}^{0}(x)\, \psi_{n_2}^{*0}(x')$$

$$\times\ V(x)$$

Now the t integral has an oscillating contribution $e^{-\frac{i}{\hbar}(E_{n_2}^{(0)}-E_{n_1}^{(0)})t}$.

To get a large contribution (proportional to $t''-t'$), from the integral we must focus on the terms with $n_1 = n_2$.

These give

$$-\frac{i\lambda}{\hbar} \oint \sum_n \left[\int_{-\infty}^{+\infty} dx\, \psi_n^{*0}(x) V(x) \psi_n^{0}(x) \right]$$

$$\times (t''-t') \times e^{-\frac{i}{\hbar} E_n^{(0)}(t''-t')} \psi_n^{0}(x'') \psi_n^{*0}(x')$$

Adding the first term

$$K_0 = \sum_n e^{-\frac{i}{\hbar} E_n^{(0)}(t''-t')} \psi_n^{0}(x'') \psi_n^{*0}(x')$$

we get:

$$K_V = \sum_n \left(1 - \frac{i\lambda}{\hbar} V_{nn}(t''-t')\right) e^{-\frac{i}{\hbar} E_n^{(0)}(t''-t')} \psi_n^{0}(x'') \psi_n^{*0}(x')$$

$$= \sum_n e^{-\frac{i}{\hbar}(E_n^{(0)} + \lambda V_{nn})(t''-t')} \psi_n^{0}(x'') \psi_n^{*0}(x')$$

and hence we can read off

$$\delta E_n = \lambda V_{nn}.$$

Doing things more carefully we can extract the wave-fn shift (from $n_1 \neq n_2$ terms) and even higher-order terms in perturbation theory.