Lecture 2 - Diagrammatic expansion for systems with pair interactions

08 February 2023 14:00

Lecture 1 summary:

$$\hat{H}\,|\alpha\rangle = \varepsilon_\alpha |\alpha\rangle \Leftrightarrow (\varepsilon^+ - \hat{H})\hat{G}_{(\varepsilon)} = \hat{I}$$

$$G(\underline{r},\underline{r}';\varepsilon) = \langle \underline{r}'|\, G(\varepsilon)\,|\underline{r}\rangle$$

F-L integral:

$$G_0(\underline{r},\underline{r}';\varepsilon) = -i\langle \bar{\psi}(\underline{r})\,\psi(r')\rangle_0$$

$$\equiv -\frac{i}{Z}\int \mathcal{D}\bar{\psi}\mathcal{D}\psi\ \bar{\psi}(\underline{r})\,\psi(\underline{r}')\,e^{iS_\varepsilon}$$

$$S_\varepsilon^+ = \int \bar{\psi}(\underline{r},\varepsilon)\,(\underset{\varepsilon+i\delta}{\underset{\equiv}{\varepsilon^+}} - \hat{H})\,\psi(\underline{r},\varepsilon)\,d\underline{r}$$

$$G_0^+(\underline{r},\underline{r}';\varepsilon) = \sum \frac{\bar{\psi}(\underline{r}')\,\psi(\underline{r})}{\varepsilon - \varepsilon_\alpha + i\delta} \qquad \text{(Lehman's representation)}$$

$\hat{H} \to \hat{H} - \mu\hat{N}$ → to go to the grand canonical ensemble

$\Downarrow$

$\varepsilon_\alpha \to \varepsilon_\alpha - \mu$

$$G_0^+(\underline{r},\underline{r}';\varepsilon) = \sum_\alpha \frac{\bar{\psi}(\underline{r}')\,\psi(\underline{r})}{(\varepsilon-\mu) - \varepsilon_\alpha + i\delta}$$

Next step: introducing the causal GF to be able to make FT to the t-representation is such a way that $e^{-i\varepsilon t}$ doesn't lead to divergence:

$$\hat{G}_0^{\pm} \to \underset{\text{causal}}{\hat{G}_0} = \sum_\alpha \frac{1}{(\varepsilon-\mu) - \varepsilon_\alpha + i\delta\,\mathrm{sgn}(\varepsilon-\mu)}$$

$$\hat{G}_0 = \begin{cases} G_0^+ \equiv G_0^R \ (\text{retarded}) & \text{for } \varepsilon > \mu \\ G_0^- \equiv G_0^A \ (\text{advanced}) & \text{for } \varepsilon < \mu \end{cases}$$

The FT from ε to t is now well defined:

$$S = \int d\underline{r}\, d\varepsilon\ \bar{\Psi}(\underline{r},\varepsilon)\left[\varepsilon - \mu + i\delta\, \mathrm{sgn}(\varepsilon-\mu) - \hat{H}\right]\psi(\underline{r},\varepsilon)$$

Parceval's theorem

$$= \int \underbrace{d\underline{r}\, dt}_{\equiv dx}\ \bar{\Psi}\underbrace{(\underline{r},t)}_{x \equiv (\underline{r},t)}\ \left(i\partial_t - \hat{H} - \mu\right)\psi(\underline{r},t)$$

Relations to observables:

LDoS: $\nu(\underline{r},\varepsilon) = \frac{i}{2\pi}\left(G^R - G^A\right)(\underline{r},\varepsilon) = \frac{1}{\pi}\mathrm{Im}\, G^R(\underline{r},\varepsilon)$

$$\langle \hat{A} \rangle = \int \bar{\Psi}(\underline{r},t)\, \hat{A}\, \psi(\underline{r},t)\, d\underline{r}$$

$$= \lim_{t\to+0} \int \hat{A}\ G(\underline{r},\underline{r};t)\, d\underline{r} =$$

$$= \lim_{t\to+0} \frac{1}{Z} \int \bar{\Psi}(\underline{r},t)\, \hat{A}\, \psi(\underline{r},t)\, e^{iS}\, \mathcal{D}\bar{\psi}\mathcal{D}\psi$$

Average density, $\rho(\underline{r},t) = \sum_i \delta(\underline{r}-\underline{r}_i)$

fixed

$$\langle \rho(\underline{r},t) \rangle = \langle \bar{\Psi}(\underline{r},t)\psi(\underline{r},t)\rangle = i \lim_{t\to+0} G(\underline{r},\underline{r};t)$$

Pair interaction

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{quadratic } H} + \hat{H}_{int}$$

$$\hat{H}_{int} = \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j) =$$

sum over particles

$$= \frac{1}{2} \int d\mathbf{r}\, d\mathbf{r}' \underbrace{\sum_i \delta(\mathbf{r} - \mathbf{r}_i)}_{\rho(\mathbf{r})} \underbrace{\sum_j \delta(\mathbf{r} - \mathbf{r}_j)}_{\rho(\mathbf{r}')} V(\mathbf{r} - \mathbf{r}')$$

(up to the spurious self-interaction, $i = j$)

$$= \frac{1}{2} \int d\mathbf{r}\, d\mathbf{r}' \, \bar{\psi}(\mathbf{r},t) \psi(\mathbf{r},t) V(\mathbf{r} - \mathbf{r}') \bar{\psi}(\mathbf{r}',t) \psi(\mathbf{r}',t)$$

$$= \frac{1}{2} \int d\mathbf{r}\, d\mathbf{r}' \, \bar{\psi}(\mathbf{r},t) \bar{\psi}(\mathbf{r}',t) V(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}',t) \psi(\mathbf{r},t)$$

$$= \frac{1}{2} \int dx\, dx' \, \bar{\psi}(x) \bar{\psi}(x') V(x - x') \psi(x') \psi(x)$$

where $V(x - x') \equiv V(\mathbf{r} - \mathbf{r}') \delta(t - t')$

The leap of faith:

Introduce $S = S_0 + S_{int}$, and

$$G(x, x') \equiv G(\mathbf{r}, \mathbf{r}'; t - t') = -i \langle \bar{\psi}(x) \psi(x') \rangle$$

where $\langle \ldots \rangle = \frac{1}{Z} \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \, (\ldots) \, e^{iS}$

Here $S_0 = \int dx \, \bar{\psi}(x) \left(i \partial_t - \hat{H}_0 - \mu \right) \psi(x)$

$$S_{int} = \frac{1}{2} \int dx\, dx' \, \bar{\psi}(x) \bar{\psi}(x') V(x - x') \psi(x') \psi(x)$$

We can only calculate Gaussian integrals:
we'll get them by expanding

$$e^{iS} = e^{iS_0 + iS_{int}} = e^{iS_0} \sum_{n=0}^{\infty} \frac{(iS_{int})^n}{n!}$$

By analogy with simple Gaussian integrals,

$$\int (\bar{z} z)^n e^{-|z|^2} d\bar{z}\, dz,$$

we shall calculate $\int (\bar{\varphi}\varphi)^{\text{any power}} e^{iS_0} \mathcal{D}\bar{\varphi}\mathcal{D}\varphi$

simple Gaussian we calculate using

$$e^{-(\bar{z}-\bar{h})(z-h)} = e^{-|z|^2 + \bar{h}z + \bar{z}h - \bar{h}h}$$

and using $\frac{\partial^2}{\partial\bar{h}\partial h}$ necessary number of times

We used a similar approach for G_0:

$$S_0[\bar{h},h] = S_0 + \int(\bar{\varphi}h + \bar{h}\varphi)dx$$
$$= S_0 + \bar{\varphi}\circ h + \bar{h}\circ\varphi$$

Then, we used

$$\frac{\delta h(x)}{\delta h(x_1)} = \delta(x - x_1)$$

and, on the other hand, the shift

$$\varphi \to \varphi - h$$
$$\bar{\varphi} \to \bar{\varphi} - \bar{h}$$

gave us the result

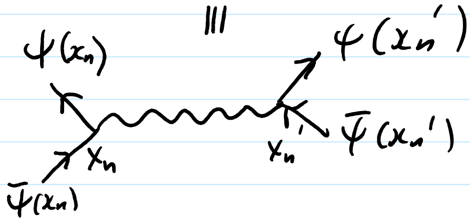
$$\frac{1}{Z}\int e^{iS_0[h]} \mathcal{D}\bar{\varphi}\mathcal{D}\varphi = e^{-\bar{h}\circ G_0\circ h}$$

$$\Rightarrow \quad G_0 = -\frac{i}{2} \int \bar{\psi}\psi \, e^{iS_0} \, D\bar{\psi} D\psi$$

Now we want to use this for multiply ψ's in pre-exponential factor.

Each $S_{int} = \frac{1}{2} \int dx_n dx_n' \, \bar{\psi}(x_n')\bar{\psi}(x_n) V(x_n - x_n') \psi(x_n)\psi(x_n')$

$\equiv$



When calculating G_1 in the 1^{st} order of the expansion we have

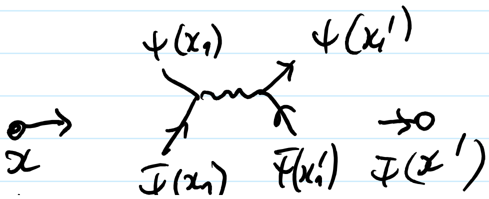
$$G(x,x') = -\frac{i}{2} \int \bar{\psi}(x)\psi(x') \underbrace{\left(\frac{i}{2}\right) \int_{x_1 x_1'} \bar{\psi}(x_1)\bar{\psi}(x_1') V(x_1 - x_1') \psi(x_1')\psi(x_1)}_{i S_{int}} e^{iS_0} D\bar{\psi} D\psi$$

This is equivalent to taking functional derivatives

$$\frac{\delta^2}{\delta \bar{h}(x_1) \delta h(x_1)} \frac{\delta^2}{\delta \bar{h}(x_1') \delta h(x_1')} e^{i \bar{h} \circ G_0 \circ h}$$

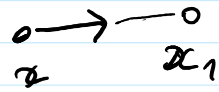
Graphically, we can account for all possible pairings of $\bar{\psi}$ & ψ, by introducing

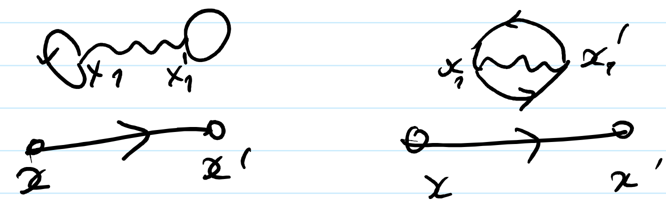
$\equiv G_0(x - x')$



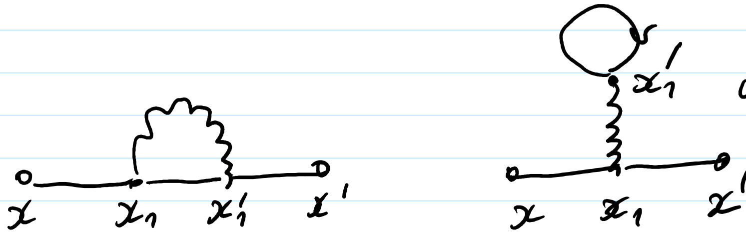
x $\quad \bar\psi(x_1) \quad \bar\psi(x_1') \quad \bar\psi(x')$

$\psi(x)$

We need to pair  to make G_0.



disconnected



connected (we can interchange $x_1 \rightleftarrows x_1'$)

$x_1 \rightleftarrows x_1'$ doubles all these, and compensates $\frac{1}{2}$

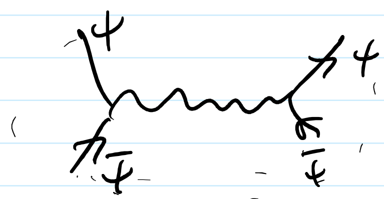
coming from $S_{int} = \frac{1}{2}\int \dots$

For fermions, any closed loop means reordering two ψ's, and hence "-1".

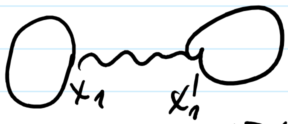
Now we need to make the same expansion in

$$\frac{1}{Z}, \quad Z = \int e^{iS} \mathcal{D}\bar\psi \mathcal{D}\psi$$

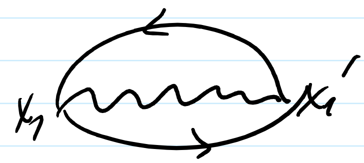
Then, in the 1^{st} order we only have



to pair:



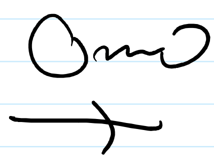
or



$\langle \bar{\psi}(x_1)\psi(x_1)\rangle \langle \bar{\psi}(x_1')\psi(x_1')\rangle$ $\qquad$ $\langle \bar{\psi}(x_1)\psi(x_1')\rangle \langle \bar{\psi}(x_1')\psi(x_1)\rangle$

$$Z = \int e^{iS_0 + iS_{int}} \mathcal{D}\bar{\psi}\mathcal{D}\psi \xrightarrow{1st.\,order} \int iS_{int}\, e^{iS_0} \mathcal{D}\bar{\psi}\mathcal{D}\psi$$

Then, as this expansion comes from the denominator, the sign is opposite to what we had in



Remember: $\langle \bar{\psi}(x)\psi(x')\rangle \neq 0$ as it comes from $\dfrac{\delta^2}{\delta\bar{h}\,\delta h}$

Something like $\langle \bar{\psi}\bar{\psi}\rangle = 0$, as it breaks the symmetry.

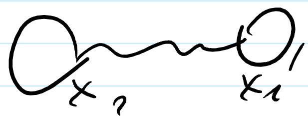
Similarly, $\int z^2 e^{-|z|^2} d\bar{z}\,dz = 0$

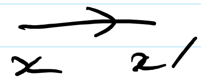
as $z = |z| e^{i\varphi}$

$z^2 = |z|^2 e^{2i\varphi}$ which is killed by the angular integration.

Alternatively, we write 1^{st} order as

$$\underbrace{\bar{\psi}(x)\psi(x')}\ \bar{\psi}(x_1)\bar{\psi}(x_1')\underbrace{\psi(x_1')}\psi(x_1)\ \tfrac{1}{2}V(x_1-x_1')$$





This pairing comes from acting by

$$\frac{\delta^2}{\delta h(x_1)\delta\bar{h}(x_1)}\ \frac{\delta^2}{\delta h(x_1')\delta\bar{h}(x_1')}$$

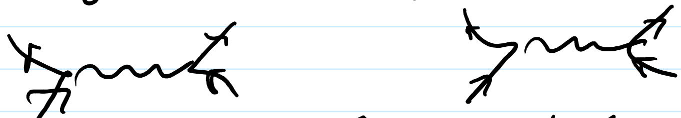
In the 2^{nd} order, we have

$$\frac{1}{2!}\left(iS_{int}\right)^2 = \frac{1}{2!}\int dx_1 dx_1'(\ldots)\int dx_2 dx_2'(\ldots)$$

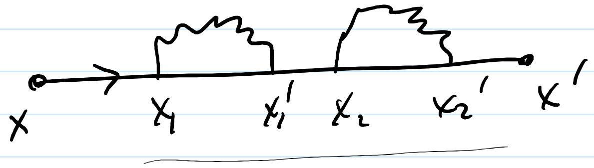
Interchanging $x_1 \rightleftarrows x_2$ compensates $\frac{1}{2!}$.

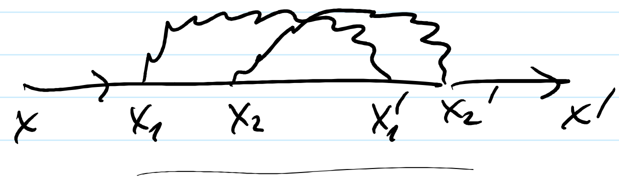
In the n^{th} order, making all the permutations cancels $\frac{1}{n!}$.

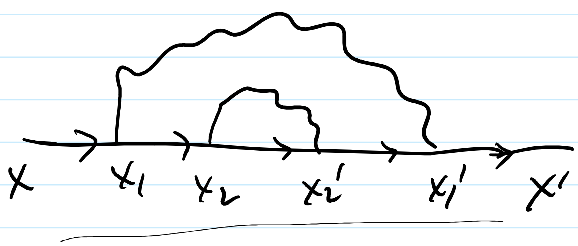
Similarly, $x_n \rightleftarrows x_n'$ cancels $\frac{1}{2}$ coming in the S_{int}.

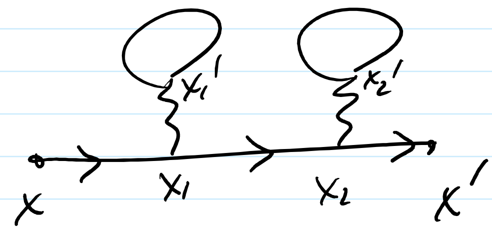
$\to$  so we need to make all connected pairs in the 2^{nd} order

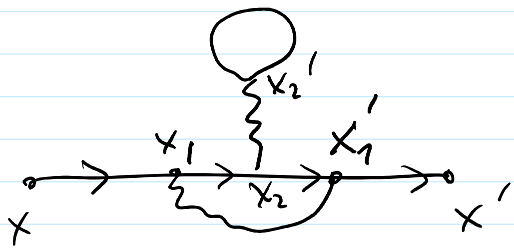
Let's try:

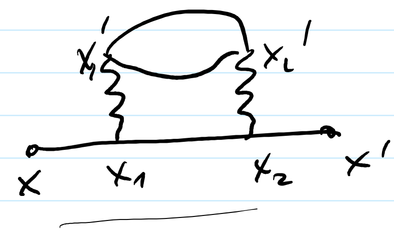


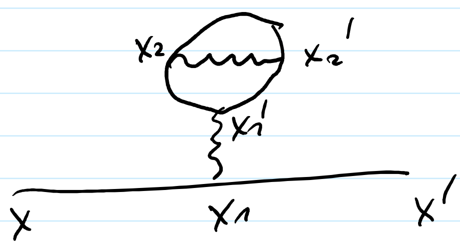










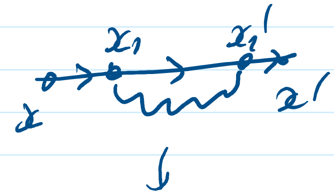


Most important is the cancellation of $\frac{1}{n!}$

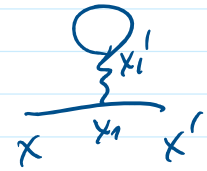
The absence of numerical factors would allow us a graphical diagrammatic summation.

What are the diagrams analytically?

$$G(x,x') = G_0(x,x') +$$



$$+ \int dx_1 dx_1' \, V(x_1 - x_1') \, G_0(x - x_1) \, G_0(x_1 - x_1') \, G_0(x_1' - x')$$

$+$ 

$$+ \int dx_1 dx_1' \, V(x_1 - x_1') \, G_0(x - x_1) \, G_0(x_1 - x') \, G_0(0)$$

Expressions like that are simplified if we can make a FT from the real to the momentum space.

We use the homogeneity by introducing

$$G(q) \equiv G(\underline{p}, \varepsilon) = \int G(x) \, e^{iqx} \, dx$$

$$G(x) = \int G(q) e^{-iqx} \frac{dq}{(2\pi)^{d+1}}$$

Substituting all $G(x - x')$ by the above integrals would give us a couple of δ-functions coming from $\int e^{-iqx} \frac{dq}{(2\pi)^{d+1}} \equiv \delta(x)$