Lecture 6: Bold diagrammatic Monte-Carlo

In the last lecture, we have seen the use of a Monte-Carlo method to resum contributions to the partition function order-by-order for the perturbative expansion of an interacting quantum theory.

The method could sum over all diagrams at a given order by formulating the result as a determinant over all contractions of the relevant correlators. As this is quite efficient, such expansions can be summed up to high order. Notable applications include, besides quantum impurity models, the half-filled Fermi-Hubbard model. However, we also saw that a sign-problem needed to be removed, which is possible only in specific situations.

Furthermore, we did not make use of analytic insight into the character of the perturbative expansion.

- For instance, we know that only connected diagrams contribute to the expectation values of observables, while the disconnected pieces cancel against the normalization factor $1/Z$.
- Likewise, when there are divergent contributions, higher order terms cannot be neglected. Instead, we have to consider a renormalization of the theory, which can be done by re-summing infinite series of diagrams.

These two properties are exploited by the Bold Diagrammatic Monte-Carlo approach, which explicitly

- considers connected diagrams only
- enables re-summations of infinite sums of diagrams.

BDMC for the unitary Fermi-Gas

I will follow: K. v. Houcke et al. arxiv: 1305.3901

The model: Spinful fermions with contact interactions

$$\mathcal{H} = \underbrace{\hat{H}_0 - \sum_\sigma \mu_\sigma \hat{N}_\sigma}_{\hat{K}_0} + \hat{H}_1$$

$$= \overbrace{\sum_\sigma \int^\Lambda \frac{d^3k}{(2\pi)^3} (\varepsilon_k - \mu_\sigma)\, \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma}}^{\hat{K}_0} + g_0 \int d^3r\, \hat{n}_\uparrow(r) \hat{n}_\downarrow(r)$$

For convenience, we have introduced an UV cut-off Λ, and $g_0 = g_0(a_s)$ to be fixed, later.

Bare Fermion Green's function:

$$G_\sigma(p,\tau) = -\langle T_\tau\, \hat{c}_{p\sigma}(\tau)\, \hat{c}^\dagger_{p\sigma}(0) \rangle_0$$

We can calculate this exactly using the Eq. of motion for $\hat{c}$:

$$\hbar \partial_\tau \hat{c}_{p\sigma}(\tau) = [\hat{K}_0, \hat{c}_{p\sigma}(\tau)]$$

$$= e^{+\frac{\tau}{\hbar}\hat{K}_0} \underbrace{[K_0, \hat{c}_{p\sigma}]}_{-(\varepsilon_p - \mu)\hat{c}_{p\sigma}} e^{-\frac{\tau}{\hbar}\hat{K}_0}$$

$$= -(\varepsilon_p - \mu)\, \hat{c}_{p\sigma}$$

by integration

$$\hat{c}_{p\sigma}(\tau) = \hat{c}_{p\sigma}\, e^{-\frac{\varepsilon_p - \mu}{\hbar}\tau}$$

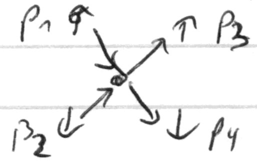
and we have

$$G_\sigma(p,\tau) \stackrel{\text{c}}{=} -e^{-\frac{\varepsilon_p - \mu}{\hbar}\tau} \times \begin{cases} 1 - n^0_p, & \tau > 0 \\ -n^0_p, & \tau > 0. \end{cases}$$

or, in frequency space $G_\sigma(p, i\omega_n) = \dfrac{1}{i\omega_n - (\varepsilon_p - \mu)}$

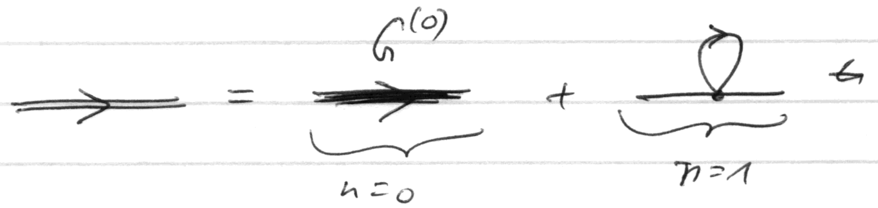
The dressed Fermion Propagator

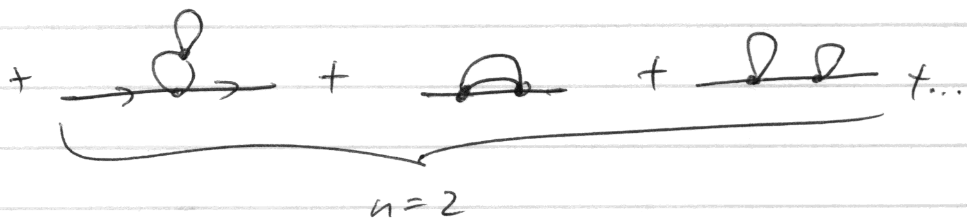
In the standard perturbative expansion in H_1, terms at n^{th} order in perturbation theory include n vertices of the form



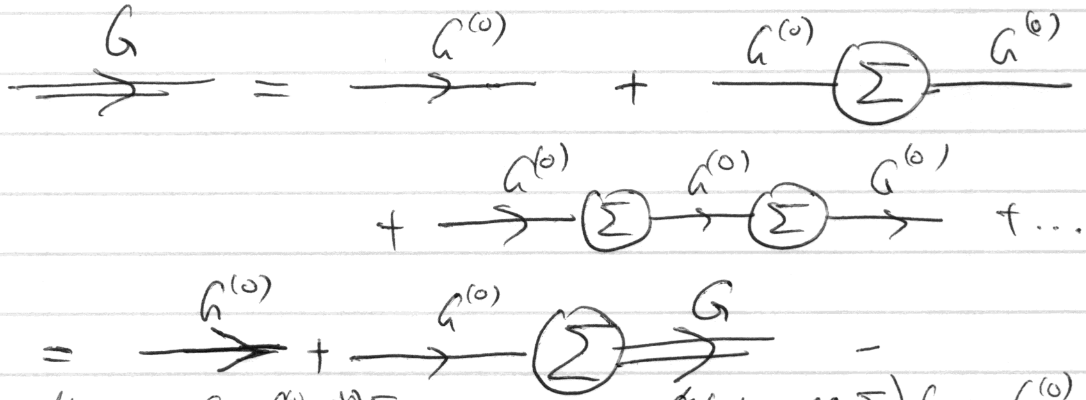
and implied momentum conservation $p_1+p_2=p_3+p_4$

Only connected diagrams contribute:





In the standard resummation, we identify 1PI diagrams as contributions to the self-energy, and diagrams can contain multiple insertions thereof:



reading $G = G^{(0)} + G^{(0)}\Sigma G \Rightarrow \cancel{G}(1 - G^{0}\Sigma)G = G^{(0)}$

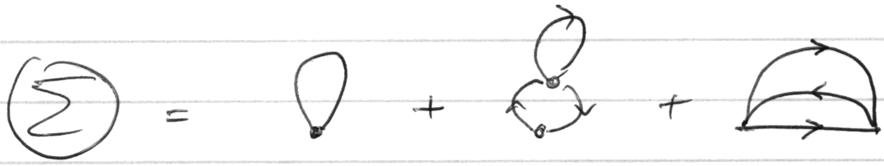
$$G^{0(-1)} = G^{0^{-1}} G G^{-1} = (G^{0})^{-1}\left(G^{(0)} + G^{(0)}\Sigma G\right)G^{-1} = G^{-1} + \Sigma$$

$$G = \left((G^{(0)})^{-1} - \Sigma\right)^{-1}.$$

We can explicitly invert these operators in the frequency representation, where

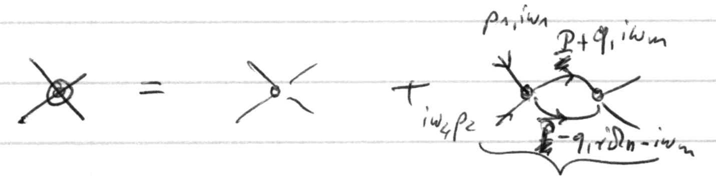
$$G_\sigma(p, i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_p - \mu) - \Sigma(p, i\omega_n)}.$$

Now, the expansion for Σ must exclude any diagrams that are one particle reducible, i.e., which can be cut in two by severing a single line. To second order, we have terms remaining:



Two-particle scattering and the vertex-function:

Let us consider two-particle scattering at order 2:



$$\bar{P} = \frac{p_1 + p_2}{2}$$

$$i\Omega_n = i\omega_1 + i\omega_2$$

$$\mu = \tfrac{1}{2}(\mu_\uparrow + \mu_\downarrow)$$

$$= -\sum_m \int \frac{d^3q}{(2\pi)^3} \underbrace{G_\uparrow^{(0)}(\bar{p}+q, \underbrace{i\omega_m}_{=z})\, G_\downarrow^{(0)}(\bar{p}-q, i\Omega_n - \underbrace{i\omega_m}_{=z})}_{I(z)}$$

$$= -\int \frac{d^3q}{(2\pi)^3} \oint_C \frac{dz}{2\pi i}\, g(z)\, I(z), \quad \text{with } g = \frac{\beta}{e^{\beta z}+1}$$

$$= (\ldots \text{ contour integration} \ldots)$$

$$= \int^{\Lambda} \frac{d^3q}{(2\pi)^3} \frac{1 - n_\uparrow^{(0)}(\bar{p}+q) - n_\downarrow^{(0)}(\bar{p}-q)}{i\Omega_n + 2\mu - \varepsilon_{\bar{p}+q} - \varepsilon_{\bar{p}-q}}$$

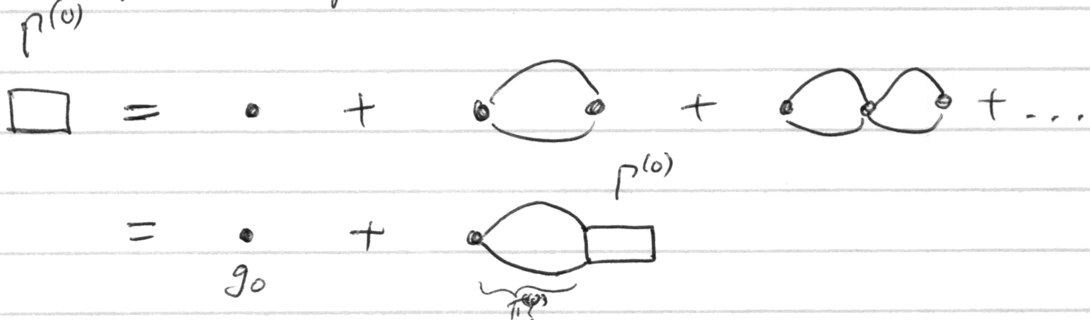
$$\propto -\int^{\Lambda} \frac{d^3q}{q^2} \longrightarrow \text{divergent!}$$

⑤

$\Rightarrow$ We have to regularise the vertex-term by adding a suitable counter-term

$$+\int \frac{d^3q}{q^2}$$

It is then possible to resum the series of bubbles: (amputating external legs)



resulting in a Dyson-type equation for the T-matrix

$$\Gamma^{(0)} = g_0 + g_0\, \Pi^{(0)}\, \Gamma^{(0)}$$

or

$$\boxed{\Pi^{(0)}(\bar{P};\Omega_n) = \frac{1}{g_0} - \frac{1}{\Gamma^{(0)}(P;\Omega_n)}}$$

Formally, our renormalization proceeds by fixing the bare coupling constant according to

$$\frac{1}{g_0} = \frac{m}{4\pi\hbar a_s} - \int \frac{d^3q}{(2\pi)^3}\, \frac{1}{q^2}$$

such that ~~the~~ we can find $\Gamma^{(0)}$ as the finite expression

$$\frac{1}{\Gamma^{(0)}(\bar{P}, i\Omega_n)} = \frac{m}{4\pi\hbar a_s} - \int \frac{d^3q}{(2\pi)^3}\left[\frac{1 - n_\uparrow^{(0)}(\bar{p}+q) - n_\downarrow^{(0)}(\bar{p}-q)}{i\Omega_n + 2\mu - \frac{\bar{p}^2}{4} - q^2} + \frac{1}{q^2}\right]$$

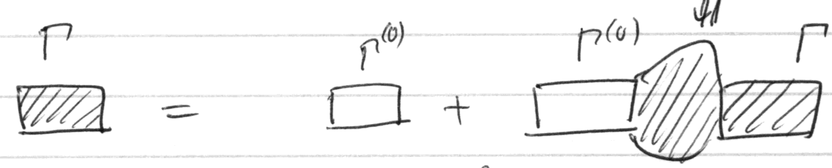
as the integrand in the previous expression vanishes as $q \to \infty$ we can now drop the cut-off function and take $\Lambda \to \infty$.

Taking into account the particle-particle ladder, via the bubble resummation, we need to exclude those terms also from the self-energy.

~~Terms~~

Bold pair-propagator:

We now want to go beyond simple bubbles and define a bold pair-propagator that includes more general polarization-terms:



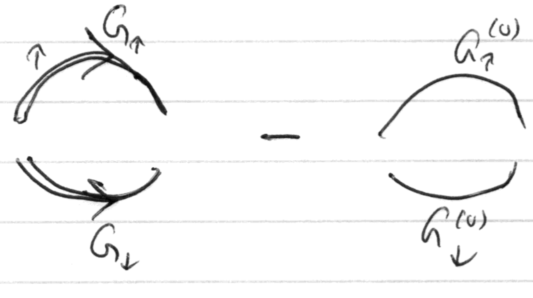
leading to get another Dyson-equation:

notation $P = 2\bar{p}$

$$\frac{1}{\Gamma(\bar{p}, \Omega_n)} = \frac{1}{\Gamma^{(0)}(\bar{p}, \Omega_n)} - \Pi(\bar{p}, \Omega_n)$$

The only subtlety occurs at order 1 for $\Pi^{(1)}$, where we already included the bare fermion bubble, which we need to subtract to make things consistent, i.e.

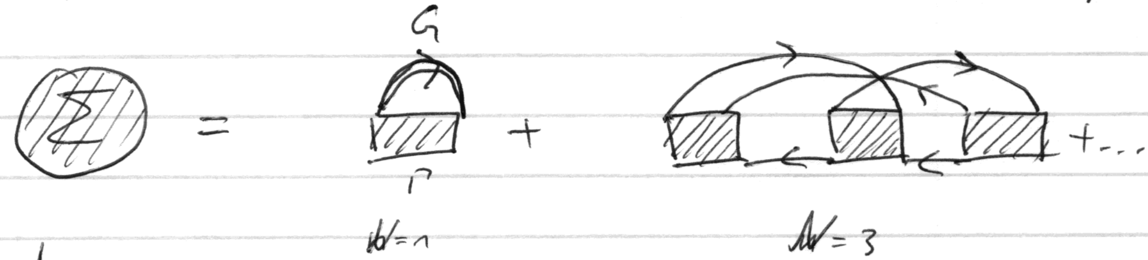
$\Pi^{(1)}(\bar{p}, \tau) =$



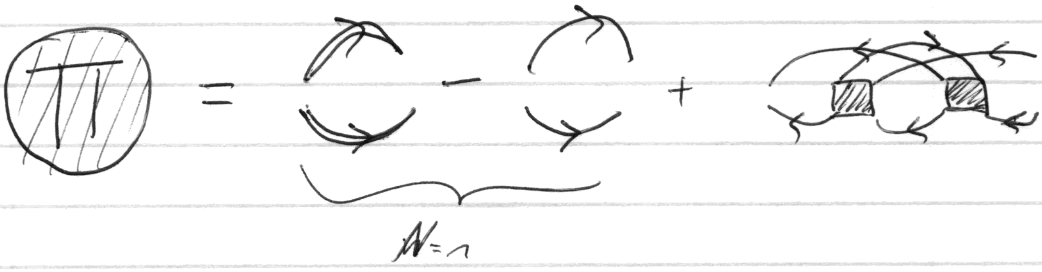
Skeleton Diagrams

Having defined the dressed pair- and fermion-propagators, we need to sum only over the class of diagrams which does not contain any self-energy insertions of Fermion-lines, or equivalently polarization-insertions on the pair-propagator

the first two contributions arise at order $N=1$ and 3, resp:



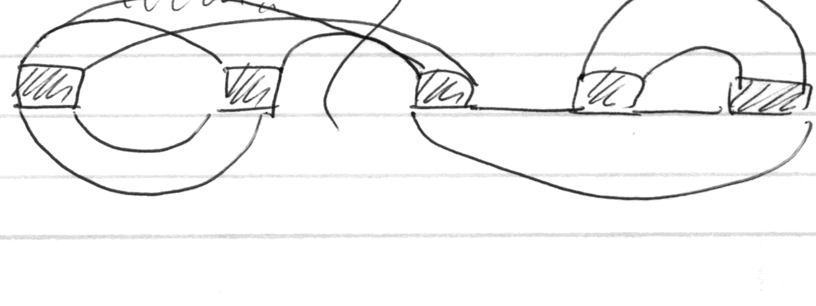
and



The structure of the terms to be included is such that they can be derived from closed & connected diagrams by cutting a fermion-line (Σ) or pair-propagator (Π).
Simultaneously the mother diagram has to be two-particle irreducible (2PI)

At order N, there are N (Σ) or $(N-1)$ (Π) vertices

e.g.



How to do Monte-Carlo on these Diagrams?

1) sample closed 2PI diagrams

2) "cut" one line to get weights for Σ / Π.

3) Use the self-consistency equations from the Dyson equation to update our knowledge of the propagator and restart the sampling for Σ, Π with the new estimates.

Notations:

internal momenta $X \equiv (q_1, \dots, q_N ; \tau_3, \dots, \tau_{2N})$

external variables $Y = (p ; \tau_1, \tau_2)$

observable $Q(Y) = \Sigma$ or Π

- expand $Q(Y)$ in some basis of functions $g(Y)$ and compute overlaps

$$A_{Q,g} \equiv \int dY \, Q(Y) \, g(Y)$$

by perturbative expansion in diagrams

$$= \sum_{\substack{T \in S_Q \\ \uparrow}} \int dX \, dY \, \mathcal{D}(\underbrace{T, X, Y}_{C}) \, g(Y)$$

allowed diagram topologies.

and a configuration $C = (T, X, Y)$

We want to solve the integral by sampling with a weight function

$$w(C) = |\mathcal{D}(C)| \cdot R(C)$$

where $R(C)$ is an arbitrary reweighting function.

Using a markov process to generate configurations C_i, observables are represented as

$$\mathcal{A}_{Q,g} = Z \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \mathcal{A}_{Q,g}(C_i)$$

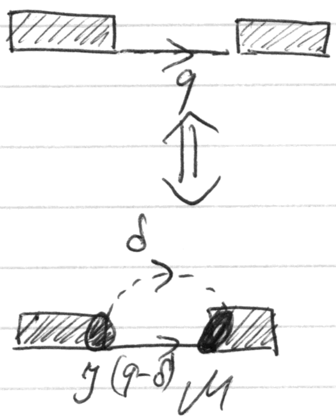
with $\mathcal{A}_{Q,g}(C_i) = \dfrac{\operatorname{sgn}(\mathcal{D}(C))\, g(Y)}{R(C)} \cdot \underbrace{1\!\!1_{\mathcal{T}\in S_Q}}_{\text{'mask' for physical diagrams}}$

and $Z = \int dC\, w(C)$ can be obtained in the same MC process.

How to sample diagram topologies?

Basic idea: introduce unphysical diagrams with a 'worm'-line that can carry some excess momentum.

Move 1: Create / Delete Worm



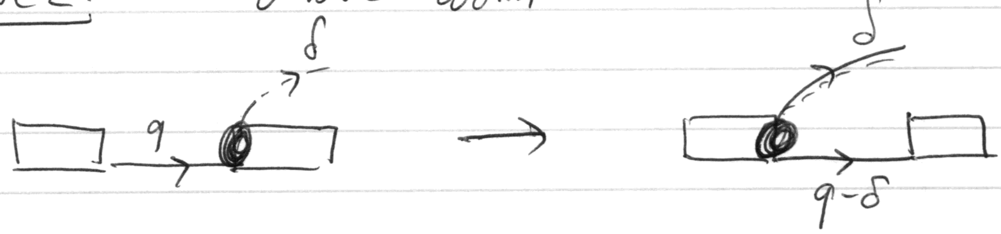
invent a propagator for the worm $C(\delta)$ to assign this some weight

$\Rightarrow$ easy to evaluate acceptance ratio

$$R_{create} = \frac{p_{delete}}{p_{create}} \frac{6N}{N_{Links} W(\delta)} \frac{|G_\sigma(q \pm \delta, \tau)| \, C(\delta)}{|G_\sigma(q,\tau)|}$$

where $W(\delta)$ is the probability distribution from which δ was drawn.

Move 2: Move Worm

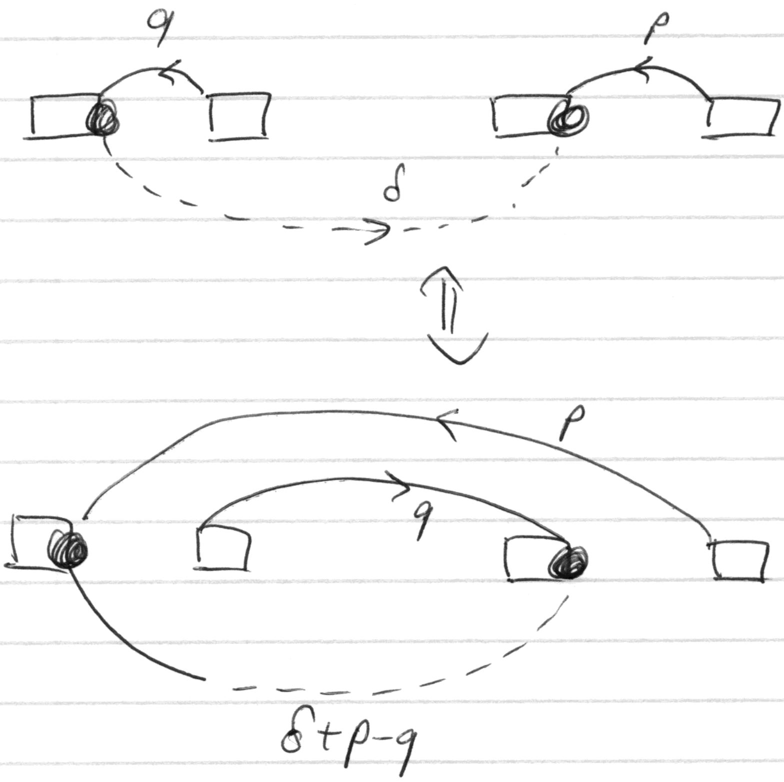


Worms can move along any of the three lines attaching to the vertex on which they are located.

$$R_{move} = \frac{|G_\sigma(q \pm \delta, \tau)|}{|G_\sigma(q,\tau)|}$$

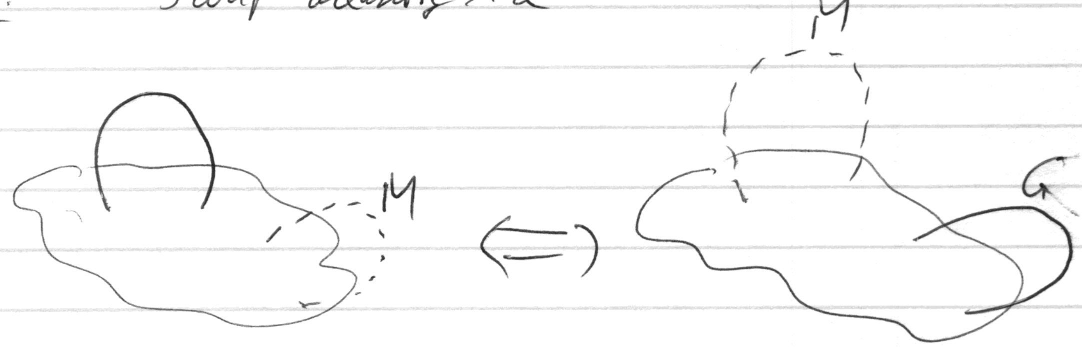
Once a worm-line is present, we can change the diagram-topology, for instance by

Move 4: Reconnect



Another move which changes topology is the choice of measurement line = line to be cut to generate a self-energy.

Move 5: Swap measuring line



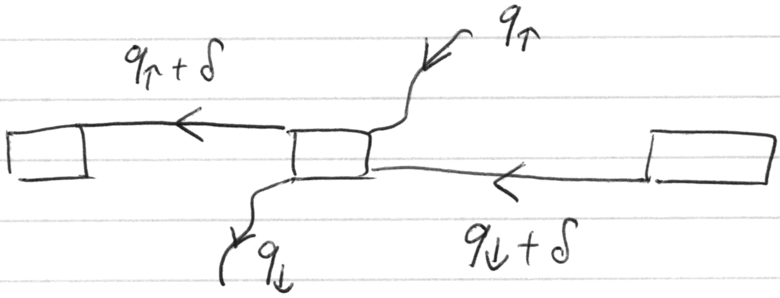
This move also changes topology.

Finally, we need to allow changes in the order of the diagram:

Move 6: Add-Remove

Again, we use the presence of a worm-line to enable us to make new connections:

Remove $\Uparrow$ $\Downarrow$ Add



- This set of moves is complemented by a few additional ones, but it should be sufficient to illustrate the general idea.
- Diagrams need to be checked for 2PI
- For further details, and for a discussion of the convergence properties, please see the preprint.

arxiv: 1305.3901