Bold Diagrammatic Monte Carlo:
A new approach for strongly correlated fermions

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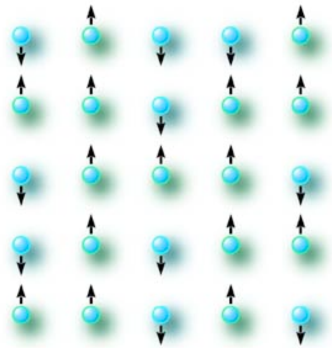
DMFT comparison: Emanuel Gull (Columbia U), Lode Pollet (ETH Zürich), Matthias Troyer (ETH Zürich)

Goal: unbiased method for solving strongly correlated fermions

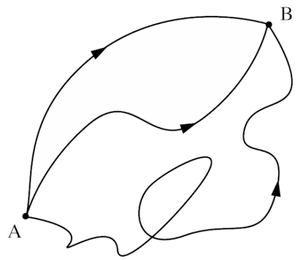
Sign problem

Classical



$$Z = \sum_x e^{-\beta E(x)}$$

Quantum



$$\mathrm{Tr}\left[e^{-\beta \hat{H}}\right] = \sum_\sigma W(\sigma)$$

Conventional solution:

$$\langle A \rangle = \frac{\sum_\sigma A(\sigma) W(\sigma)}{\sum_\sigma W(\sigma)} = \frac{\sum_\sigma A(\sigma) sign(\sigma) |W(\sigma)|}{\sum_\sigma sign(\sigma) |W(\sigma)|} = \frac{\langle A \cdot sign \rangle_{|W|}}{\langle sign \rangle_{|W|}}$$

SIGN PROBLEM:

$$\langle sign \rangle_{|W|} \sim e^{-\#\beta V}$$

Goal: unbiased method for solving strongly correlated fermions

sign-problem

Variational methods

+ universal
- mostly used at T=0
- systematic errors
- finite-size extrapolation

Determinant (diagrammatic) MC

+ "solves" $n_{i\sigma} = n_{i\,-\sigma}$ case
- CPU expensive
- not universal
- finite-size extrapolation

Cluster DMFT methods

+ universal
- cluster size extrapolation

Diagrammatic MC

+ universal
- diagram-order extrapolation

Computational complexity Is exponential : $\exp\{\#\xi\}$

Cluster DMFT

$$\xi = \left(\frac{\varepsilon_F}{T}\right) L^D$$

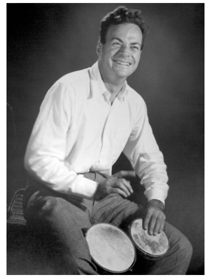
linear size

Diagrammatic MC

$$\xi = N$$

diagram order

Reminder: Feynman diagrams



$$G_\sigma(\mathbf{p},\tau) \equiv -\langle \mathrm{T}\, c_{\mathbf{p},\sigma}(\tau)\, c^\dagger_{\mathbf{p},\sigma}(0)\rangle$$

$$c_{\mathbf{p},\sigma}(\tau) \equiv e^{\tau(H-\mu N)} c_{\mathbf{p},\sigma}\, e^{-\tau(H-\mu N)}$$

Extract observables from Green's functions:

$$G_\sigma(\mathbf{p},\tau=0^-) = \langle c^\dagger_{\mathbf{p},\sigma} c_{\mathbf{p},\sigma}\rangle = n_\sigma(\mathbf{p})$$

$$\sum_{\sigma=\uparrow,\downarrow} \int \frac{d\mathbf{p}}{(2\pi)^3}\, n_\sigma(\mathbf{p}) = n$$

Feynman Diagrams: graphical representation for the high-order perturbation theory

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{H}_1 \\ -G_\sigma(\mathbf{p},\tau) &= \sum_{m=0}^{\infty} \left(\frac{-1}{\hbar}\right)^m \frac{1}{m!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_m \langle T_\tau \hat{H}_1(\tau_1)\ldots \hat{H}_1(\tau_m)\hat{c}_{\mathbf{p},\sigma}(\tau)\hat{c}^\dagger_{\mathbf{p},\sigma}(0)\rangle_{\text{connected}} \end{aligned}$$

History of Diagrammatic MC: Polarons

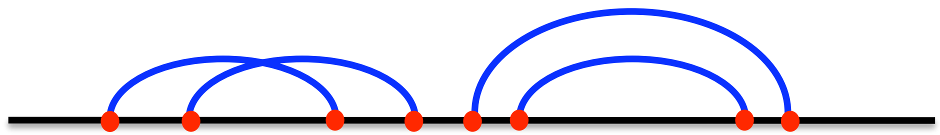
Polaron problem: $H = H_{\text{particle}} + H_{\text{environment}} + H_{\text{coupling}}$

$$\longrightarrow E(p), m_*, G(p,t), \ldots$$

Electron-phonon polarons (e.g. Frölich polaron)
= particle in bosonic environment

Prokof'ev & Svistunov (PRL1998)

$$H = \sum_{\mathbf{k}} \frac{k^2}{2} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_q b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q}} V(\mathbf{q})(b^\dagger_{\mathbf{q}} - b_{-\mathbf{q}}) a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}$$



$$N \sim 10^2$$

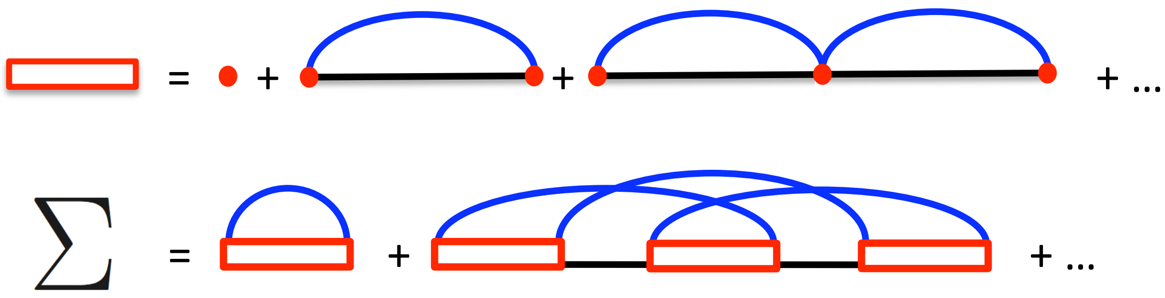
Series:
- positive definite
- convergent

History of Diagrammatic MC: Polarons

Fermi Polaron (polarized Fermi gas)
= particle in *fermionic* environment

Prokof'ev & Svistunov (PRB2008)

$$H = \frac{p^2}{2m} + H_{\text{Fermi sea}} + \int V(\mathbf{r}-\mathbf{r}')n(\mathbf{r}')d\mathbf{r}'$$



$$N_{\max} = 11$$

Bare Series:

- sign alternating
- no convergence seen

History of Diagrammatic MC: Polarons

Fermi Polaron (polarized Fermi gas)
= particle in *fermionic* environment

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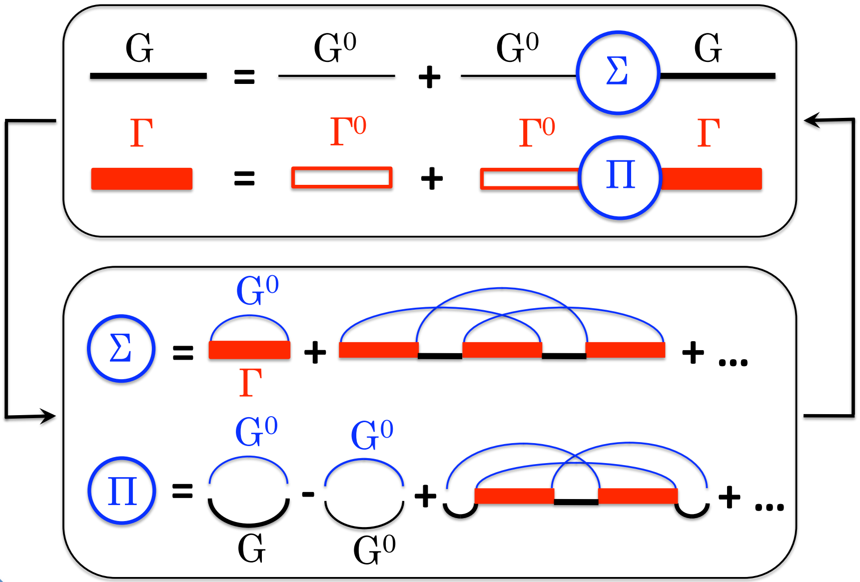
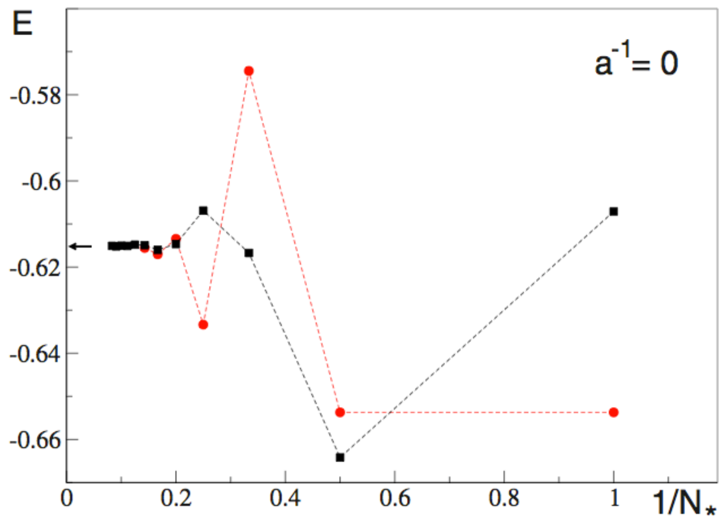
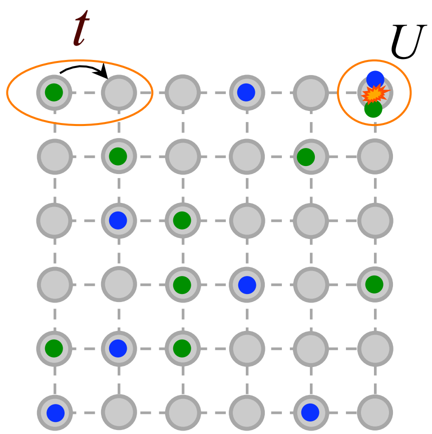
$$H = \frac{p^2}{2m} + H_{\text{Fermi sea}} + \int V(\mathbf{r}-\mathbf{r}')n(\mathbf{r}')d\mathbf{r}'$$

Bold diagrammatic MC:





Fermi-Hubbard model: $$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \hat{a}^\dagger_{i,\sigma}\hat{a}_{j,\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i,\sigma}\hat{n}_{i\sigma}$$

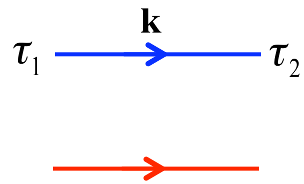


momentum representation:

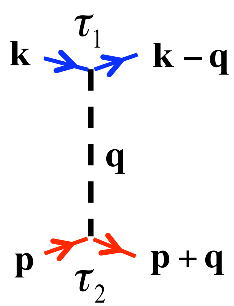
$$\hat{H} = \sum_{\mathbf{k},\sigma}(\varepsilon_{\mathbf{k}} - \mu)\hat{a}^\dagger_{\mathbf{k},\sigma}\hat{a}_{\mathbf{k},\sigma} + U\sum_{\mathbf{kpq}} \hat{a}^\dagger_{\mathbf{k-q},\downarrow}\hat{a}^\dagger_{\mathbf{p+q},\uparrow}\hat{a}_{\mathbf{p},\uparrow}\hat{a}_{\mathbf{k},\downarrow}$$

Elements of the diagrammatic expansion:

$$G^0_\sigma(\mathbf{k}, \tau_2 - \tau_1) \longrightarrow$$

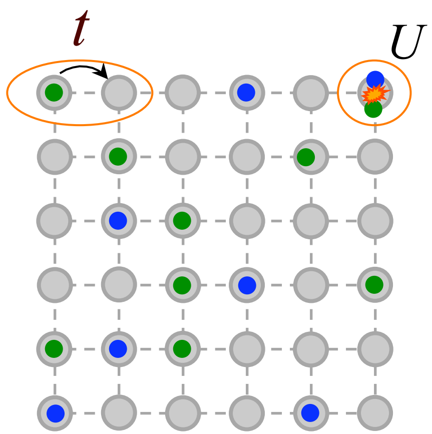


$$U\delta(\tau_1 - \tau_2) \longrightarrow$$



Fermi-Hubbard model:

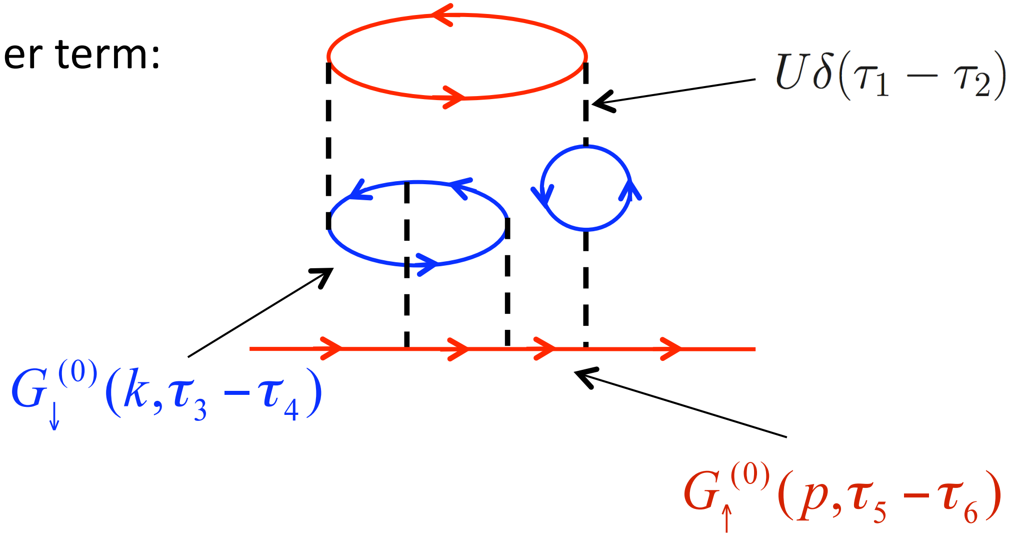
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{a}^{\dagger}_{i,\sigma} \hat{a}_{j,\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}$$



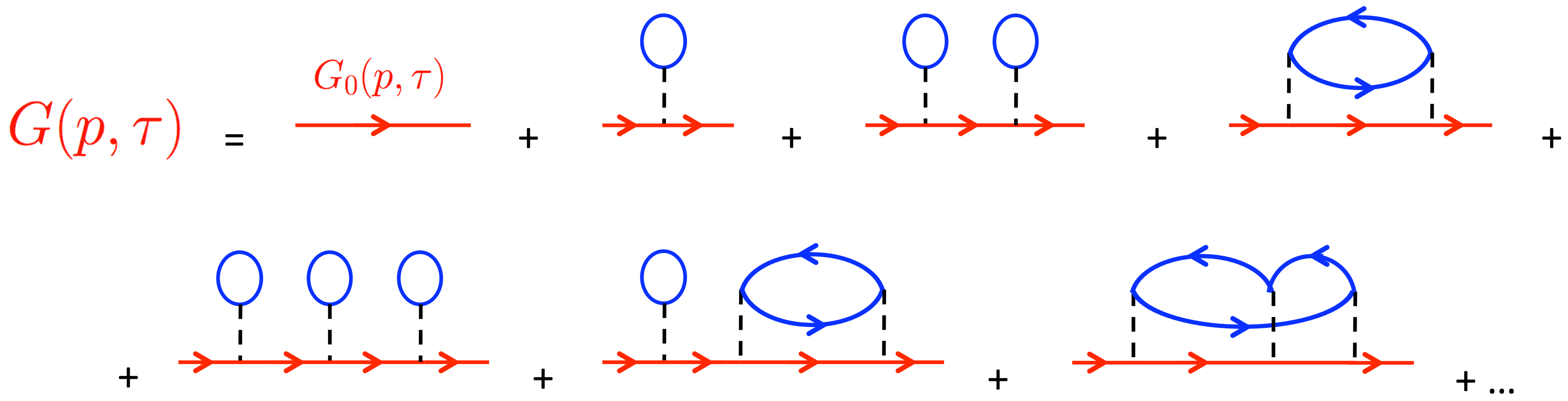
momentum representation:

$$\hat{H} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) \hat{a}^{\dagger}_{\mathbf{k},\sigma} \hat{a}_{\mathbf{k},\sigma} + U \sum_{\mathbf{kpq}} \hat{a}^{\dagger}_{\mathbf{k-q},\downarrow} \hat{a}^{\dagger}_{\mathbf{p+q},\uparrow} \hat{a}_{\mathbf{p},\uparrow} \hat{a}_{\mathbf{k},\downarrow}$$

fifth order term:



The full Green's Function: $G_\sigma(\mathbf{p},\tau) \equiv -\langle \mathrm{T}\, c_{\mathbf{p},\sigma}(\tau)\, c^\dagger_{\mathbf{p},\sigma}(0)\rangle$



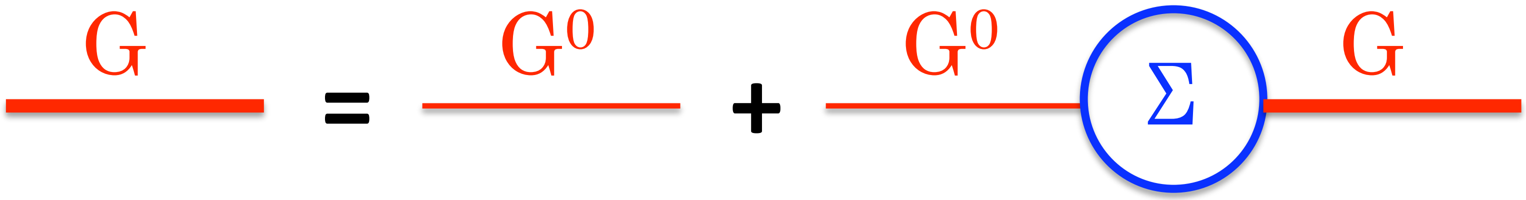
Evaluate the series in a stochastic way

(Monte Carlo sampling)

Configuration space =
(diagram order, topology and types of lines, internal variables)

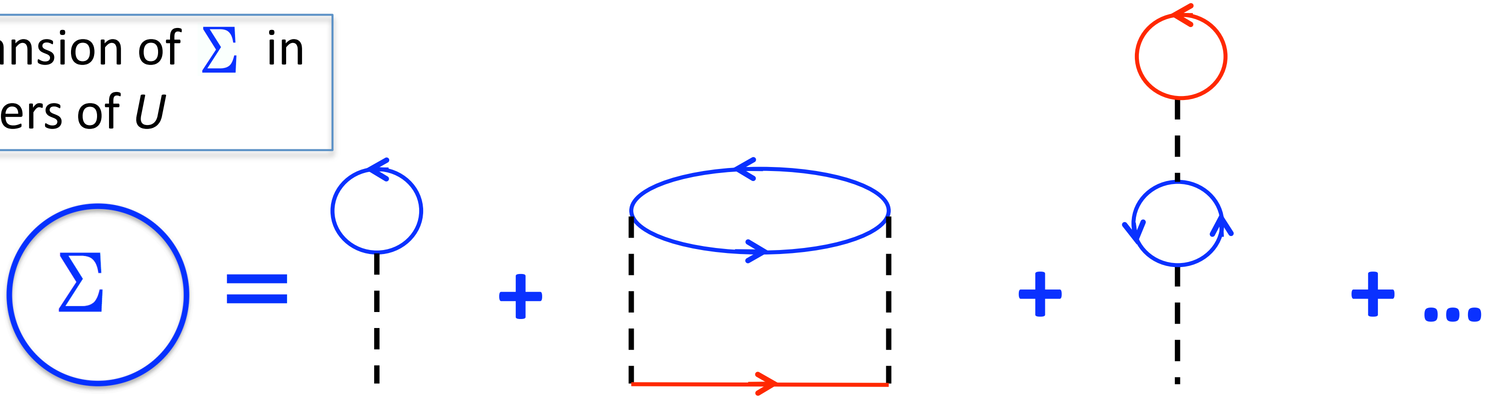
Reduce number of diagrams via partial summation (**bold** lines)

Dyson Eq.:



→ Irreducible diagrams for self-energy

Expansion of Σ in powers of U



Every analytic solution or insight into the problem can be 'built in'

- Summation of ladder diagrams
- use dressed (or bold) propagators

➔ skeleton series

- higher levels of irreducibility (e.g., fully irreducible four-point vertex)

Determinant Diagrammatic MC ⟷ Diagrammatic MC

(Dis)connected + (ir)reducible diagrams for the partition function ⟷ Irreducible diagrams for Self-energy

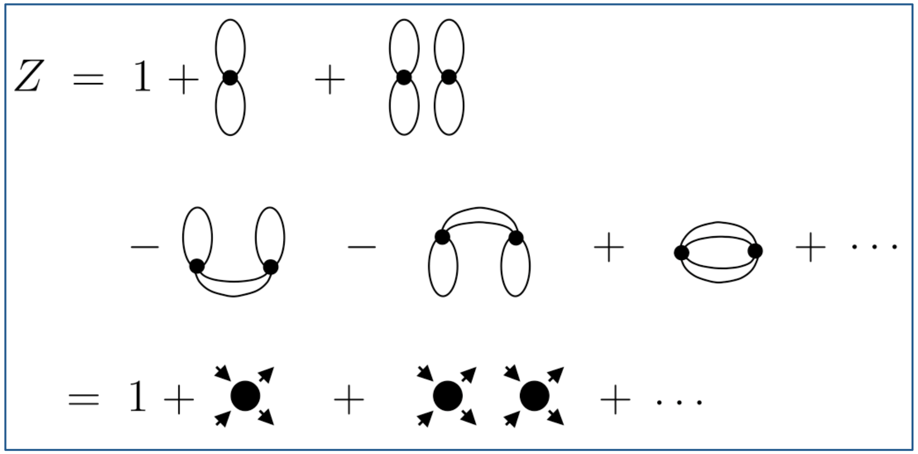
+ thermodynamic limit for free!

Rubtsov (2003); Burovski et al. (2006)

$$\exp(-\beta H) = \exp(-\beta H_0)\mathcal{T}_\tau \exp\left(-\int_0^\beta \mathrm{d}\tau H_1(\tau)\right)$$

$$H_1(\tau) = \mathrm{e}^{\tau H_0} H_1 \mathrm{e}^{-\tau H_0}$$

$$Z = \sum_{n=0}^{\infty}(-U)^n \sum_{\mathbf{x}_1\cdots\mathbf{x}_n} \int_{0<\tau_1<\tau_2<\cdots<\beta} \prod_{j=1}^{n} \mathrm{d}\tau_j \times \mathrm{tr}\left[\mathrm{e}^{-\beta H_0} \prod_{j=1}^{n} c_\uparrow^\dagger(\mathbf{x}_j\tau_j)c_\uparrow(\mathbf{x}_j\tau_j)c_\downarrow^\dagger(\mathbf{x}_j\tau_j)c_\downarrow(\mathbf{x}_j\tau_j)\right]$$



- No sign problem for balanced case
- Finite size extrapolation

sign alternation of the diagrammatic expressions
(with order, topology, and values of functions of internal variables)

Sign problem or sign blessing?

limits the max. order that can be evaluated

Series convergent/re-summable (cancellation beats factorial growth)

Dyson's collapse argument:
if changing the sign of some parameter g (e.g., coupling constant) makes the system unstable, then g = 0 is a point of non-analyticity and the expansion in powers of g has zero radius of convergence

BUT: (i) does not apply to Hubbard model and fermions in the zero-range limit (collapse is suppressed by Pauli blocking)

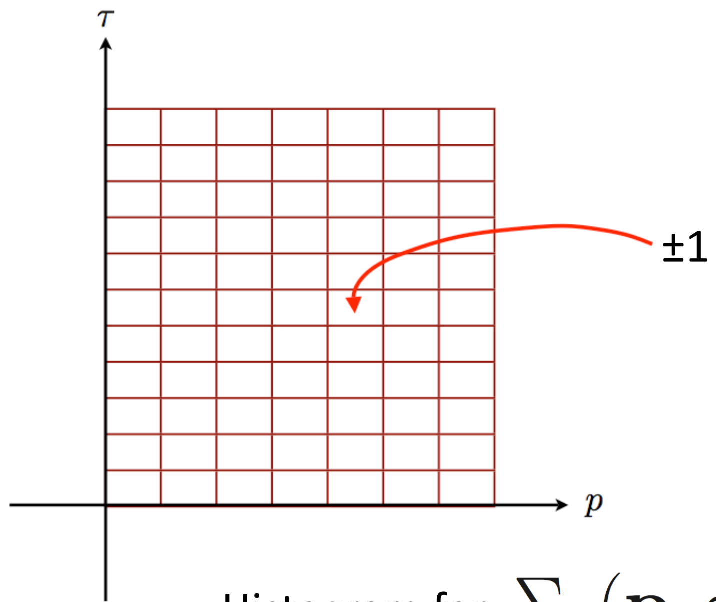
(ii) does not necessarily apply to non-perturbative skeleton series.

Diagrammatic Monte Carlo:

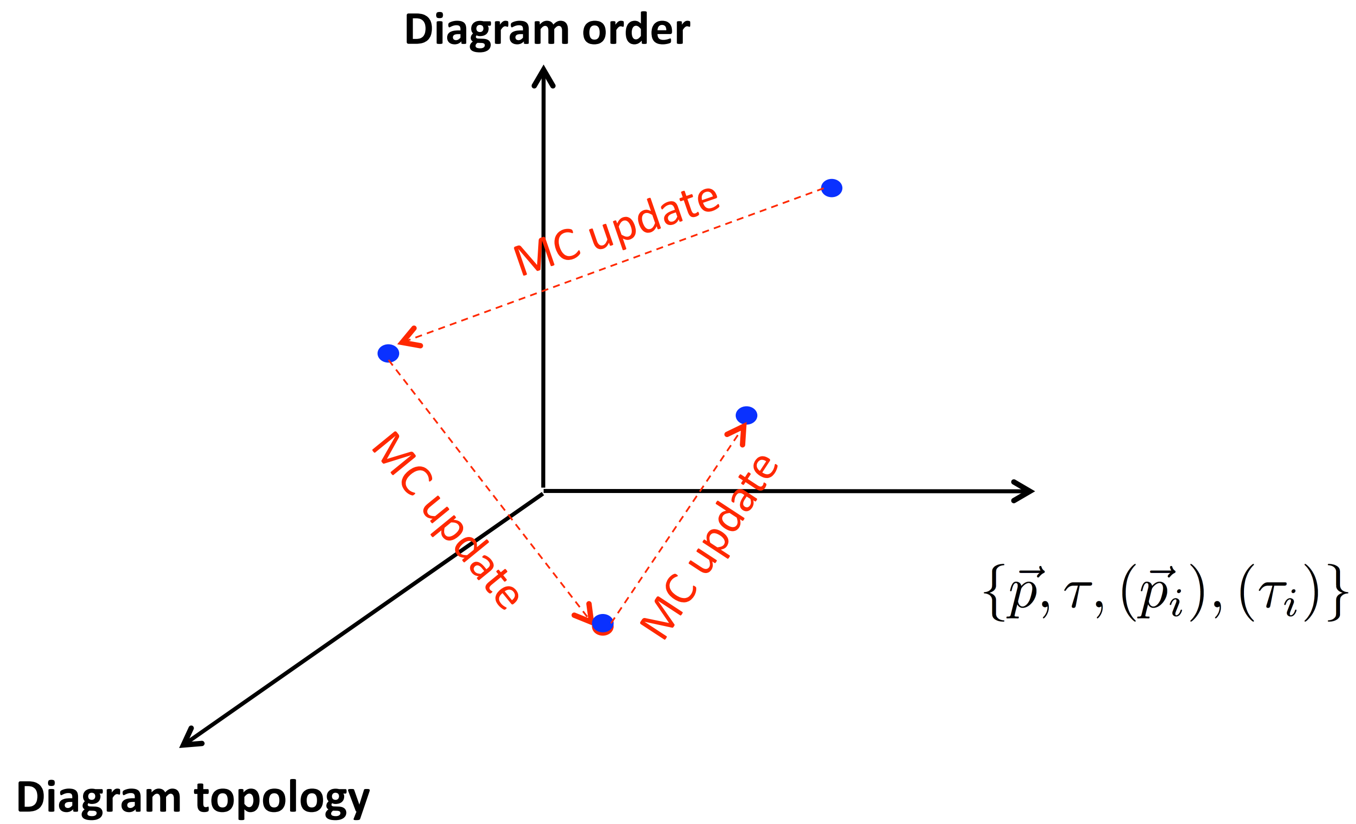
Random walk in the space of all possible diagram topologies and all values of internal and external variables.

Each configuration is visited with a probability proportional to the absolute value of its contribution to $\Sigma_\sigma(\mathbf{p},\tau)$.

After each MC update:



Histogram for $\Sigma_\sigma(\mathbf{p},\tau)$



This is NOT: write diagram after diagram, compute its value, sum

2D Fermi-Hubbard model in the Fermi-liquid regime

$U/t = 4$

$\mu/t = 1.5 \rightarrow n \approx 0.6$

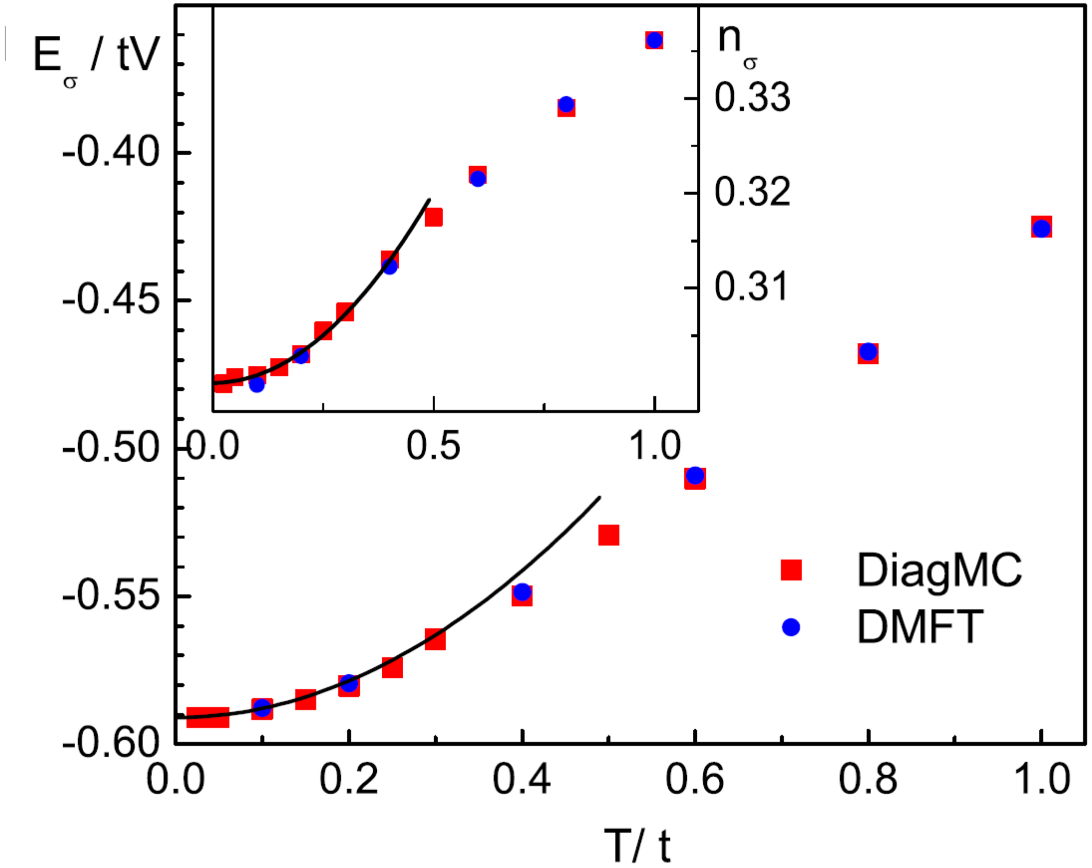
$T/t > 0.025 \sim E_F/100$

Fermi –liquid regime was reached

Bare series convergence:
yes, after order 4

$$E(T) - E(0) = (\rho_F + \rho_F' E_F)\frac{\pi^2 T^2}{6}$$

$$n(T) - n(0) = \rho_F' \frac{\pi^2 T^2}{6}$$



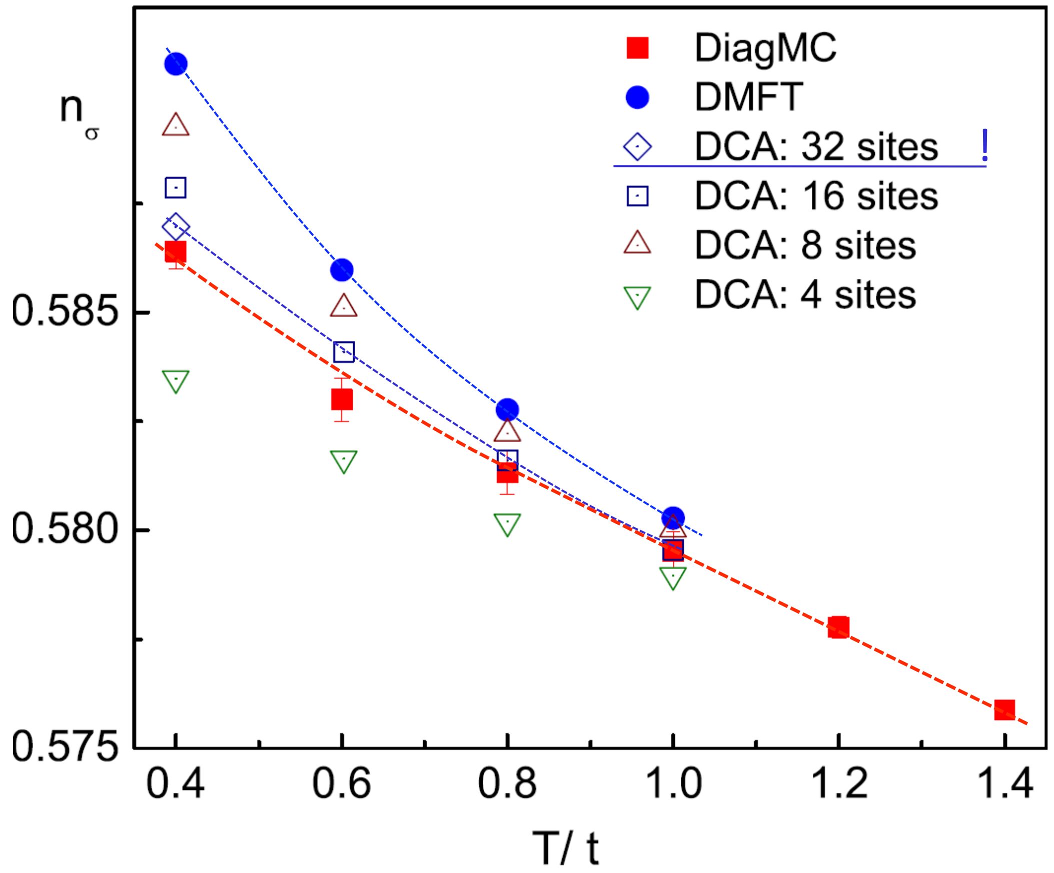
2D Fermi-Hubbard model in the Fermi-liquid regime

$U/t = 4$

$\mu/t = 3.1 \rightarrow n \approx 1.2$

$T/t \geq 0.4 \sim E_F/10$

Comparing DiagMC with cluster DMFT (DCA implementation)



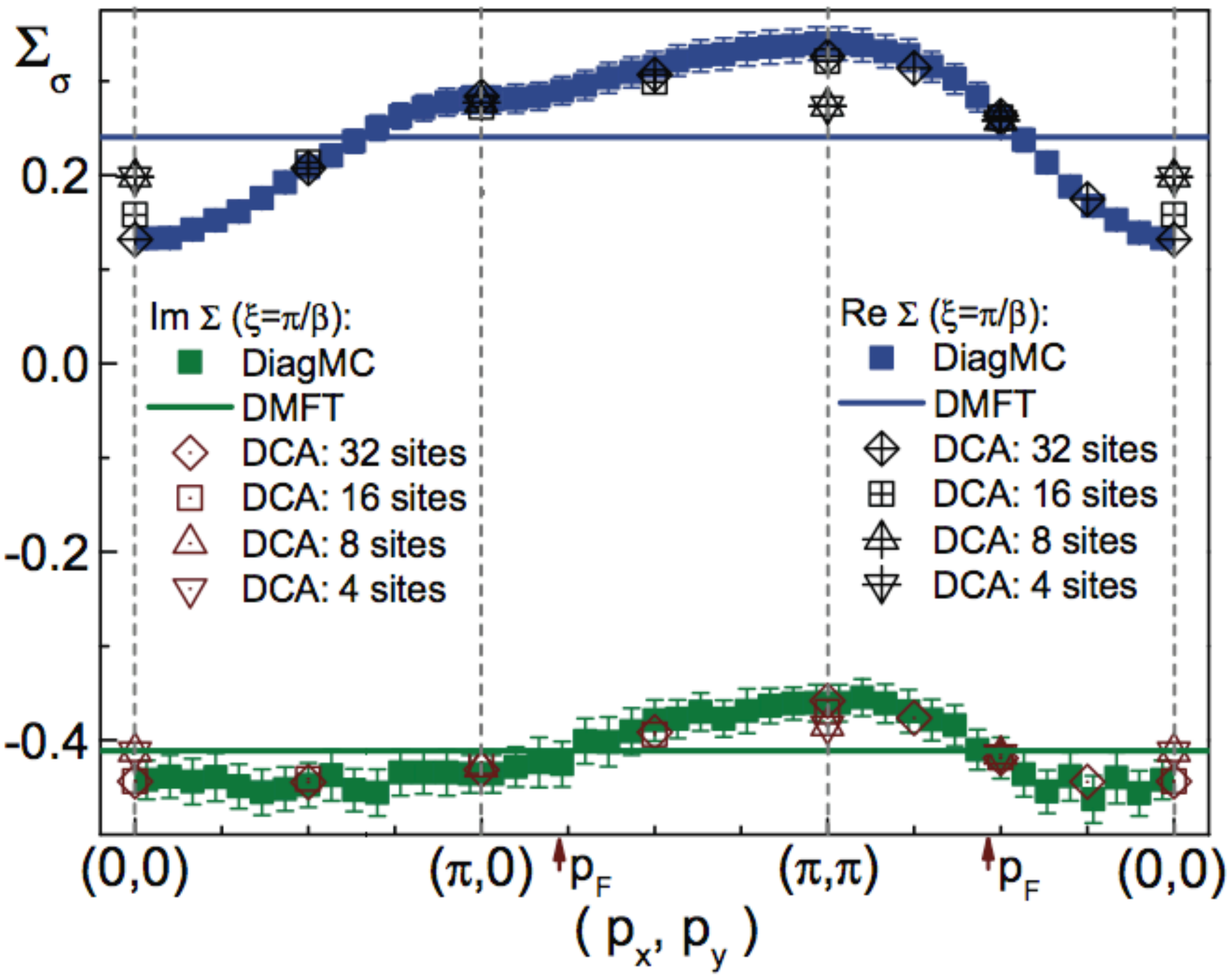
2D Fermi-Hubbard model in the Fermi-liquid regime

$U/t = 4$

$\mu/t = 3.1 \rightarrow n \approx 1.2$

$T/t \geq 0.4 \sim E_F/10$

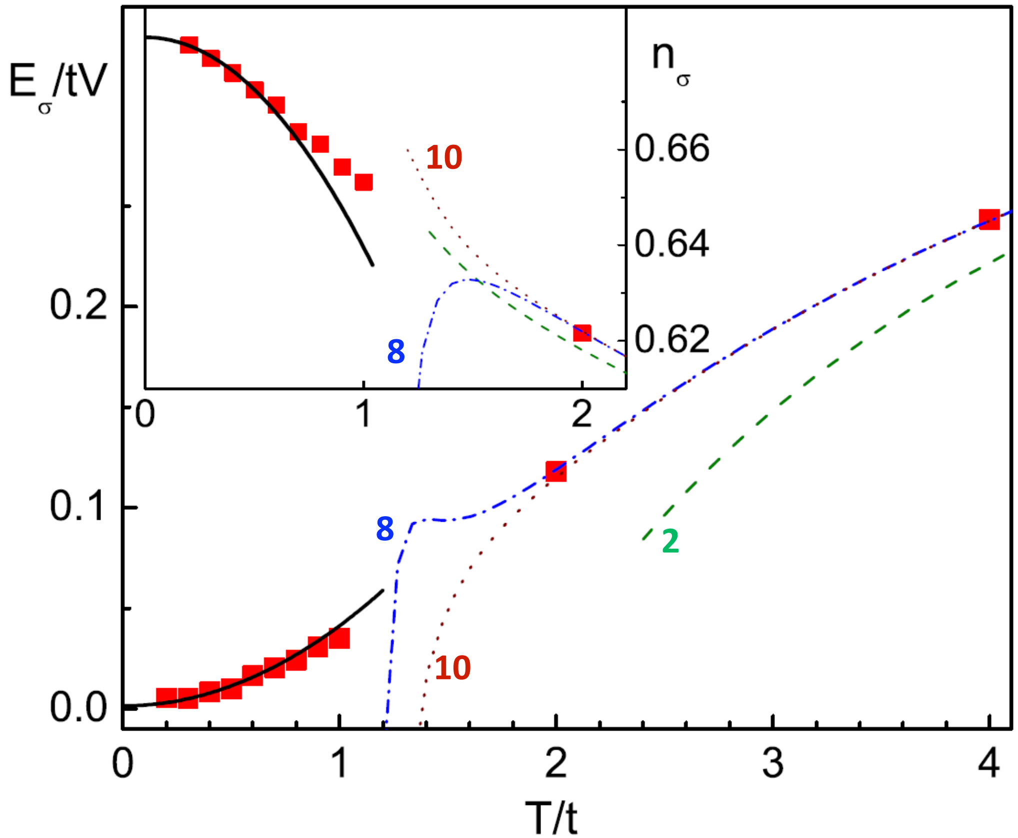
Momentum dependence of self-energy $\Sigma(\omega_0 = \pi T, p)$



3D Fermi-Hubbard model in the Fermi-liquid regime

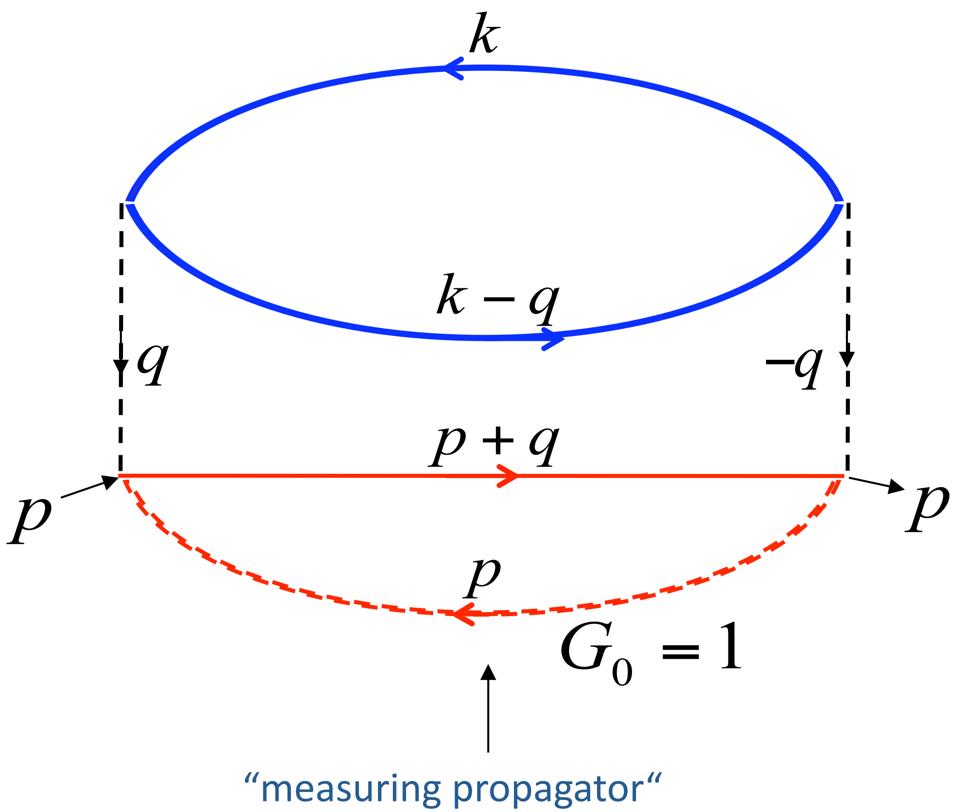
$$U/t = 4$$
$$(\mu - nU)/t = 1.5 \;\rightarrow\; n \approx 1.35$$
$$T/t \geq 0.1 \sim E_F/50$$

DiagMC *vs* high-T expansion in t/T
(up to 10-th order)



High-T expansion in t/T
fails at T/t>1 before the FL regime sets in

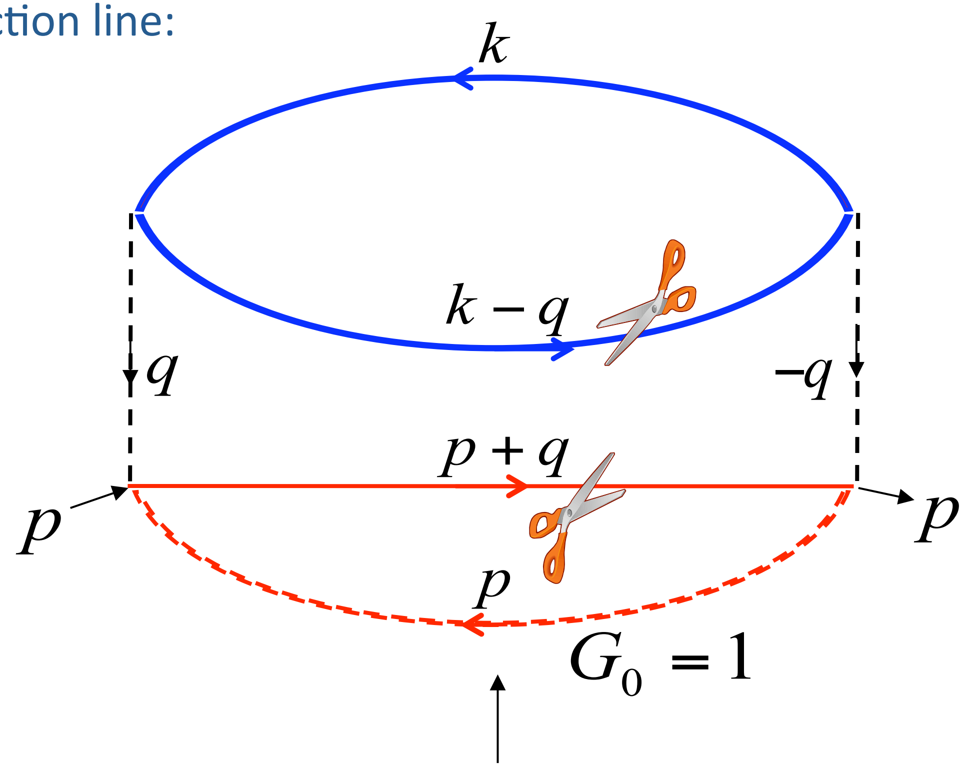
Sampling the diagram space



Global updates???

Sampling the diagram space

Adding interaction line:

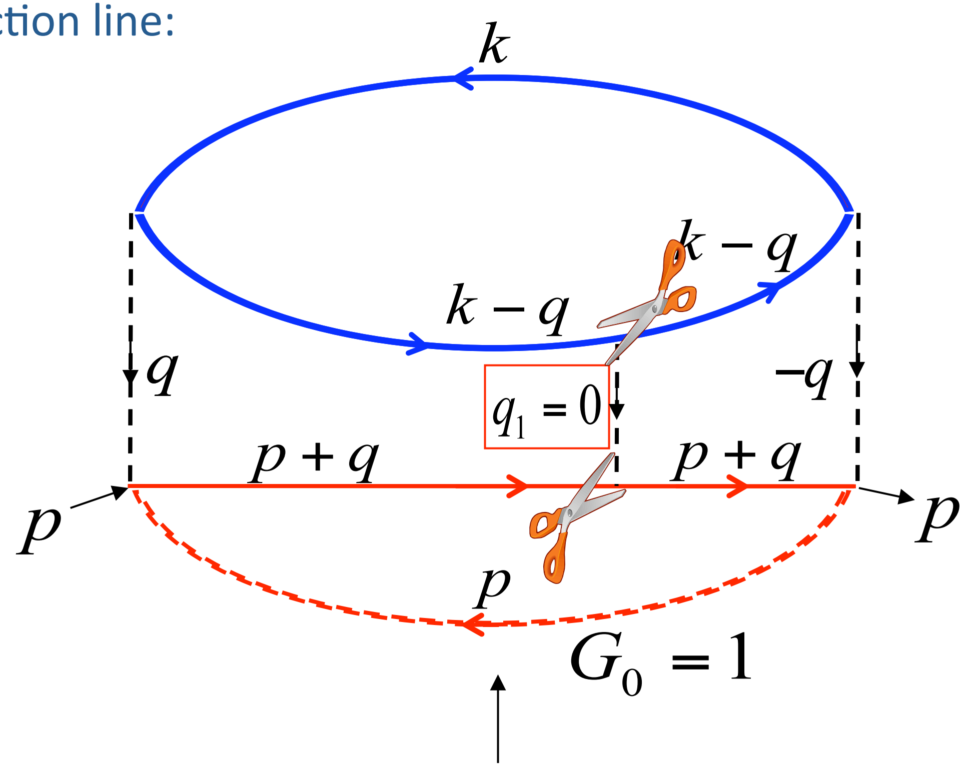


"measuring propagator"

Global updates???

Sampling the diagram space

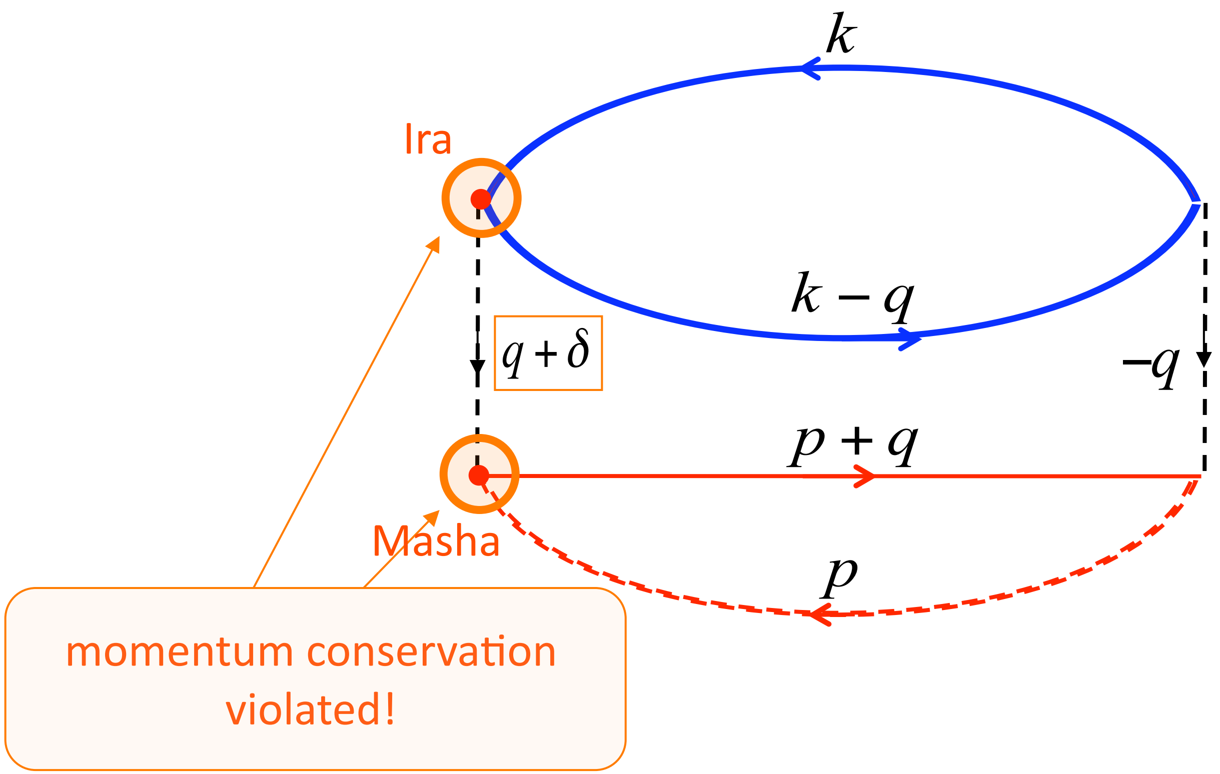
Adding interaction line:



"measuring propagator"

Global updates???

Updates



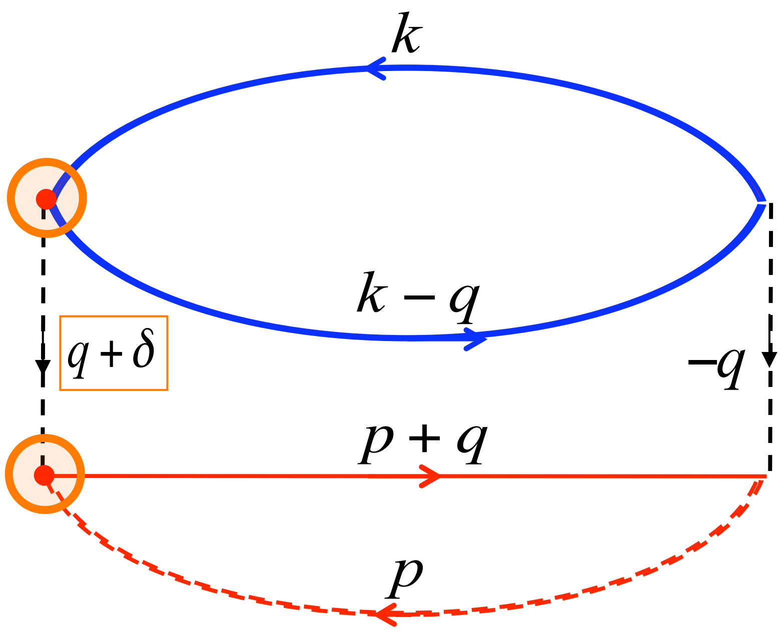
Worm ends

Perform all the changes through the worm ends!

ONLY LOCAL UPDATES

Updates

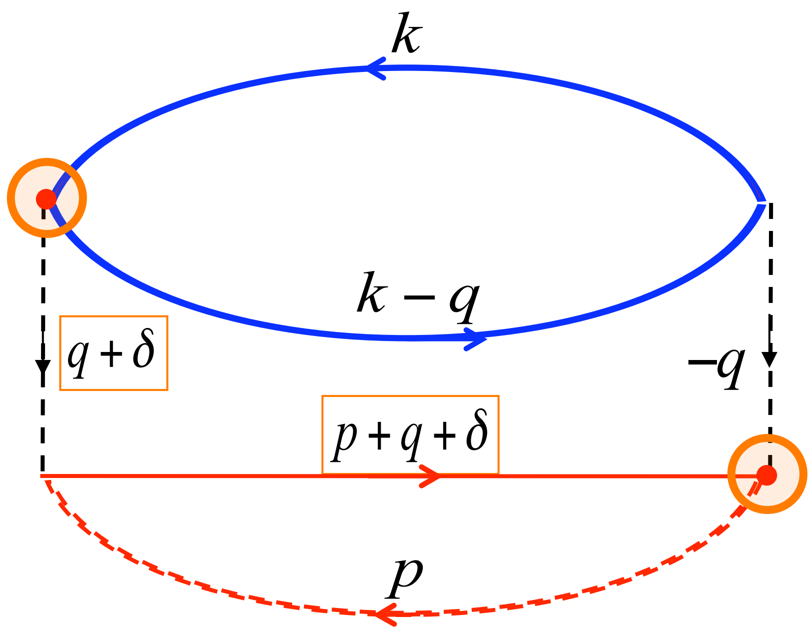
Move worms:



Do not measure Σ

Updates

Move worms:



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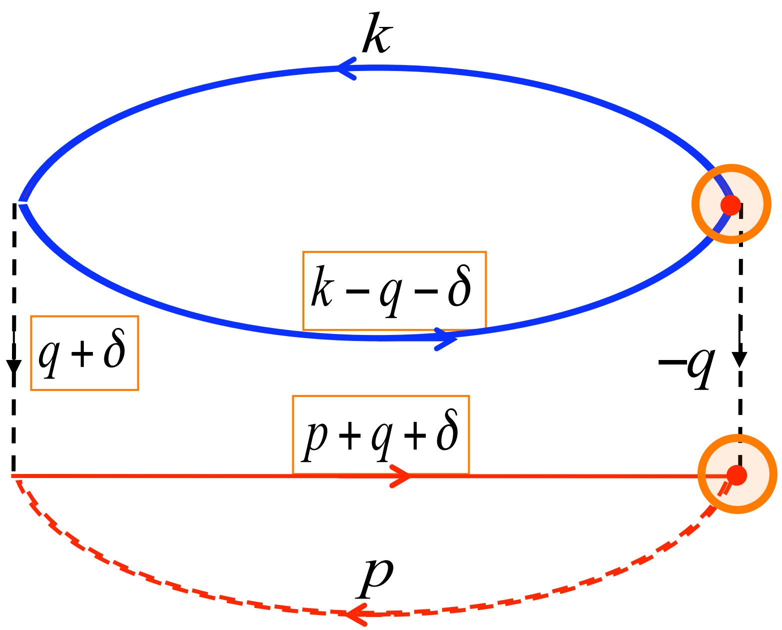

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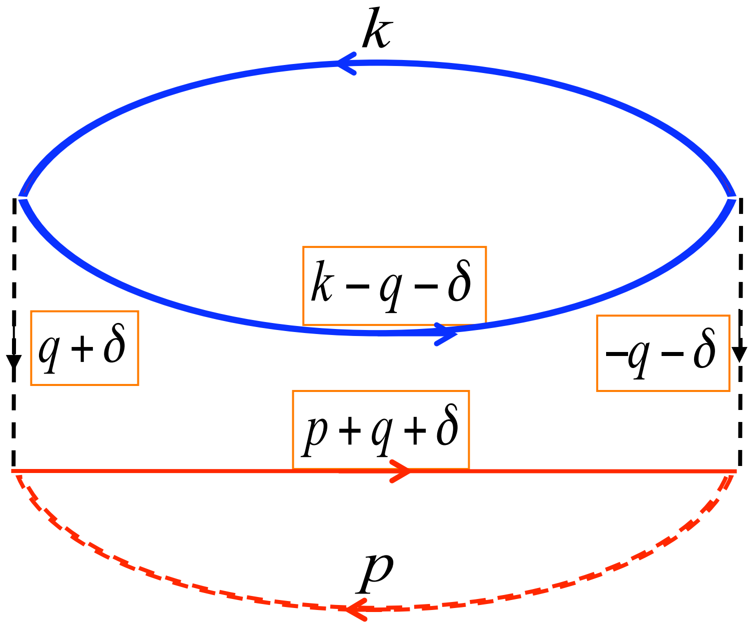
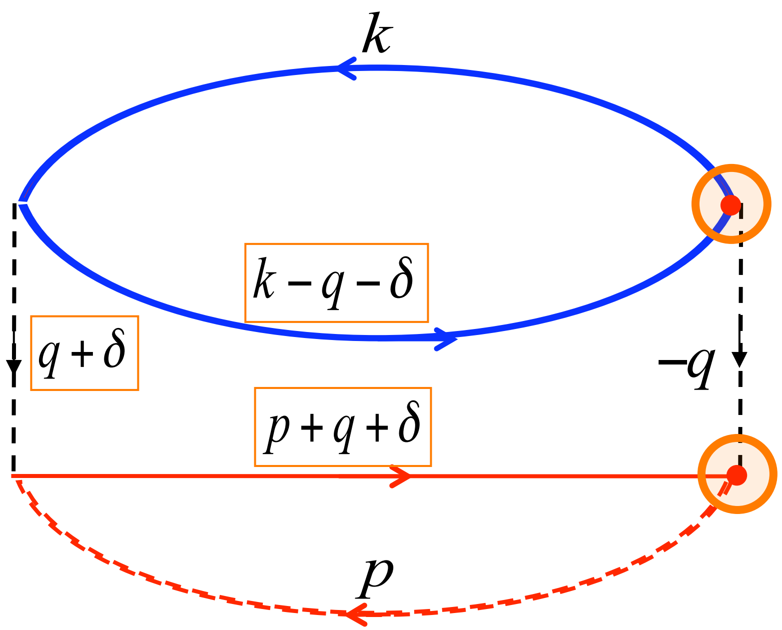


Now measure Σ

Updates

Add a vertex:



Do not measure Σ

Updates

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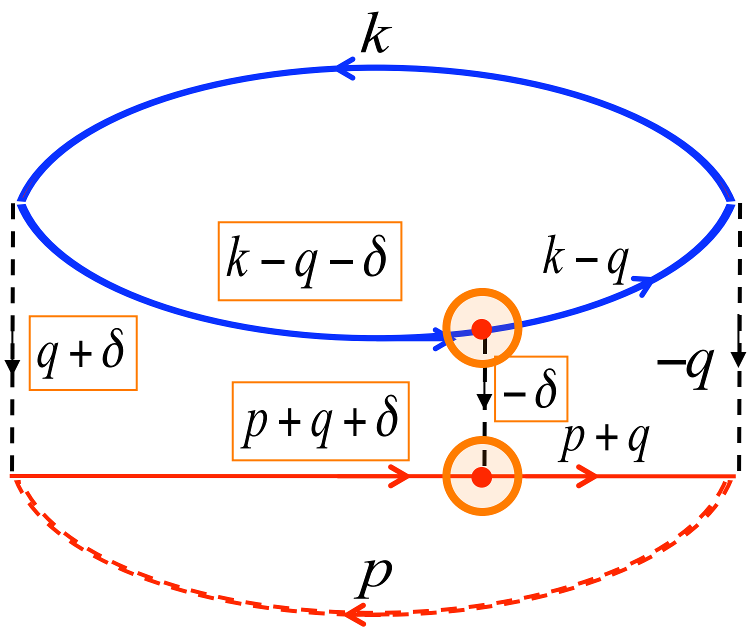

Do not measure Σ

Updates

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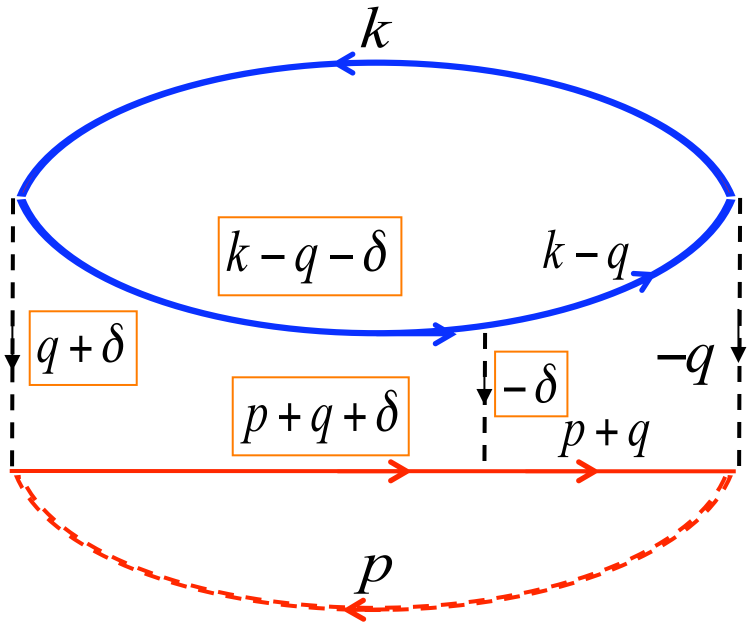
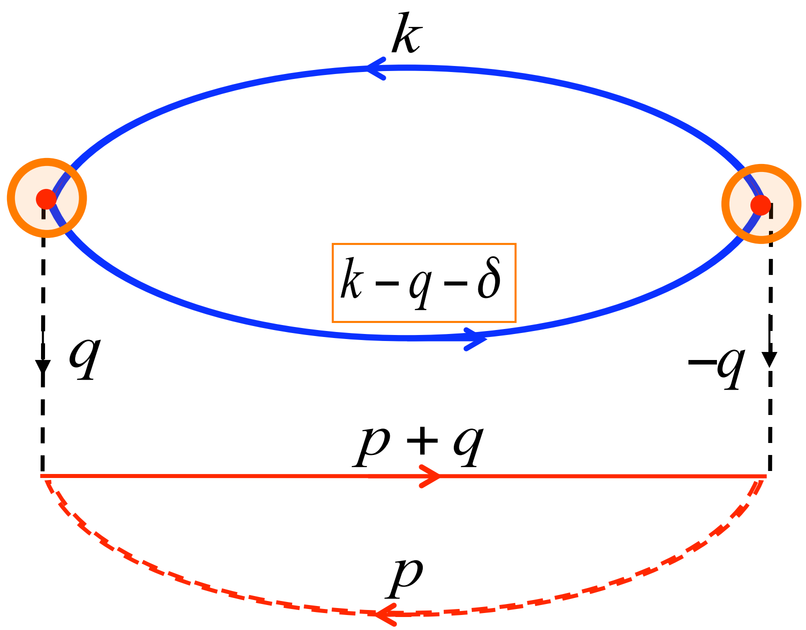


Now measure Σ

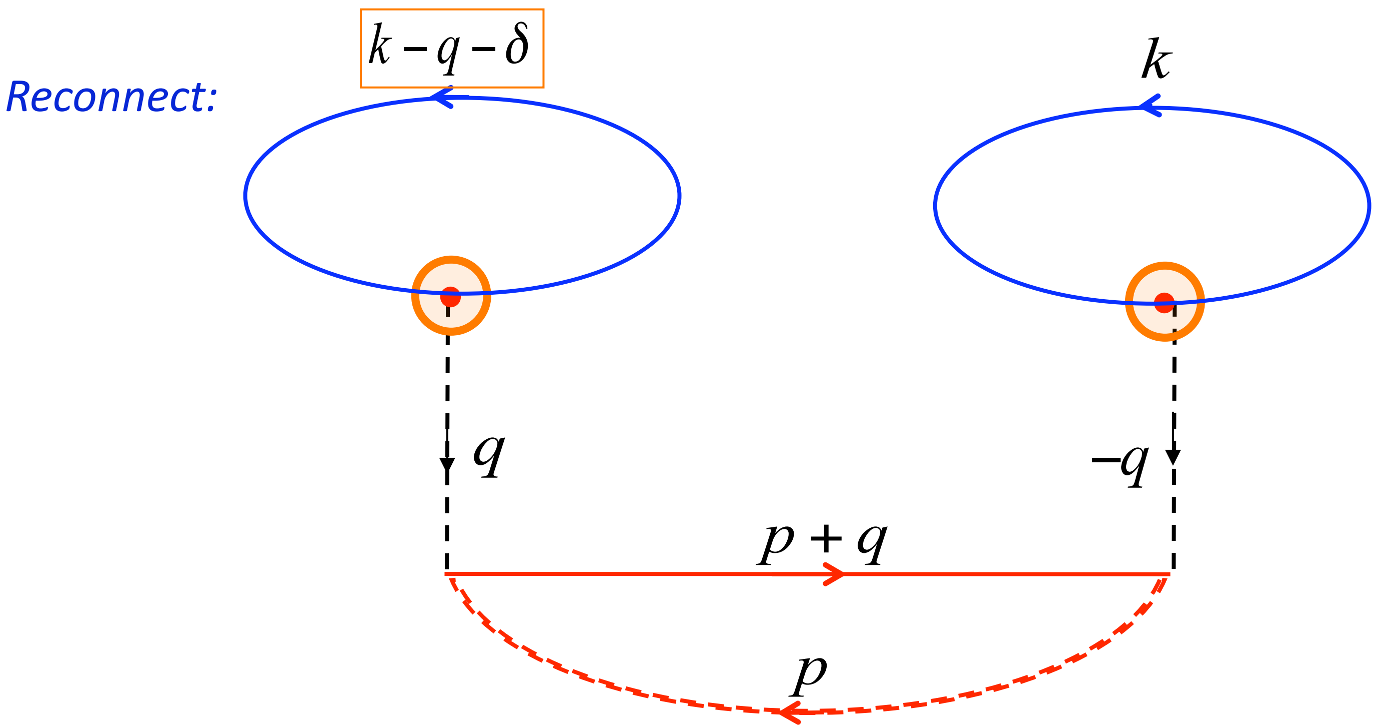
Updates

Reconnect:



Do not measure Σ

Updates



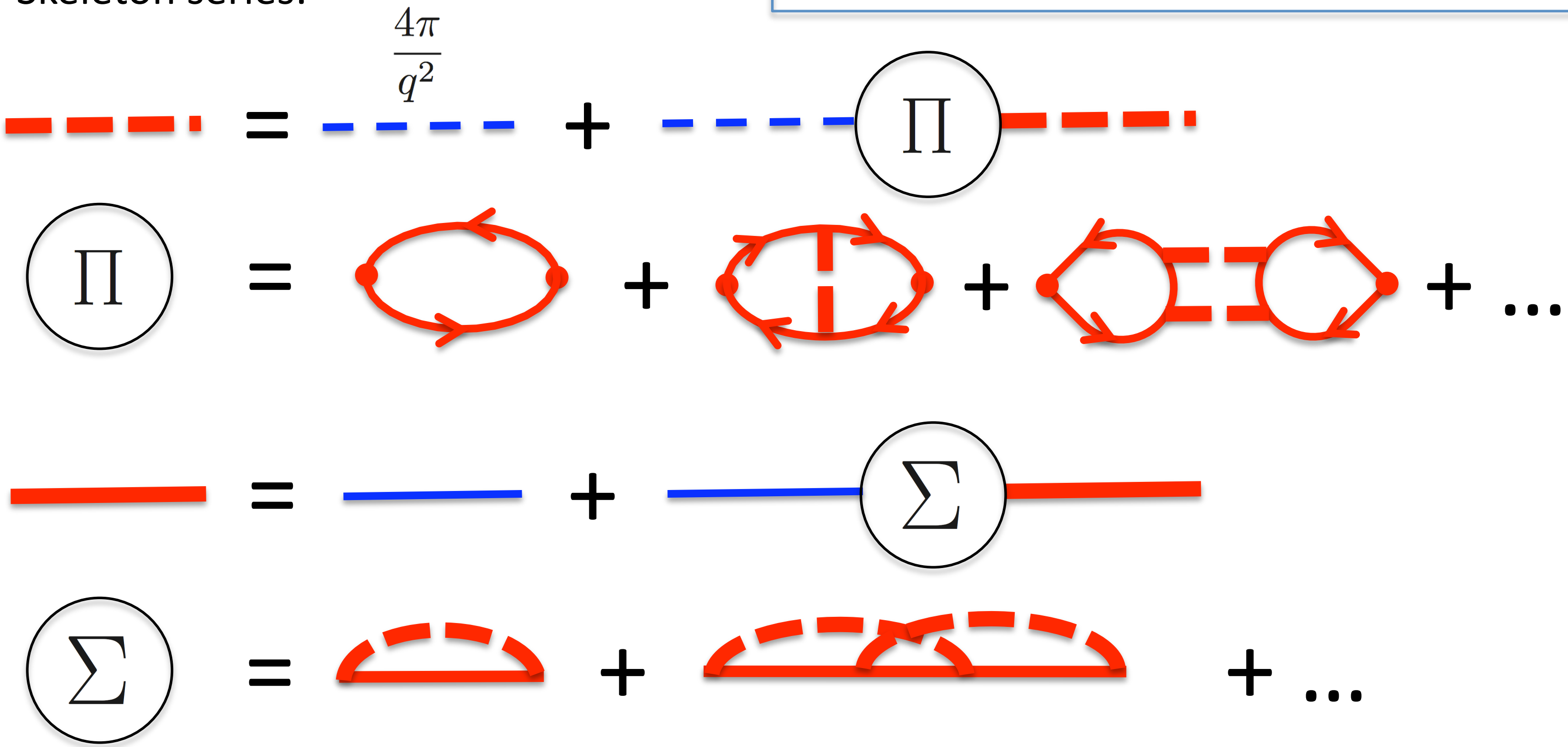
Do not measure Σ

Bold DiagMC for the electron gas

$$H = \sum_{\mathbf{k}\sigma} \left(\frac{\hbar^2 k^2}{2m} - \mu_\sigma \right) a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{1}{2V} \frac{e^2}{4\pi\epsilon_0} \sum_{\mathbf{kpq}}{}' \sum_{\sigma\sigma'} \frac{4\pi}{q^2} a^\dagger_{\mathbf{k+q},\sigma} a^\dagger_{\mathbf{p-q},\sigma'} a_{\mathbf{p},\sigma'} a_{\mathbf{k},\sigma}$$

One has to take care of screening

Skeleton series:



- DiagMC scheme for EG samples only skeleton diagrams in ergodic way (same diagrams as in QED)
- Work in progress: comparison of exchange-correlation energy with GW/DMC.

Conclusions/perspectives

- **Bold-line Diagrammatic series can be efficiently simulated.**

- combine analytic and numeric tools
- thermodynamic-limit results
- sign-problem tolerant (small configuration space)

- **Equation of state of the Hubbard model in Fermi liquid regime (bare Diagrammatic MC)**

- **Equation of state of the unitary gas (see talk by Félix Werner tomorrow)**

- **Work in progress: BEC-BCS,** bold-line implementation for the Hubbard model and the continuous electron gas or jellium model (screening version).