BOLD DIAGRAMMATIC MONTE CARLO:
From polarons to path-integrals to skeleton Feynman diagrams

Nikolay Prokofiev, Umass, Amherst

National Science Foundation
WHERE DISCOVERIES BEGIN

DARPA DSO
DEFENSE SCIENCES OFFICE

OLE
OPTICAL LATTICE EMULATOR

Tallahassee, NHMFL (January 2012)

High energy physics / Standard model

High-Tc superconductors / Hubbard model

Quantum chemistry & band structure / Coulomb gas

Quantum magnetism / Heisenberg model

Periodic Anderson & Kondo lattice models / Heavy fermion materials

…

- Introduced in mid 1960s or earlier

- Still not solved (just a reminder, today is 01/13/2012)

- Admit description in terms of Feynman diagrams

Feynman Diagrams & Physics of strongly correlated many-body systems

In the absence of small parameters, are they useful in higher orders?

N.Abel, 1828:

“Divergent series are the devil's invention...”

Yes, with sign-blessing for regularized skeleton graphs!

And if they are, how to handle millions and billions of skeleton graphs?

Steven Weinberg, Physics Today, Aug. 2011 :

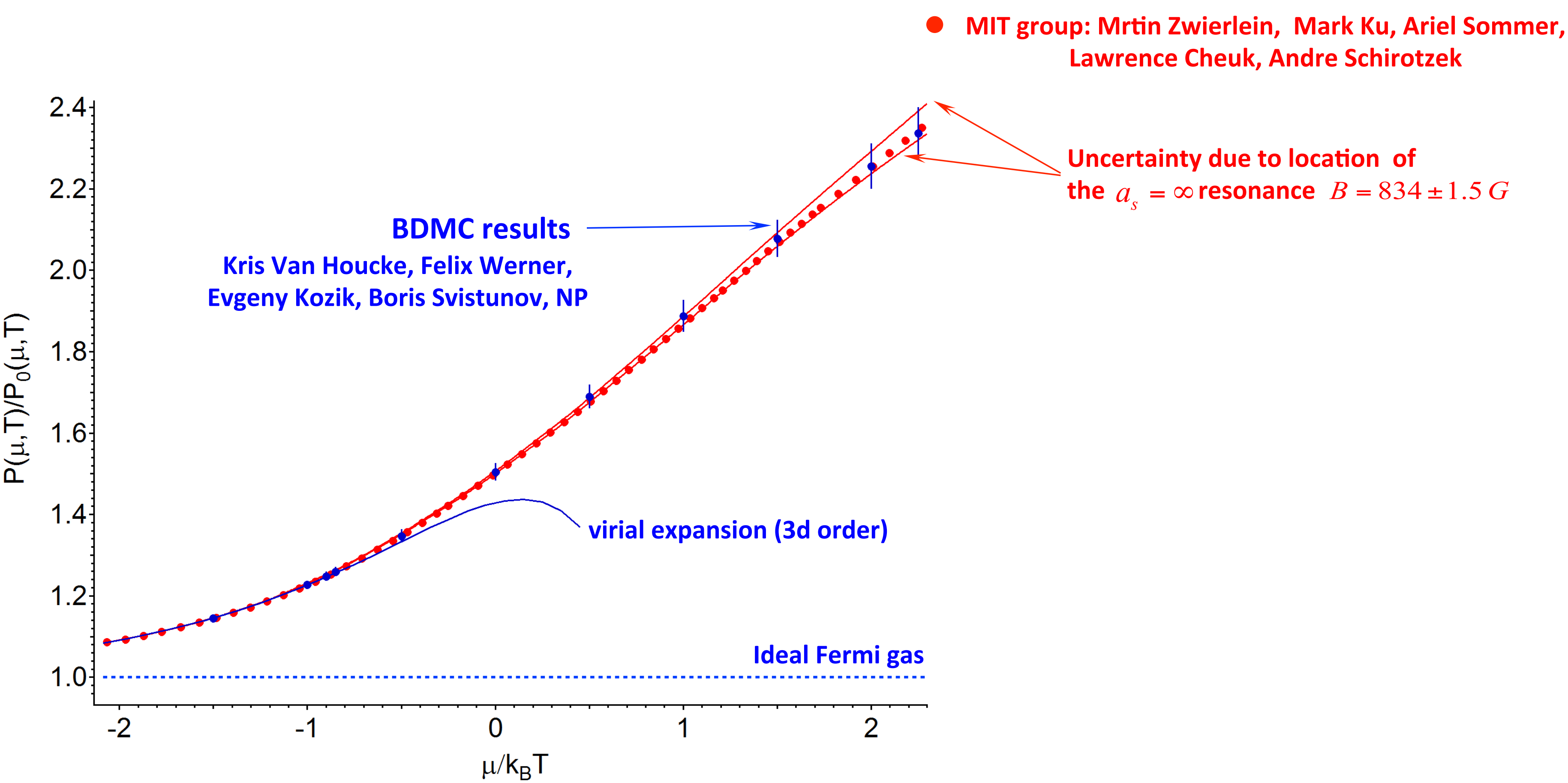
“Also, it was easy to imagine any number of quantum field theories of strong interactions but what could anyone do with them?”

Sample them with Diagrammatic Monte Carlo techniques
(teach computers rules of quantum field theory)

From current strong-coupling theories based on one lowest order skeleton graph (MF, RPA, GW, SCBA, GG_0, GG, …

Unbiased solutions beased on millions of graphs with extrapolation to the infinite diagram order

Answering Weinberg's question:
Equation of State for ultracold fermions & neutron matter at unitarity



QMC for connected Feynman diagrams NOT particles!

Sign blessing

Sign ~~problem~~

Conventional Sign-problem *vs* Sign-blessing

Sign-problem:
(diagrams for Z)

Computational complexity is exponential in system volume $t_{CPU} \propto \exp\{\# L^d \beta\}$ and error bars explode before a reliable exptrapolation to $L \to \infty$ can be made

Feynamn diagrams:
(for $\ln Z$)

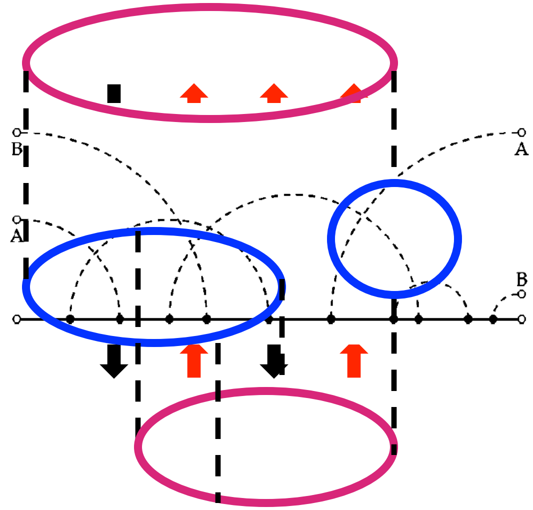
No $L \to \infty$ limit to take, selfconsistent formulation, admit analytic results and partial resummations.

Sign-blessing:
(diagrams for $\ln Z$)

Number of diagram of order n is factorial $\propto n! 2^n n^{3/2}$ thus the only hope for good series convergence properties is sign alter-nation of diagrams leading to their cancellation. Still, $t_{CPU} \propto n! 2^n n^{3/2}$ i.e. Smaller and smaller error bars are likely to come at exponential price (unless convergence is exponential).

Standard Monte Carlo setup:

- configuration space (depends on the model and it's representation)



- each cnf. has a weight factor W_{cnf} $e^{-E_{cnf}/T}$

- quantity of interest $A_{cnf} \longrightarrow \langle A \rangle = \dfrac{\sum_{cnf} A_{cnf} W_{cnf}}{\sum_{cnf} W_{cnf}}$

Statistics: $\sum_{\{states\}} e^{-E_{state}/T} O_{state}$ $\xrightarrow{\text{Monte Carlo}}$ $\sum_{\{states\}}^{MC} O_{state}$

states generated from probability distribution $e^{-E_{state}/T}$

Anything: $\sum_{\{\nu=\text{any set of variables}\}} F(\nu)\, O(\nu)$ $\xrightarrow{\text{Monte Carlo}}$ $\sum_{\{\nu\}}^{MC} e^{i\arg[F(\nu)]} O(\nu)$

states generated from probability distribution $|F(\nu)|$

Anything = **Connected Feynman diagrams, e.g. for the proper self-energy**

$\nu = \begin{cases} \text{diagram order} \\ \text{topology} \\ \text{internal variables} \end{cases}$

$\xrightarrow{\text{Monte Carlo}}$ **Answer to S. Weinberg's question**

$$\Sigma = \sum_{\nu}^{MC} sign(F(\nu))$$

Classical MC

$$Z\left(\vec{y}\right) = \iiint d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_N \; W\left(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N, \vec{y}\right)$$

the number of variables N is constant

Quantum MC (often)

$$Z\left(\vec{y}\right) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint \underbrace{\underbrace{d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_n}_{\text{Integration variables}} \; D_n\left(\xi; \vec{x}_1, \vec{x}_2, \ldots \vec{x}_n, \vec{y}\right)}$$

term order

different terms of
of the same order

Integration variables

Contribution to the answer
or weight (with differential measures!)

$$A(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_n \; D_n\left(\xi; \vec{x}_1, \vec{x}_2, \ldots \vec{x}_n, \vec{y}\right) = \sum_{\nu} D_{\nu}$$

Monte Carlo (Metropolis) cycle:

→ **Diagram** W_ν → **suggest a change** → **Accept with probability** $R_{acc} \sim \frac{W_{\nu'}}{W_\nu}$ →

Same order diagrams:

$$\frac{D_{\nu'}}{D_\nu} \sim \frac{(d\vec{x})^n}{(d\vec{x})^n} \sim O(1)$$

Business as usual

Updating the diagram order:

$$\frac{D_{\nu'}}{D_\nu} \sim \frac{(d\vec{x})^{n+m}}{(d\vec{x})^n} \sim (d\vec{x})^m \rightarrow$$ **Ooops**

Balance Equation:

If the desired probability density distribution of different terms in the stochastic sum is P_ν then the updating process has to be stationary with respect to P_ν (equilibrium condition). Often $P_\nu = W_\nu$

$$D_\nu \underbrace{\sum_{updates\ \nu \to \nu'} \Omega_\nu(\nu')\, R^{\nu \to \nu'}_{accept}}_{\text{Flux out of } \nu} = \underbrace{\sum_{updates\ \nu' \to \nu} D_{\nu'}\, \Omega_{\nu'}(\nu)\, R^{\nu' \to \nu}_{accept}}_{\text{Flux to } \nu}$$

Flux out of ν

Flux to ν

$\Omega_\nu(\nu')$ Is the probability of proposing an update transforming ν to ν'

Detailed Balance: solve equation for each pair of updates separately

$$D_\nu\, \Omega_\nu(\nu')\, R^{\nu \to \nu'}_{accept} = D_{\nu'}\, \Omega_{\nu'}(\nu)\, R^{\nu' \to \nu}_{accept}$$

Let us be more specific. Equation to solve:

$$\underbrace{D_n\left(\vec{x}_1,\ldots,\vec{x}_n\right)(d\vec{x})^n}_{D_\nu}\ \underbrace{\Omega_{n,n+m}\left(\vec{x}_1,\ldots,\vec{x}_{n+m}\right)(d\vec{x})^m}_{\Omega_\nu(\nu')}\ R_{accept}^{n\to n+m} = \underbrace{D_{n+m}\left(\vec{x}_1,\ldots,\vec{x}_{n+m}\right)(d\vec{x})^{n+m}}_{D_\nu}\ \underbrace{\Omega_{n+m,n}}_{\Omega_{\nu'}(\nu)}\ R_{accept}^{n+m\to n}$$

new variables $\vec{x}_{n+1},\ldots,\vec{x}_{n+m}$ are proposed from the normalized probability distribution

Solution:

$$R = \frac{R_{accept}^{n\to n+m}}{R_{accept}^{n+m\to n}} = \frac{D_{n+m}(x_1,\ldots,x_{n+m})}{D_n(x_1,\ldots,x_n)}\ \frac{\Omega_{n+m,n}}{\Omega_{n,n+m}(x_1,\ldots,x_{n+m})}$$

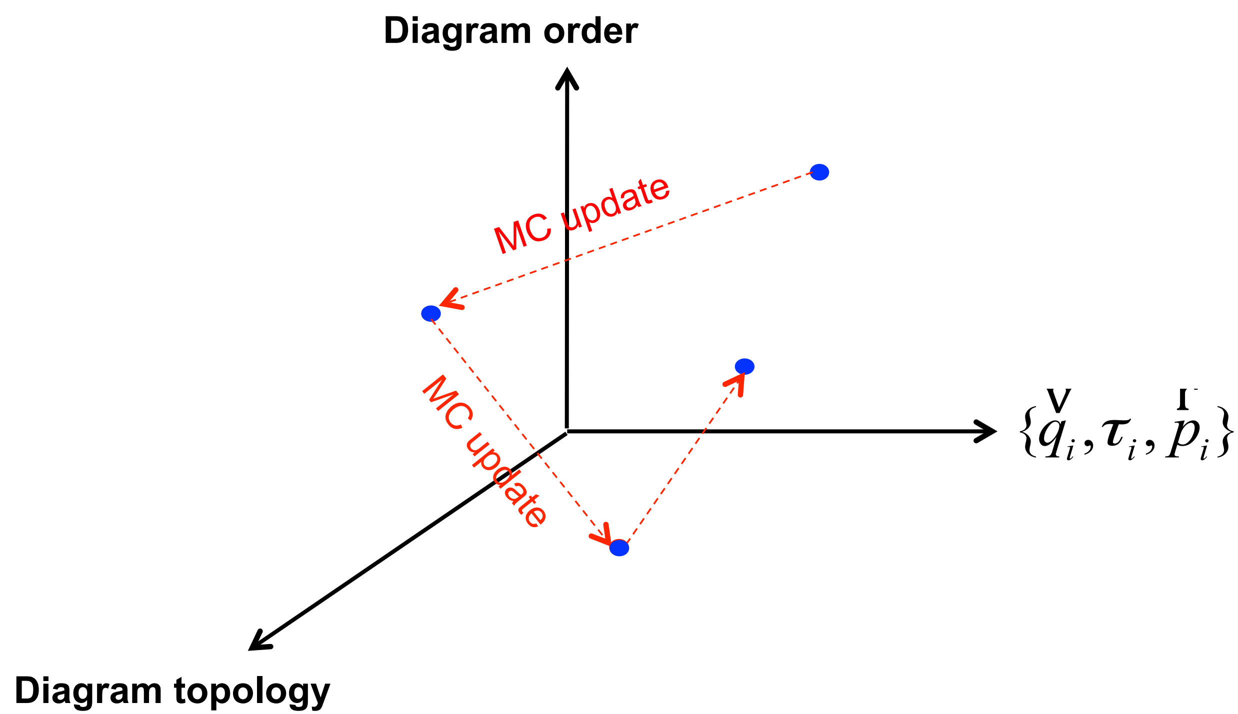
All differential measures are gone!

Efficiency rules:

- try to keep $R\sim 1$
- simple analytic function $\Omega_{n,n+m}(x_{n+1},\ldots,x_{n+m})$

ENTER

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



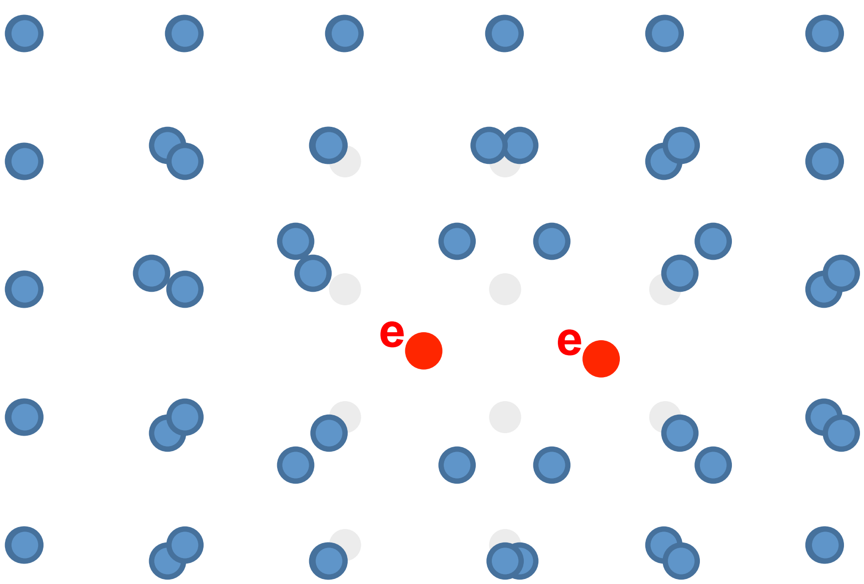
This is NOT: write/enumerate diagram after diagram, compute its value, and then sum

Polaron problem:

$$H = H_{\text{particle}} + H_{\text{environment}} + H_{\text{coupling}} \quad \longrightarrow \quad \textbf{quasiparticle}$$

$$E(p=0),\ m_*,\ G(p,t),\ \ldots$$

Electrons in semiconducting crystals (electron-phonon polarons)



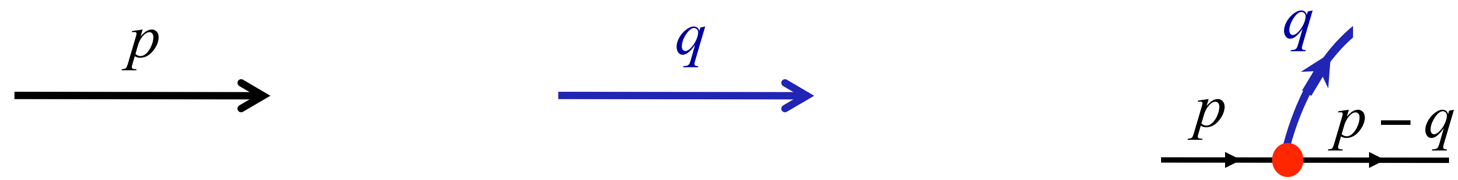
$$H = \sum_p \varepsilon(p) a_p^+ a_p + \qquad \textbf{electron}$$

$$\sum_q \omega(p)(b_q^+ b_q + 1/2) + \qquad \textbf{phonons}$$

$$\sum_{pq} \left(V_q a_{p-q}^+ a_p b_q^+ + h.c. \right) \qquad \textbf{el.-ph. interaction}$$

$$H = \sum_p \varepsilon(p) a_p^+ a_p + \sum_q \omega(p)(b_q^+ b_q + 1/2) + \sum_{pq} \left(V_q a_{p-q}^+ a_p b_q^+ + h.c. \right)$$

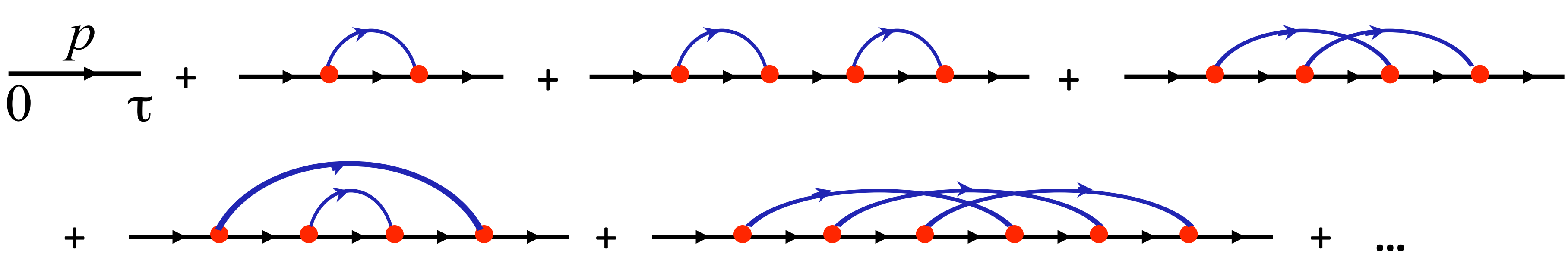
electron **phonons** **el.-ph. interaction**



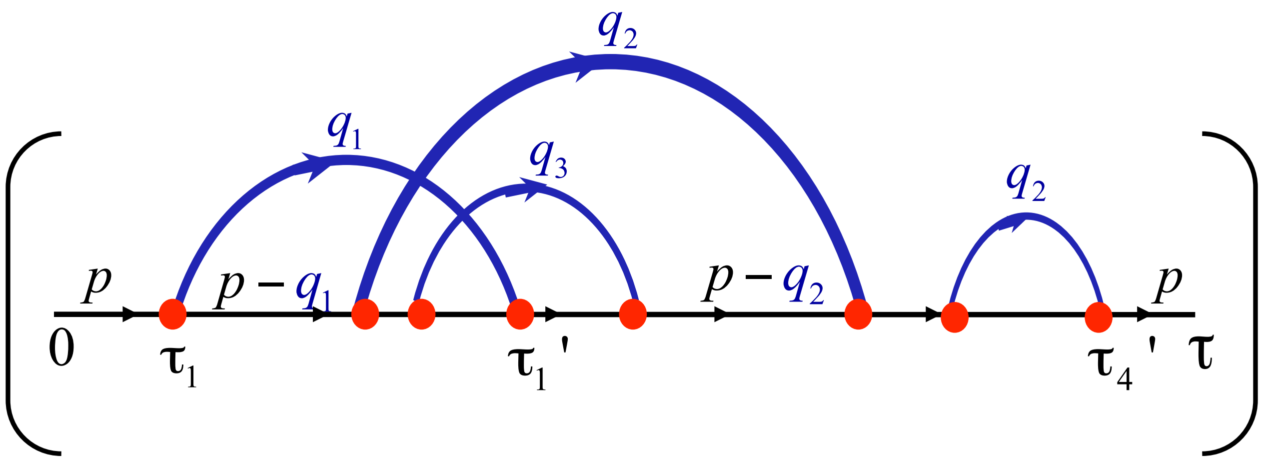
Green function: $G(p,\tau) = \langle a_p(0) a^+{}_p(\tau) \rangle = \langle a_p \; e^{-\tau H} \; a^+{}_p \; e^{\tau H} \rangle$

$=$ **Sum of all Feynman diagrams**

Positive definite series in the (p,τ) **representation**



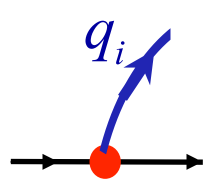
$$G(p,\tau) = \sum_{\text{Feynman digrams}}$$



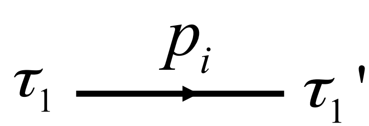
Graph-to-math correspondence:

$$G(\vec{p},\tau) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_n \; D_n(\xi; \vec{x}_1, \vec{x}_2, \ldots \vec{x}_n, \vec{p}, \tau) \text{ where } \vec{x}_i = (q_i, \tau_i, \tau_i')$$

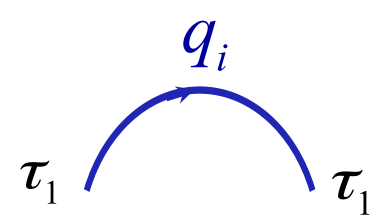
is a product of



V_{q_i}

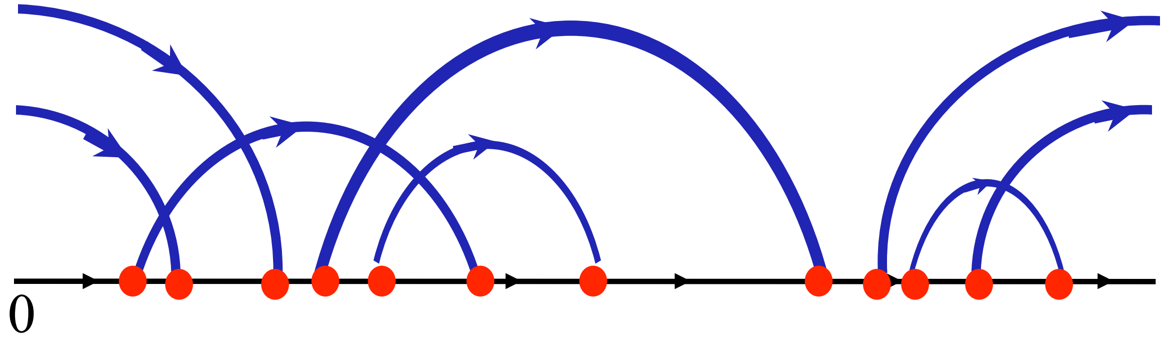


$e^{-\varepsilon(p_i)(\tau_i'-\tau_i)}$



$e^{-\omega(q)(\tau_i'-\tau_i)}$

Positive definite series in the $(\vec{p},\tau)$ representation



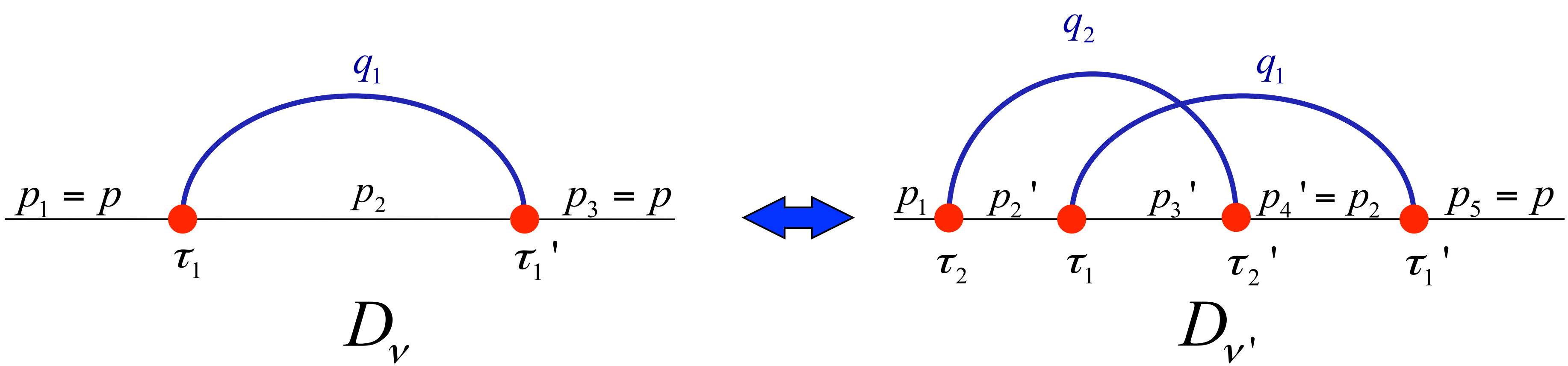
Diagrams for: $\left\langle b_{q_1}(0) b_{q_2}(0)\ a_{p-q_1-q_2}(0)\ a^{+}_{p-q_1-q_2}(\tau)\ b^{+}_{q_1}(\tau) b^{+}_{q_2}(\tau) \right\rangle$

there are also diagrams for optical conductivity, etc.

Doing MC in the Feynman diagram configuration space is an endless fun!

The simplest algorithm has three updates:

Insert/Delete pair (increasing/decreasing the diagram order)



$$D_{\nu'} / D_{\nu} = |V_{q_2}|^2 \; e^{-\omega(q_2)(\tau_2' - \tau_2)} \; e^{-(\varepsilon(p_2') - \varepsilon(p_2))(\tau_1 - \tau_2)} \; e^{-(\varepsilon(p_3') - \varepsilon(p_2))(\tau_2' - \tau_1)}$$

$$R = \frac{D_{\nu'}}{D_{\nu}} \frac{\Omega_{n+1,n}}{\Omega_{n,n+1}(x_1,\mathrm{K}\ ,x_{n+1})} = \frac{D_{\nu'}}{D_{\nu}} \frac{1}{(n+1)\,\Omega_{n,n+1}(x_1,\mathrm{K}\ ,x_{n+1})}$$

In Delete select the phonon line to be deleted at random

The optimal choice of $\Omega_{n,n+1}(x_1, \ldots, x_{n+1})$ depends on the model

Frohlich polaron: $\varepsilon = p^2/2m$, $\omega_q = \omega_0$, $V_q \sim \alpha / q$

$$D_{\nu'} / D_\nu \propto \frac{q^2}{q^2} \, e^{-\omega_0(\tau_2' - \tau_2)} \, e^{-\frac{[(p_2')^2 - p_2^2](\tau_1 - \tau_2) + [(p_3')^2 - p_2^2](\tau_2' - \tau_1)}{2m}} dq\, d\varphi\, d\theta\, d\tau^2$$

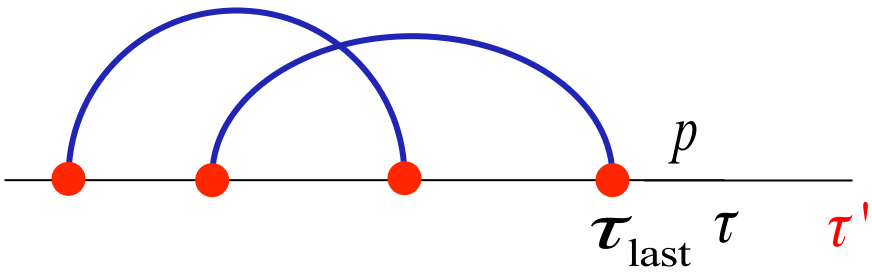
1. Select τ_2 anywhere on the interval $(0, \tau)$ from uniform prob. density

2. Select τ_2' anywhere to the left of τ_2 from prob. density $e^{-\omega_0(\tau_2' - \tau_2)}$
(if $\tau_2' > \tau$ reject the update)

3. Select q_2 from Gaussian prob. density $e^{-(q_2^2/2m)(\tau_2' - \tau_2)}$, i.e.

$$\Omega_{n,n+1}(\tau_2, \tau_2', q_2) \sim e^{-\omega_0(\tau_2' - \tau_2)} e^{-(q_2^2/2m)(\tau_2' - \tau_2)}$$

New τ :



Standard "heat bath" probability density $\sim e^{-\varepsilon(p)(\tau'-\tau_{\text{last}})}$

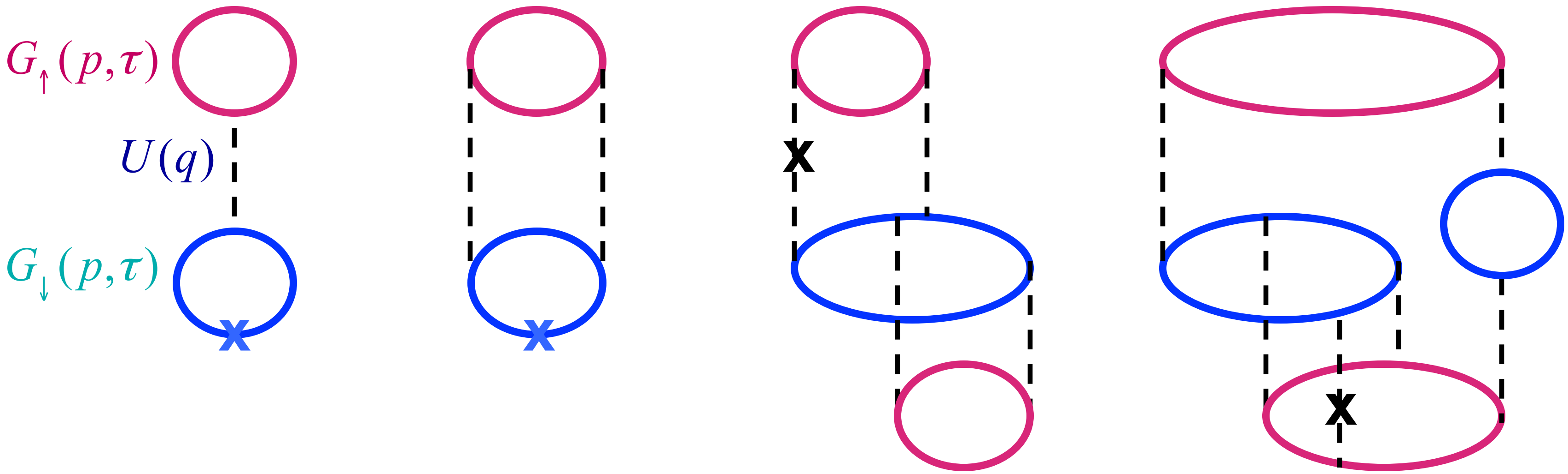
Always accepted, $R = 1$

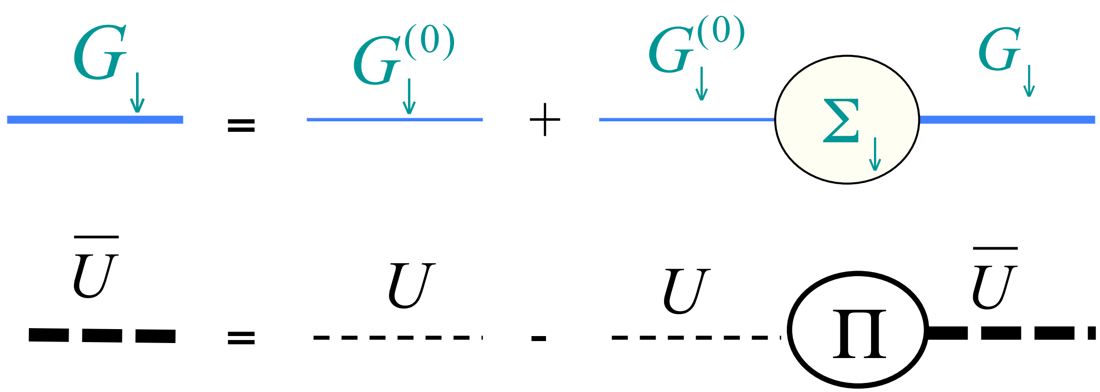
This is it! Collect statistics for $G(p,\tau)$**. Analyze it using**

$$G(p,\tau \to \infty) \to Z_p e^{-E(p)\tau}$$ **, etc.**

Diagrammatic Monte Carlo in the generic many-body setup

Feynman diagrams for free energy density



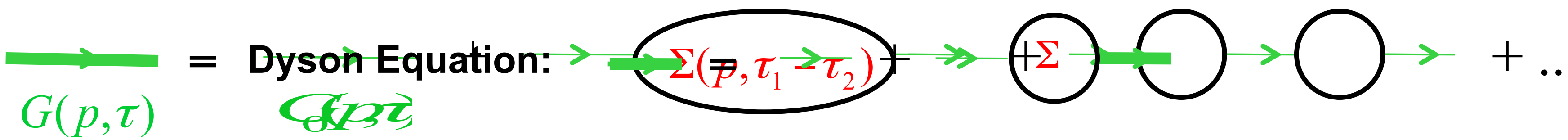


Bold (self-consistent) Diagrammatic Monte Carlo

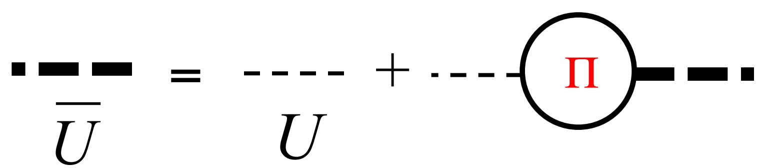
Diagrammatic technique for ln(Z) diagrams: admits partial summation and self-consistent formulation

No need to compute all diagrams for G and $\bar{U}$:

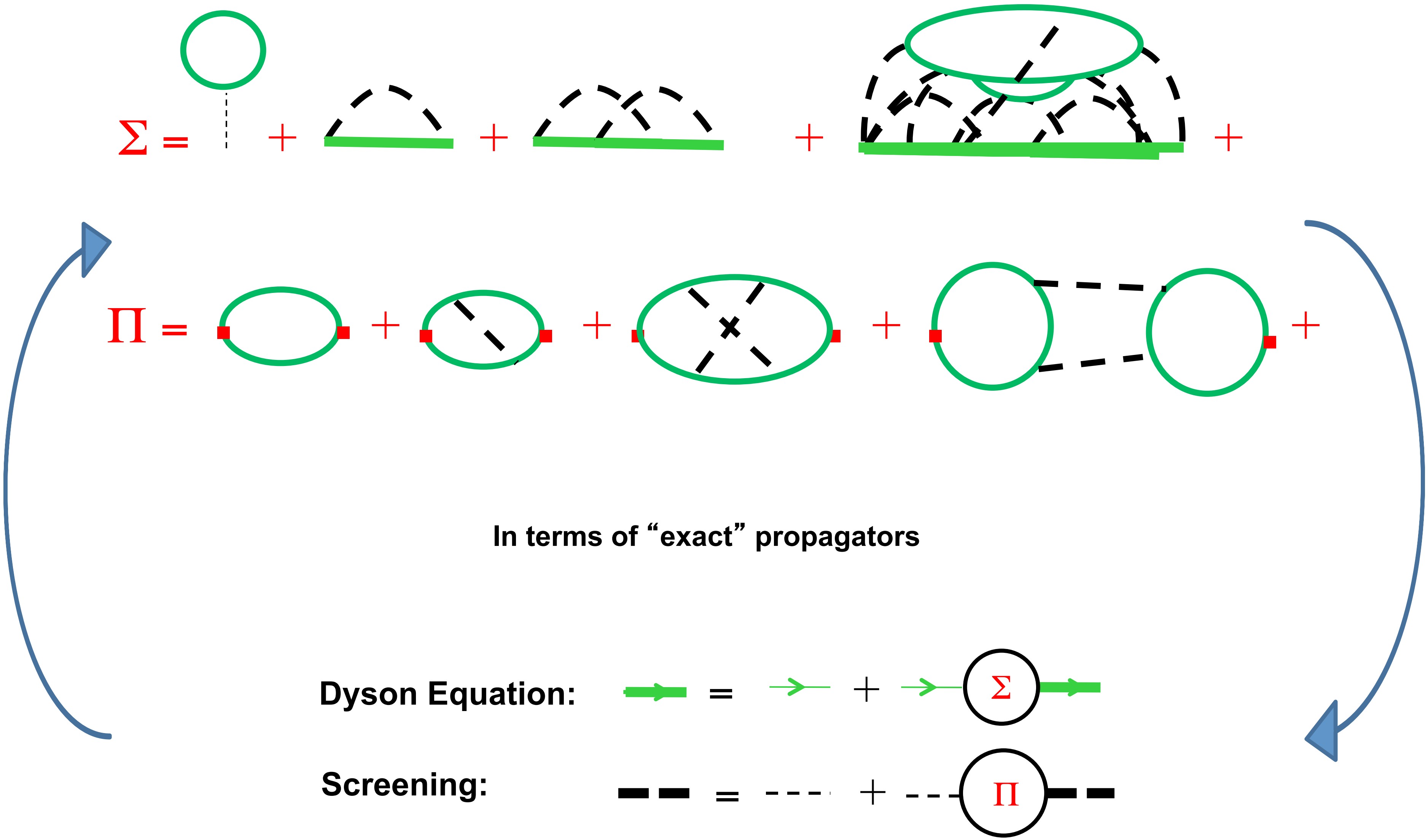
Dyson Equation:



Screening:



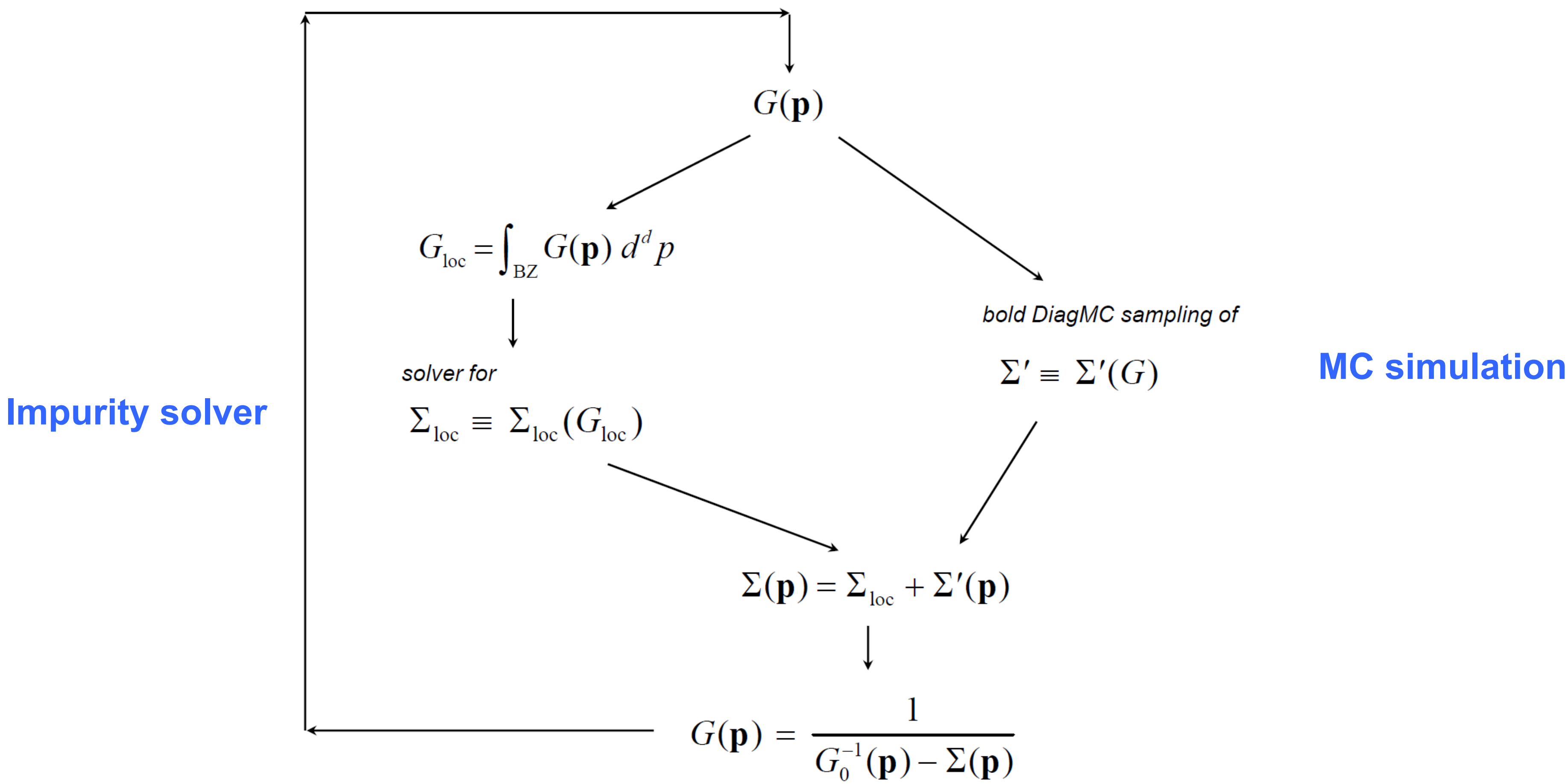
Calculate irreducible diagrams for Σ , Π , … to get G, $\bar{U}$, …. from Dyson equations


Σ =
Π =
In terms of “exact” propagators
Dyson Equation:
Σ
Screening:
Π

More tools: Incorporating DMFT solutions for Σ_{loc}

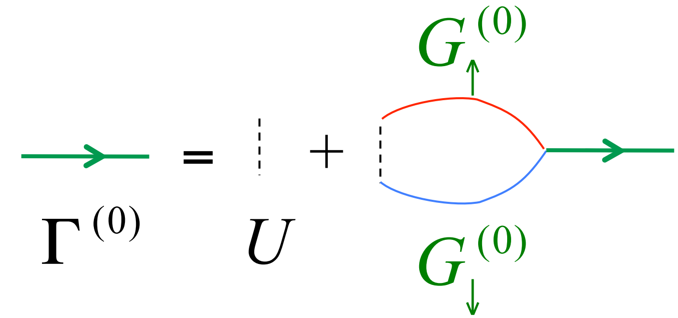
$\Sigma_{loc}[G_{loc}] =$ **all electron propagator lines in all graphs are local,** $G \rightarrow G_{loc} = G_{rr}\delta_{rr'}$

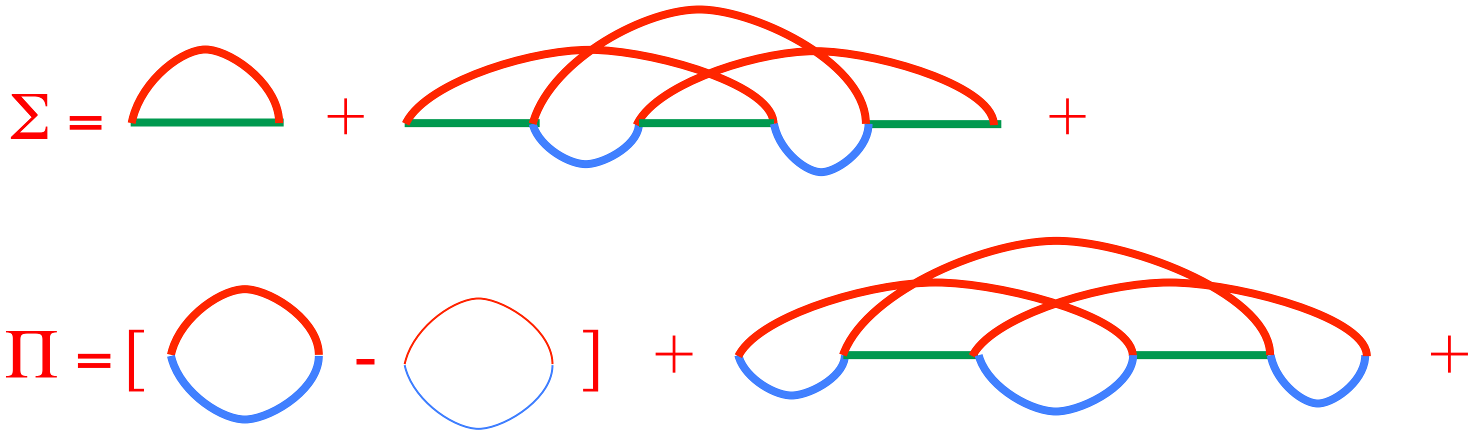
$\Sigma' =$ **at least one electron propagator in the graph is non-local, i.e. the rest of graphs**



More tools: Build diagrams using ladders:

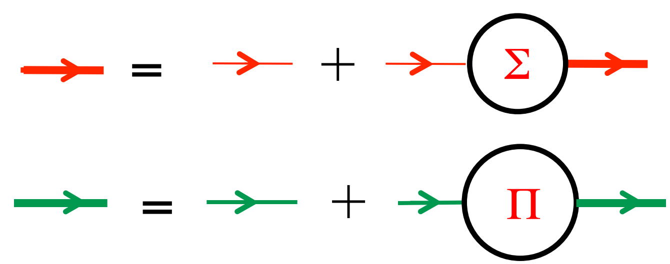
(contact potential)



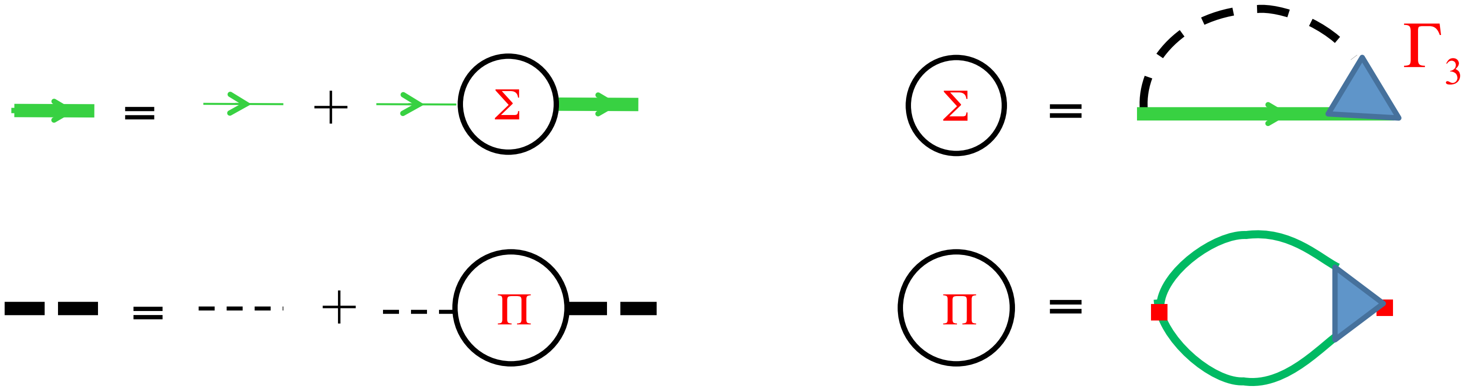


In terms of "exact" propagators

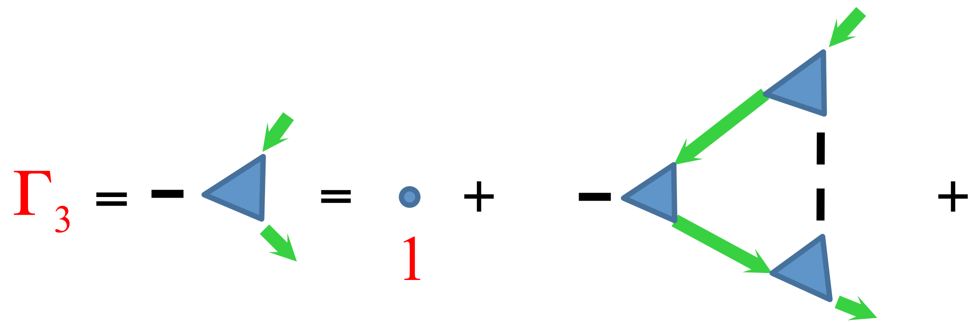
Dyson Equations:

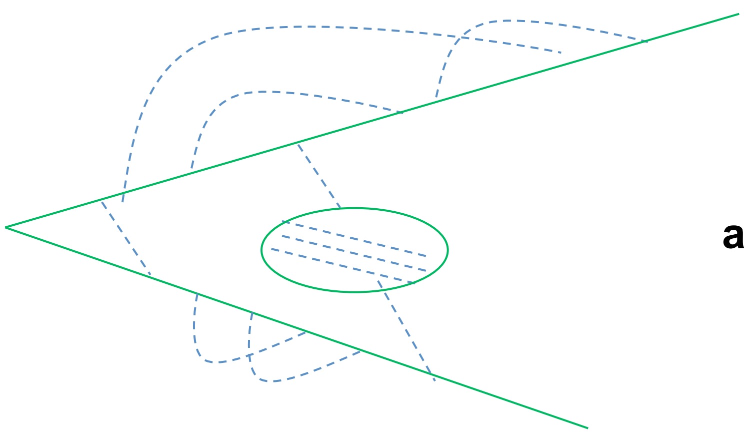


Fully dressed skeleton graphs (Heidin):

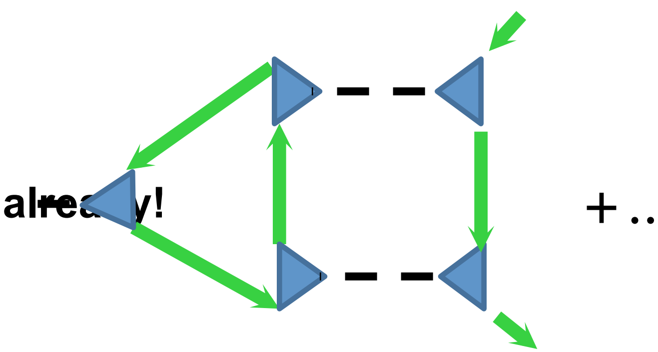


Irreducible 3-point vertex:





all accounted for already!

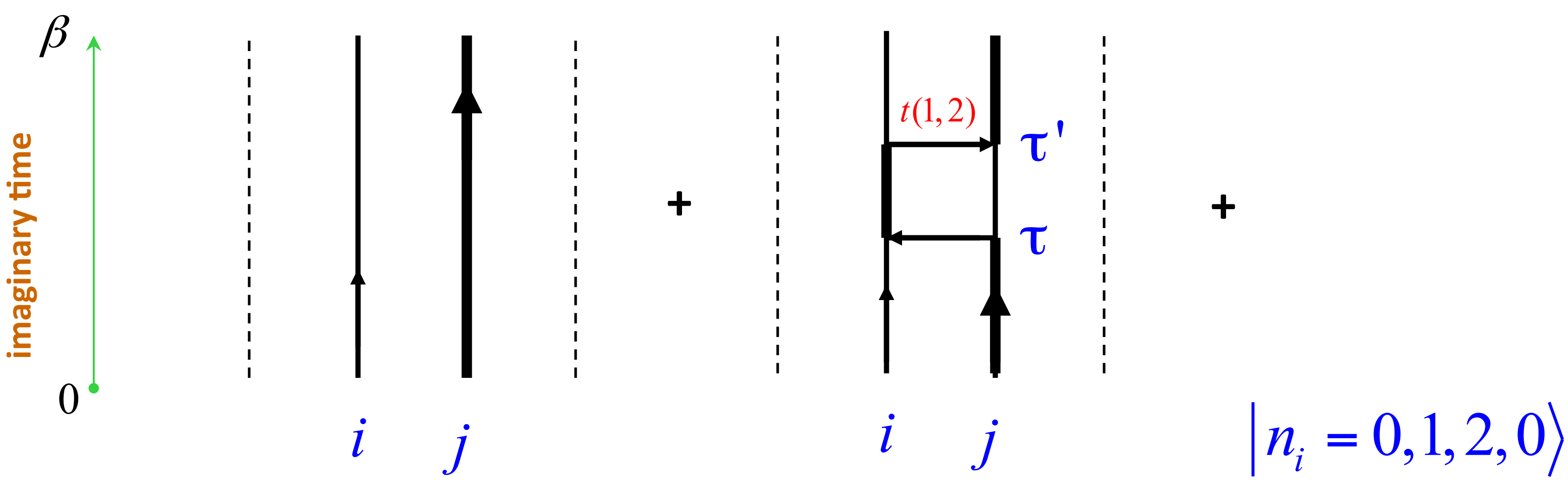


$$H = H_0 + H_1 = \sum_{ij} U_{ij} n_i n_j - \sum_i \mu_i n_i \;\; - \sum_{<ij>} t(n_i, n_j) b_j^+ b_i$$

Lattice path-integrals for bosons and spins are "diagrams" of closed loops!

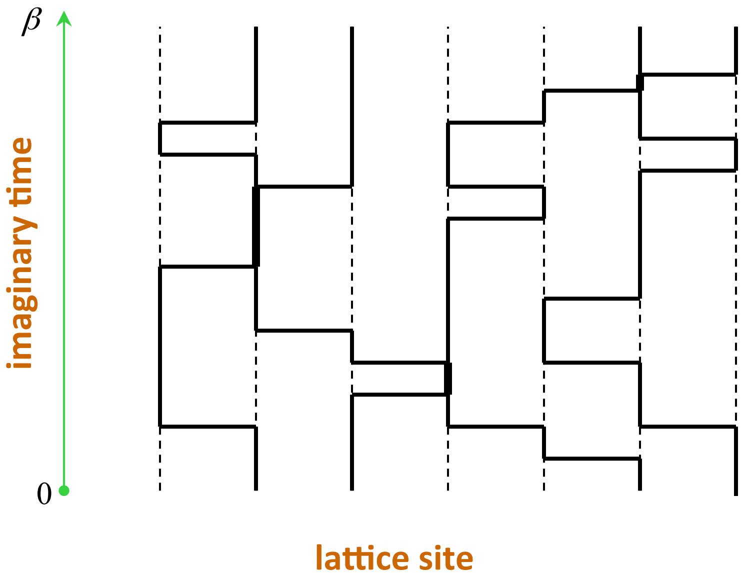
$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \mathrm{Tr}\, e^{-\beta H_0}\, e^{-\int_0^\beta H_1(\tau)\, d\tau}$$

$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_0^\beta \int_\tau^\beta H_1(\tau)\, H_1(\tau)\;\; d\tau\, d\tau' + \ldots \right\}$$



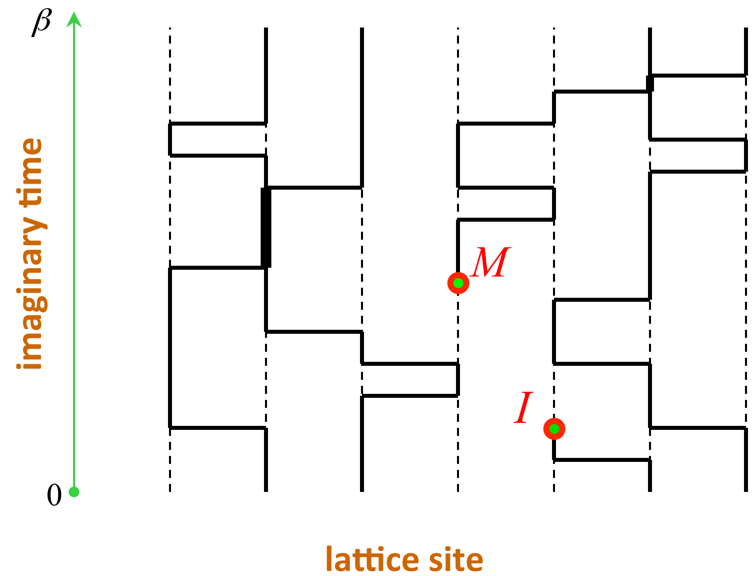
Diagrams for

$$Z = \mathrm{Tr}\, e^{-\beta H}$$



Diagrams for

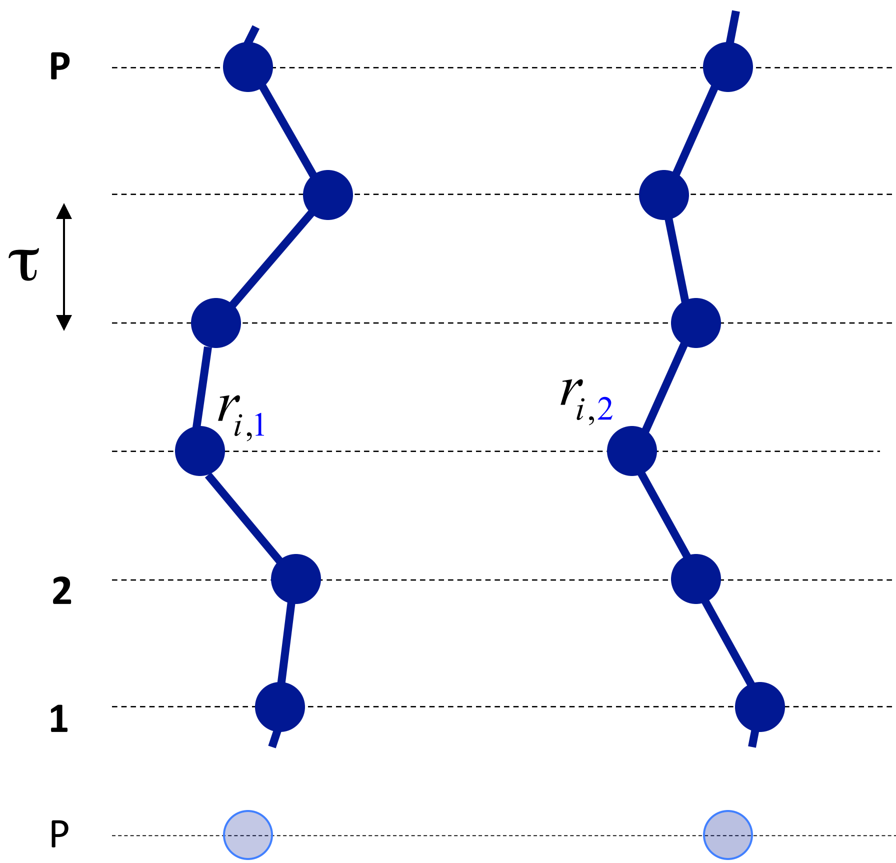
$$G_{IM} = \mathrm{Tr}\, T_\tau\, b_M^\dagger(\tau_M)\, b_I(\tau_I)\, e^{-\beta H}$$



The rest is conventional worm algorithm in continuous time

$$Z = \iiint dR_1 \ldots dR_P \exp\left\{ -\sum_{i=1}^{P=\beta/\tau} \left(\frac{m(R_{i+1} - R_i)^2}{2\tau} + U(R)\tau \right) \right\}$$

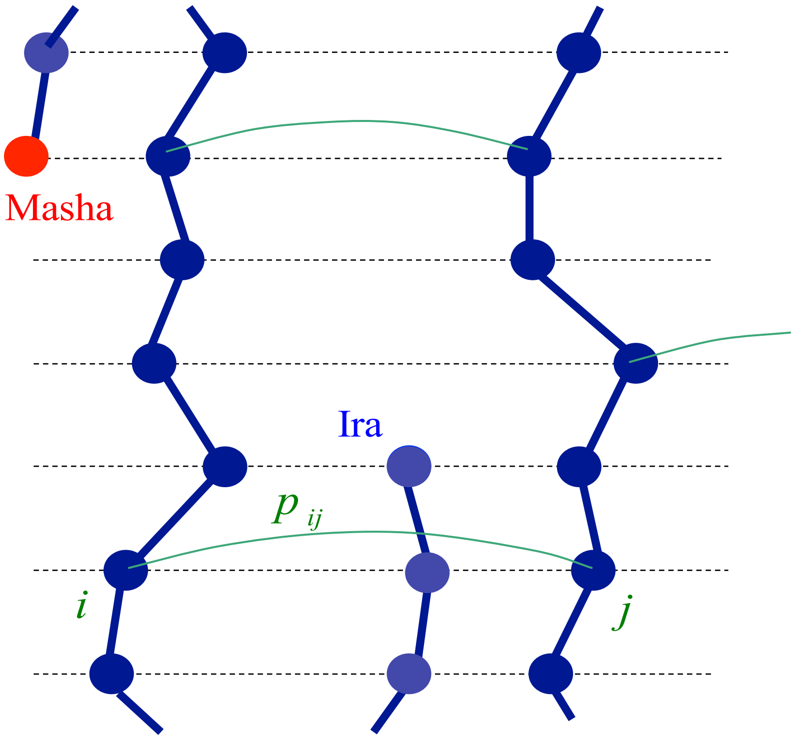
Path-integrals in continuous space are "diagrams" of closed loops too!



$$R_i = (r_{i,1}, r_{i,2}, \ \ldots, r_{i,N})$$

Diagrams for the attractive tail in $U(r)$:

If $-\tau \sum_{j\neq i}^{N} U(r_j - r_i)\ \theta(|r_j - r| - r_c) << 1$ and N>>1 all the effort is for something small !



$$e^{-V(r_{ij})\tau} \equiv 1 + (e^{-V(r_{ij})\tau} - 1) = 1 + p_{ij}$$

statistical interpretation

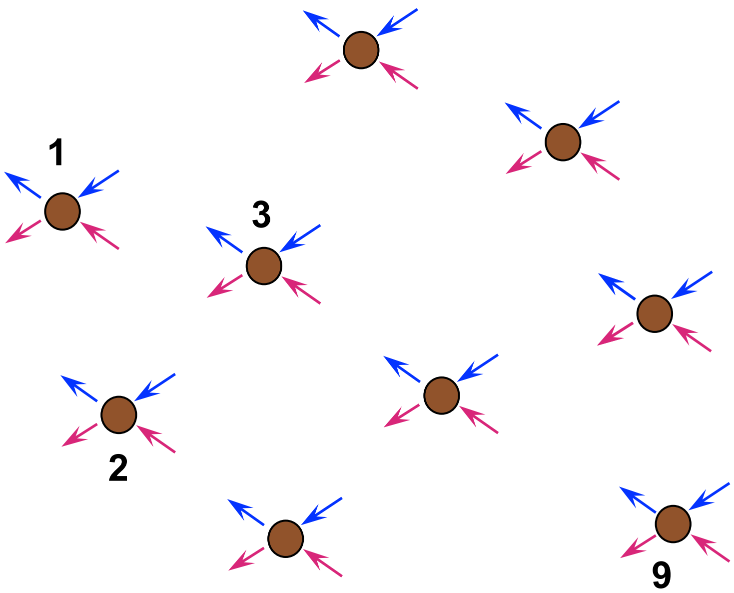
ignore $V(r_{ij})$ **: stat. weight** 1

Account for $V(r_{ij})$ **: stat. weight p**

Faster than conventional scheme for N>30, scalable (size independent) updates with exact account of interactions between all particles

Other applications: Continuous-time QMC solves (impurity solvers) are standard DMC schemes

Fermions with contact interaction



$$\nu = \{ n; \mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2; \ldots; \mathbf{r}_n, \tau_n \}$$

$$\det G_{ij} = \begin{vmatrix} G_{11} & G_{12} & \ldots & G_{1p} \\ G_{21} & G_{22} & \ldots & G_{2p} \\ \ldots & \ldots & \ldots & \ldots \\ G_{p1} & G_{p2} & \ldots & G_{pp} \end{vmatrix}$$

$$Z = \sum_{p=0}^{\infty} \int \ldots \int (d\vec{r} d\tau)^p (-U)^p \det G_{\uparrow}(\vec{x}_i, \vec{x}_j) \det G_{\downarrow}(\vec{x}_i, \vec{x}_j)$$

Rubtsov (2003)

+ more in A. Millis' s talk

Skeleton diagrams up to high-order: do they make sense for $g \geq 1$?

NO

Diverge for large g even if are convergent for small g.

Dyson: Expansion in powers of g is asymptotic if for some (e.g. complex) g one finds pathological behavior.

Electron gas: $e \rightarrow i\,e$

Bosons: $U \rightarrow -U$

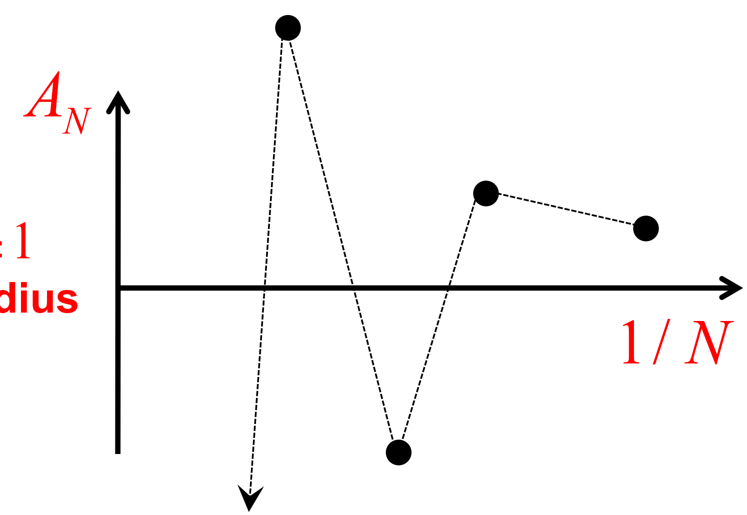
[collapse to infinite density]

Math. Statement: # of skeleton graphs

$\propto 2^n n^{3/2} n! \rightarrow$

asymptotic series with zero conv. radius (n! beats any power)

Asymptotic series for $g \geq 1$ with zero convergence radius



Skeleton diagrams up to high-order: do they make sense for $g \geq 1$?

YES

Divergent series outside of finite convergence radius can be re-summed.

Dyson:

- **Does not apply to the resonant Fermi gas and the Fermi-Hubbard model at finite T.**
- **not known if it applies to skeleton graphs which are NOT series in bare g: cf. the BCS answer (one lowest-order diagram) $\Delta \propto e^{-1/g}$**
- **Regularization techniques**

# of graphs is $\propto 2^n n^{3/2} n!$

but due to sign-blessing they may compensate each other to accuracy better then $1/n!$ leading to finite conv. radius

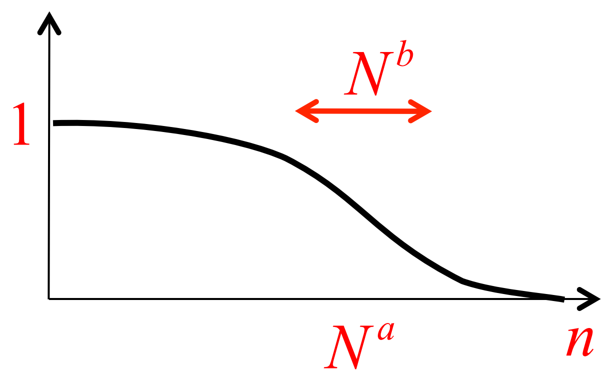
Re-summation of divergent series with finite convergence radius.

Example: $A = \sum_{n=0}^{\infty} c_n = 3 - 9/2 + 9 - 81/4 + \ \ldots = $ бред какой то

Define a function $f_{n,N}$ **such that:**

$f_{n,N} \to 1 \ \text{ for } \ n << N$

$f_{n,N} \to 0 \ \text{ for } \ n > N$



$f_{n,N} = e^{-n^2/N}$ (Gauss)

$f_{n,N} = e^{-\varepsilon n \ln(n)}$ (Lindeloef)

Construct sums $A_N = \sum_{n=0}^{\infty} c_n f_{n,N}$ **and extrapolate** $\lim_{N\to\infty} A_N$ **to get** A