



The Abdus Salam
International Centre for Theoretical Physics



1929-16

Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry

21 January - 1 February, 2008

Diagrammatic Monte Carlo.

N. Prokofiev

University of Massachusetts, Amherst

DIAGRAMMATIC MONTE CARLO: From polarons to path-integrals to generic many-body setup

Nikolay Prokofiev, Umass, Amherst

Nearly all work on algorithms
was done in collaboration with

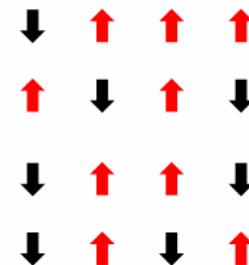
Boris Svistunov
UMass, Amherst



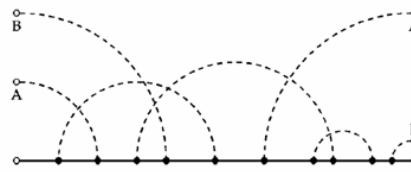
Trieste, January 2008

Standard Monte Carlo setup:

(depends on the model
and it's representation)



- configuration space



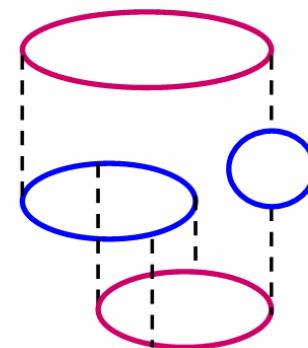
- each cnf. has a weight factor

$$W_{cnf}$$

$$e^{-E_{cnf}/T}$$

- quantity of interest

$$A_{cnf} \longrightarrow \langle A \rangle = \frac{\sum_{cnf} A_{cnf} W_{cnf}}{\sum_{cnf} W_{cnf}}$$



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

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

Anything: $\sum_{\{x=\text{any set of variables}\}} F(x) O(x)$ $\xrightarrow{\text{Monte Carlo}}$ $\sum_{\{x\}}^{MC} O(x)$

states generated from probability distribution $F(x)$

Anything = $\xrightarrow{\text{Connected Feynman diagrams, e.g. for the proper self-energy}}$ relief for
 $x = \left\{ \begin{array}{l} \text{diagram order} \\ \text{topology} \\ \text{internal variables} \end{array} \right.$



Classical MC

$$Z(\vec{y}) = \iiint d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_N W(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N, \vec{y})$$

the number of variables N is constant

Quantum MC (often)

$$Z(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_n W_n(\xi; \vec{x}_1, \vec{x}_2, \dots, \vec{x}_n, \vec{y})$$

term order

different terms of
of the same order

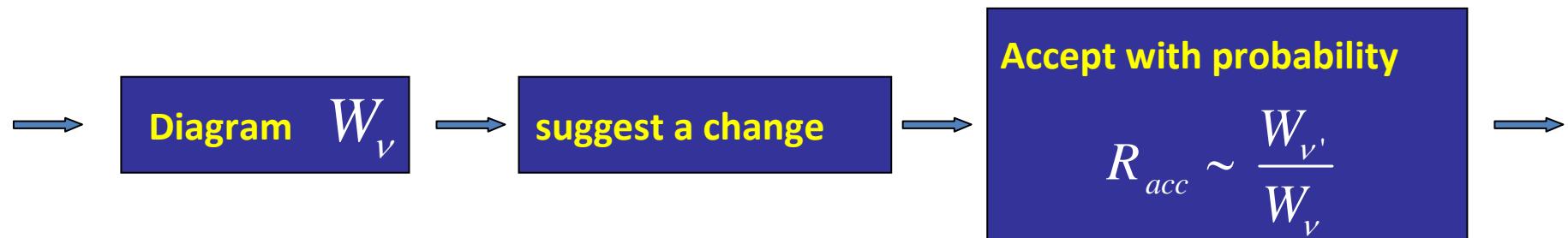
Integration variables

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

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graph TD; Z["Z(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_n W_n(\xi; \vec{x}_1, \vec{x}_2, \dots, \vec{x}_n, \vec{y})"]; Z -- "term order" --> n0["n=0"]; Z -- "different terms of the same order" --> xi["\xi"]; Z -- "Integration variables" --> xiInt["d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_n"]; Z -- "Contribution to the answer or weight (with differential measures!)" --> weight["W_n(\xi; \vec{x}_1, \vec{x}_2, \dots, \vec{x}_n, \vec{y})"];
```

$$A(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_n D_n(\xi; \vec{x}_1, \vec{x}_2, \dots, \vec{x}_n, \vec{y}) = \sum_v D_v$$

Monte Carlo (Metropolis) cycle:



Same order diagrams:

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

Business as usual

Updating the diagram order:

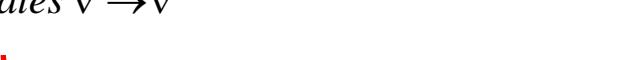
$$\frac{D_{v'}}{D_v} \sim \frac{(d\vec{x})^{n+m}}{(d\vec{x})^n} \sim (d\vec{x})^m \rightarrow \text{Ooops}$$

Balance Equation:

If the desired probability density distribution of different terms in the stochastic sum is P_v , then the updating process has to be stationary with respect to P_v (equilibrium condition). Often $P_v = W_v$

$$W_v \sum_{\text{updates } v \rightarrow v'} U_v(v') R_{accept}^{v \rightarrow v'} = \sum_{\text{updates } v' \rightarrow v} W_{v'} U_{v'}(v) R_{accept}^{v' \rightarrow v}$$


Flux out of v


Flux to v

$U_v(v')$ Is the probability density of proposing an update transforming v to v'

Detailed Balance: solve equation for each pair of updates separately

$$W_v U_v(v') R_{accept}^{v \rightarrow v'} = W_{v'} U_{v'}(v) R_{accept}^{v' \rightarrow v}$$

Let us be more specific. Equation to solve:

$$W_n(\vec{x}_1, \dots, \vec{x}_n)(d\vec{x})^n U_{n,n+m}(\vec{x}_1, \dots, \vec{x}_{n+m})(d\vec{x})^m R_{accept}^{n \rightarrow n+m} = W_{n+m}(\vec{x}_1, \dots, \vec{x}_{n+m})(d\vec{x})^{n+m} U_{n+m,n} R_{accept}^{n+m \rightarrow n}$$

W_v
 $U_v(v')$
 W_v
 $U_{v'}(v)$

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

Solution:

$$R = \frac{R_{accept}^{n \rightarrow n+m}}{R_{accept}^{n+m \rightarrow n}} = \frac{W_{n+m}(x_1, \dots, x_{n+m})}{W_n(x_1, \dots, x_n)} \frac{U_{n+m,n}}{U_{n,n+m}(x_1, \dots, x_{n+m})}$$

All differential measures are gone!

Efficiency rules:

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

ENTER

Polaron problem:

$$H = H_{\text{particle}} + H_{\text{environment}} + H_{\text{coupling}} \rightarrow \text{quasiparticle}$$

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

Electrons in semiconducting crystals (electron-phonon polarons)

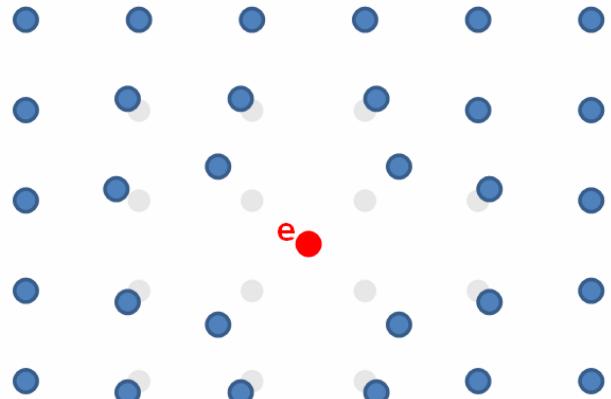


Fig.1

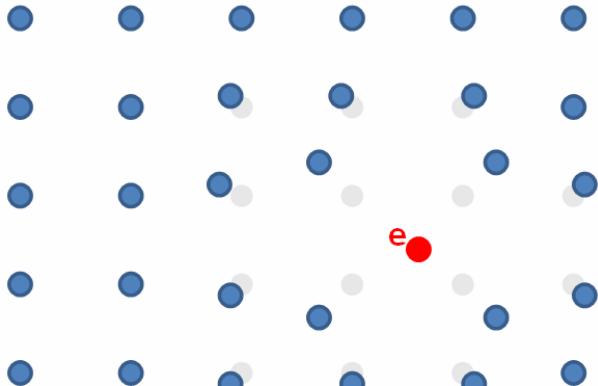


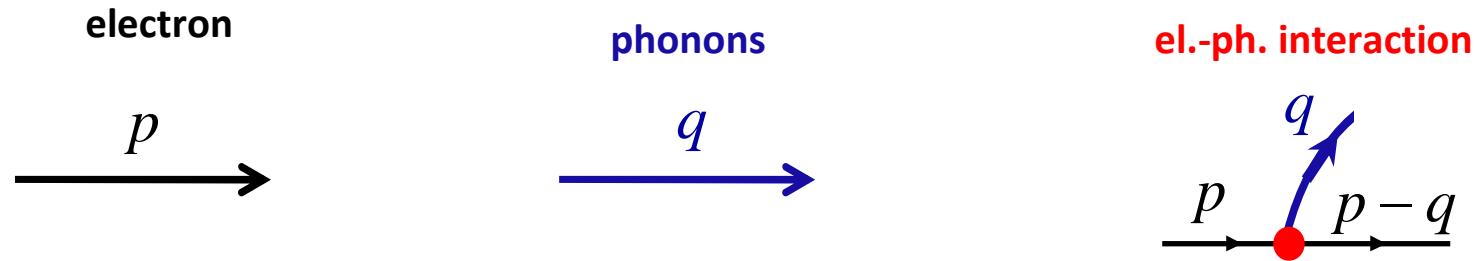
Fig.2

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

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

$$\sum_{pq} (V_q a_{p-q}^+ a_p b_q^+ + h.c.) \quad \text{el.-ph. interaction}$$

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



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

$$G(p, \tau) = 0 \xrightarrow[\tau]{p} + 0 \xrightarrow[\tau_1]{p} \xrightarrow[p-q]{p} \xrightarrow[\tau_2]{p} \tau + \dots$$

The diagram shows the definition of the Green function $G(p, \tau)$ as a sum of Feynman diagrams. The first term is a bare electron propagator $0 \xrightarrow[\tau]{p}$. The second term is a diagram with a vertex at τ_1 , a loop with momentum q connecting two vertices at τ_1 and τ_2 , and a bare electron propagator $\xrightarrow[p-q]{p}$. Subsequent terms represent higher-order corrections.

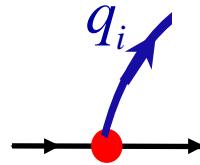
= Sum of all Feynman diagrams

$$G(p, \tau) = \sum_{\text{Feynman diagrams}} \left[\text{Diagram} \right]$$

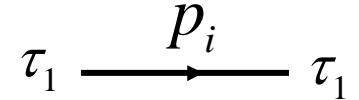
Graph-to-math correspondence:

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

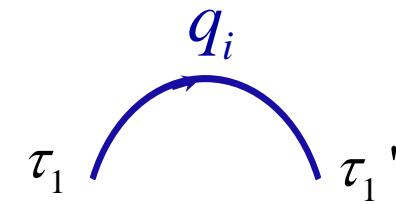
is a product of



$$V_{q_i}$$

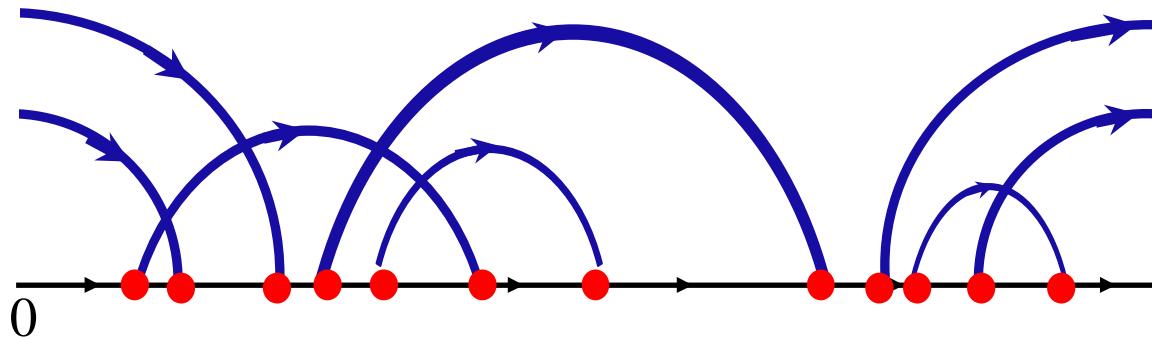


$$e^{-\varepsilon(p_i)(\tau_i' - \tau_i)}$$



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

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



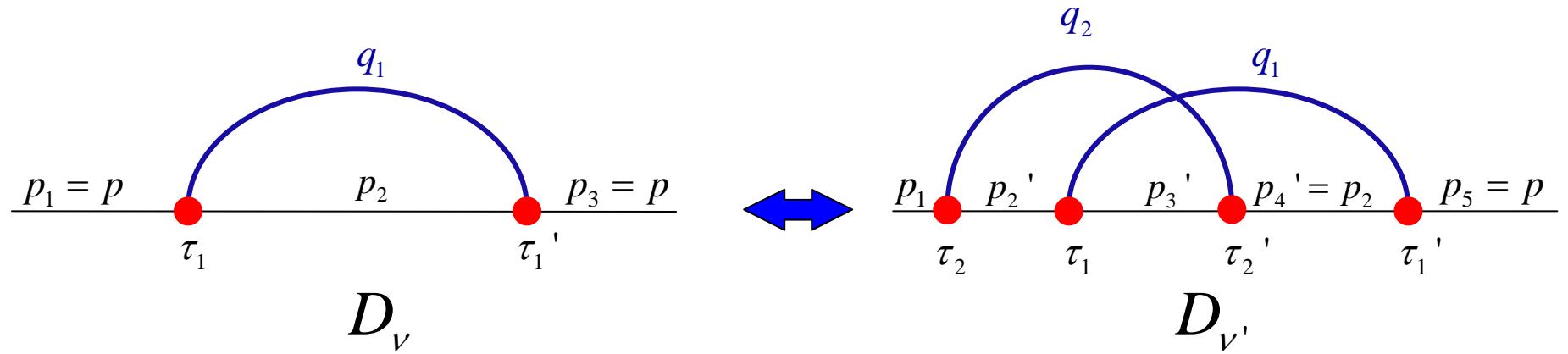
Diagrams for: $\langle b_{q_1}(0)b_{q_2}(0) \ a_{p-q_1-q_2}(0) \ a_{p-q_1-q_2}^+(\tau) \ b_{q_1}^+(\tau)b_{q_2}^+(\tau) \rangle$

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)



$$D_{v'} / D_v = |V_{q_2}|^2 e^{-\omega(q_2)(\tau_2' - \tau_2)} e^{-(\epsilon(p_2') - \epsilon(p_2))(\tau_1 - \tau_2)} e^{-(\epsilon(p_3') - \epsilon(p_2))(\tau_2' - \tau_1)}$$

$$R = \frac{D_{v'}}{D_v} \frac{U_{n+1,n}}{U_{n,n+1}(x_1, \dots, x_{n+1})} = \frac{D_{v'}}{D_v} \frac{1}{(n+1) U_{n,n+1}(x_1, \dots, x_{n+1})}$$

In Delete select the phonon line to be deleted at random

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

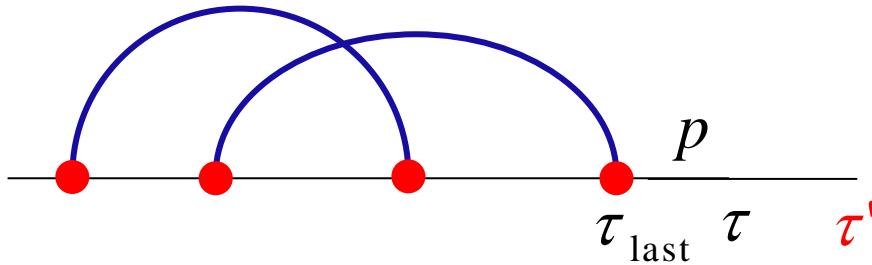
Frohlich polaron: $\varepsilon = p^2 / 2m$, $\omega_q = \omega_0$, $V_q \sim \alpha / q$

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

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.

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

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

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

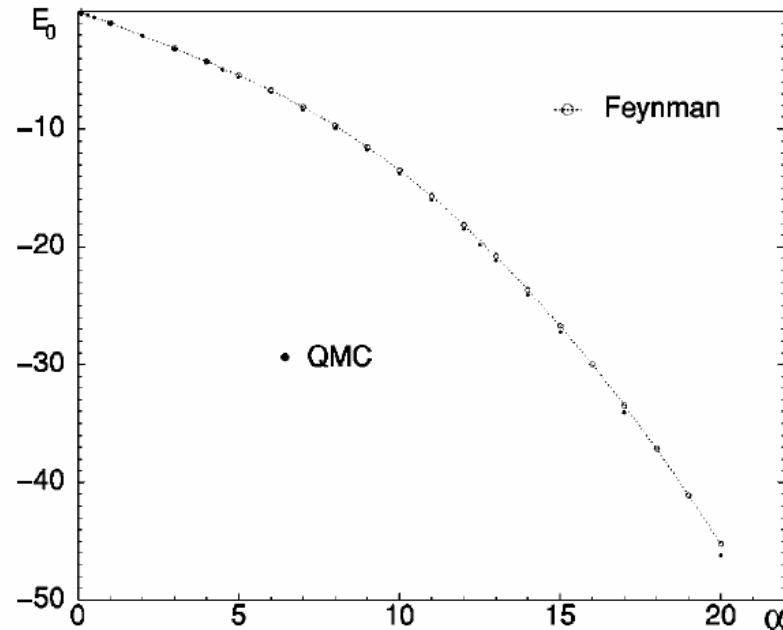


FIG. 4. Bottom of the polaron band E_0 as a function of α . The error bars are much smaller than the point size.

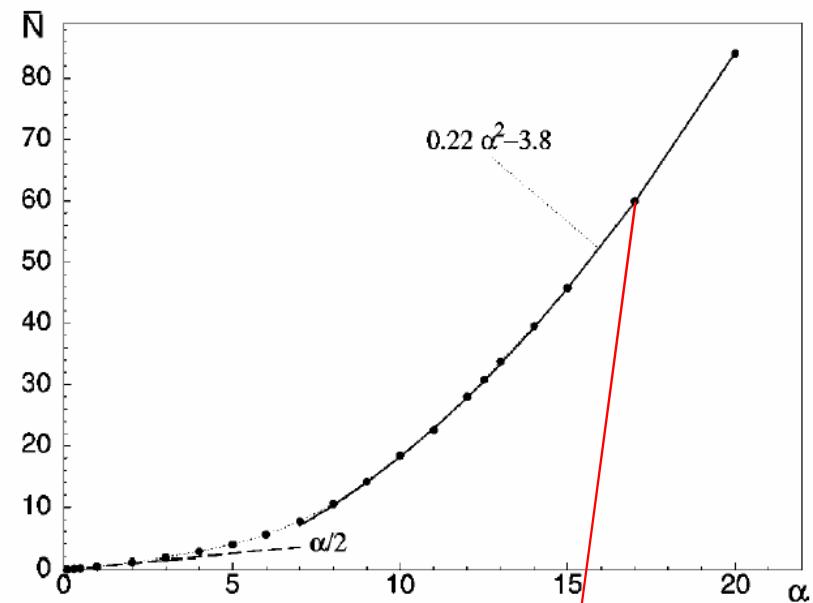
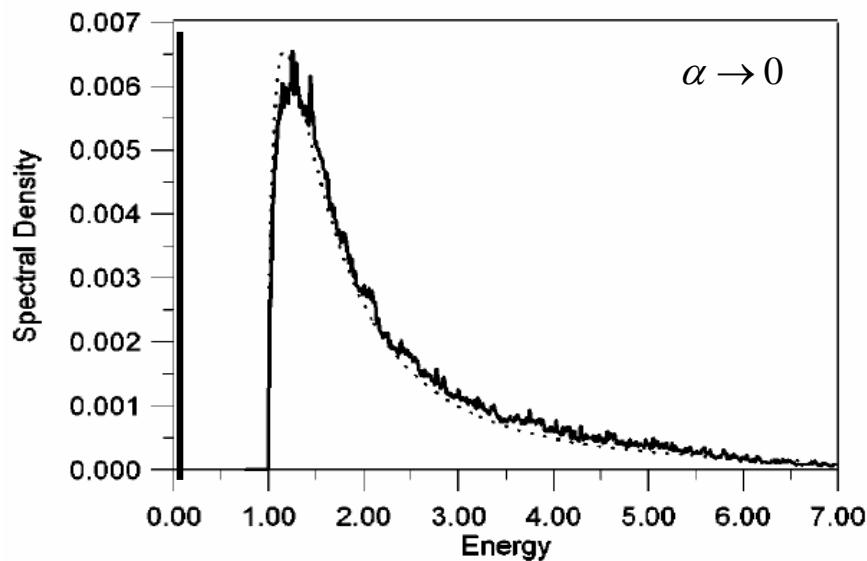
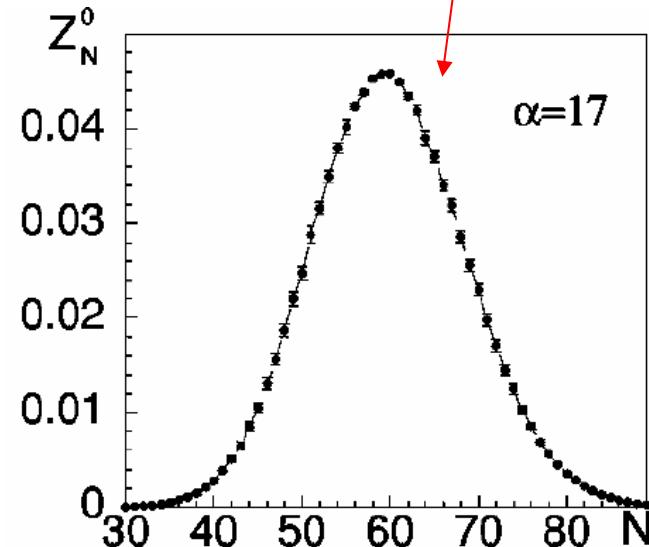


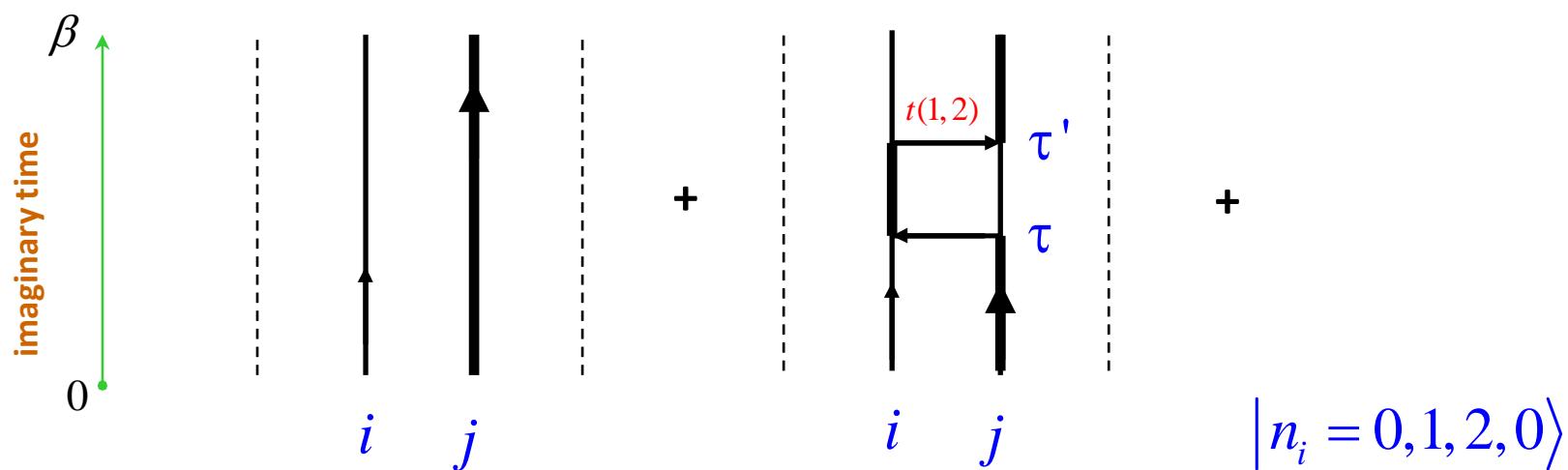
FIG. 8. The average number of phonons in the polaron ground state as a function of α . Filled circles are the MC data (calculated to the relative accuracy better than 10^{-3}), the dashed line is the perturbation theory result (4.1), and the solid line is the parabolic fit for the strong coupling limit.



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

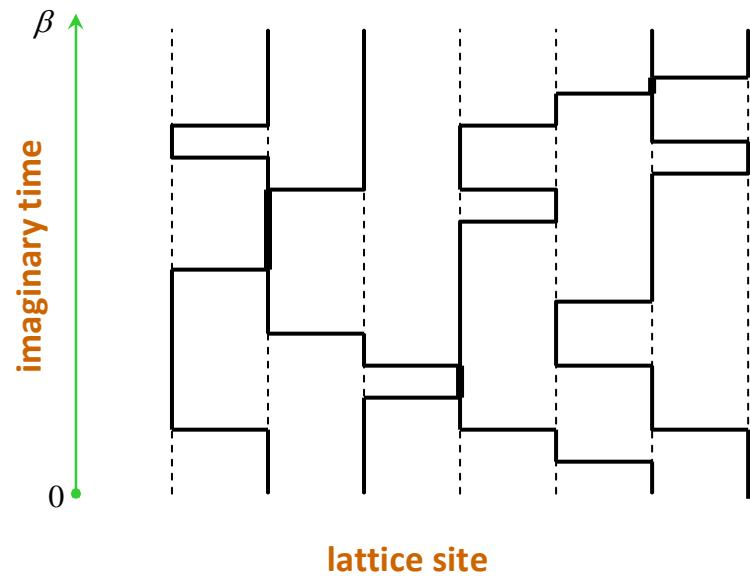
Lattice path-integrals for bosons and spins are “diagrams” of closed loops!

$$\begin{aligned} Z &= \text{Tr } e^{-\beta H} \equiv \text{Tr } e^{-\beta H_0} e^{-\int_0^\beta H_1(\tau) d\tau} \\ &= \text{Tr } e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau) d\tau + \int_0^\beta \int_\tau^\beta H_1(\tau) H_1(\tau') d\tau d\tau' + \dots \right\} \end{aligned}$$



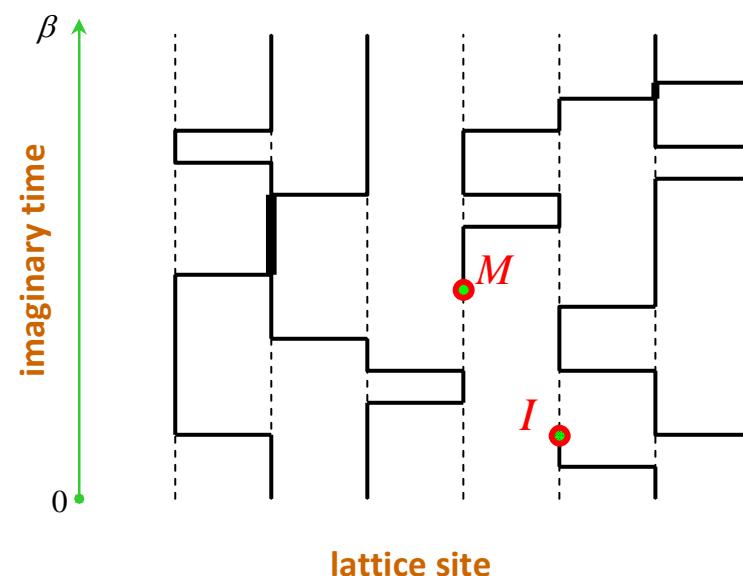
Diagrams for

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



Diagrams for

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



The rest is conventional worm algorithm in continuous time

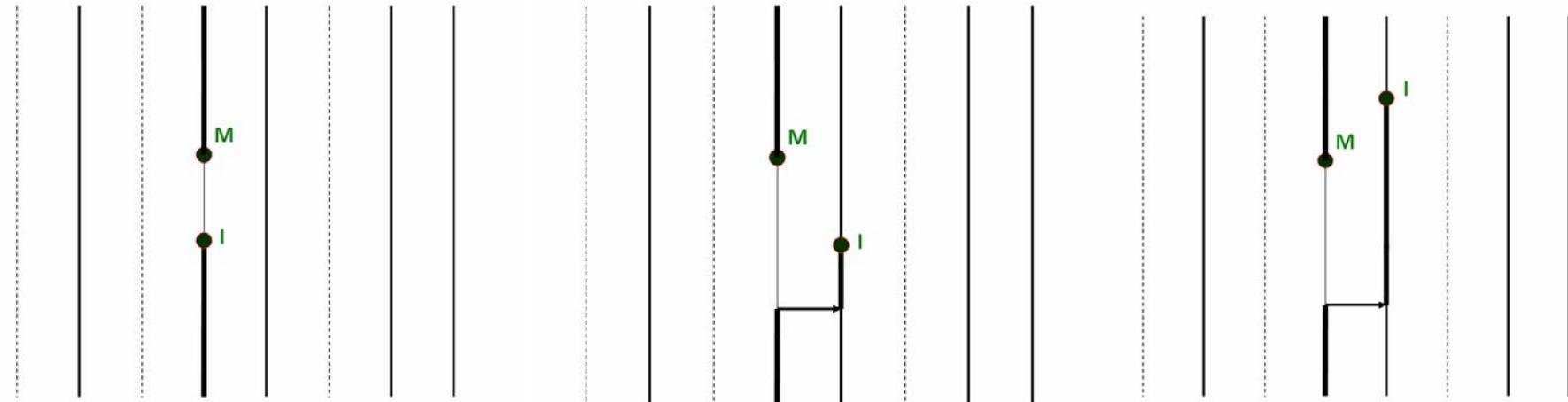


Fig. 1

Fig. 2

Fig. 3

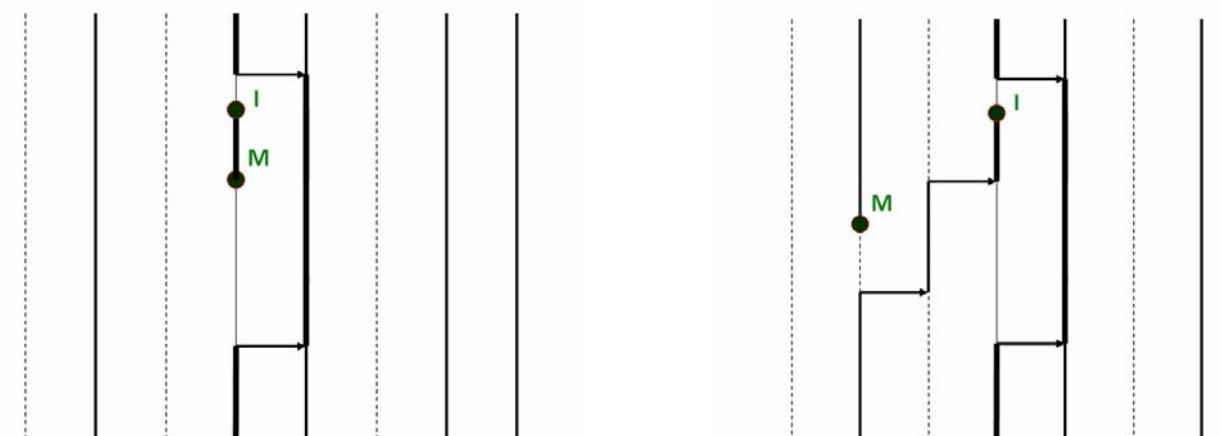
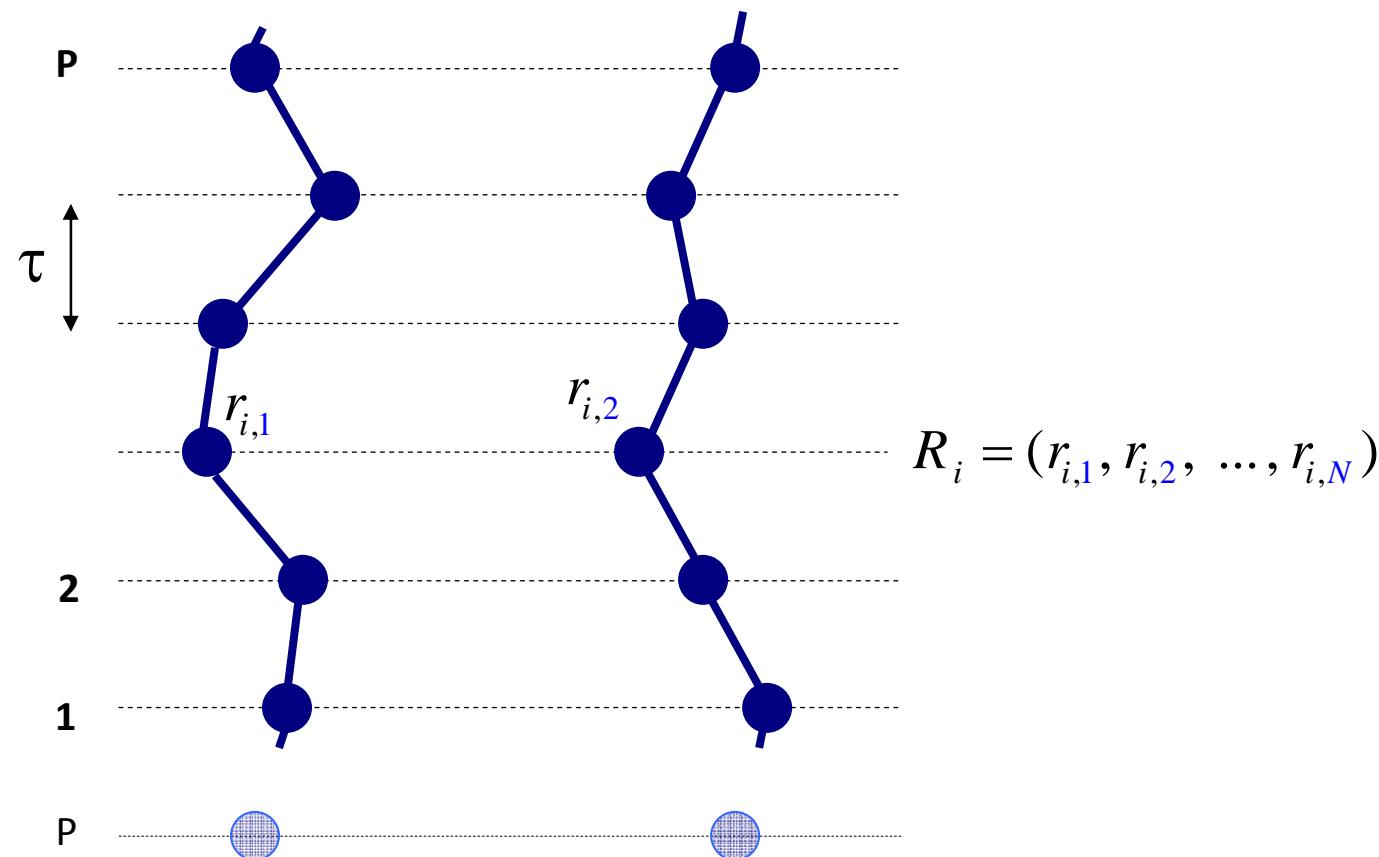


Fig. 4

Fig. 5

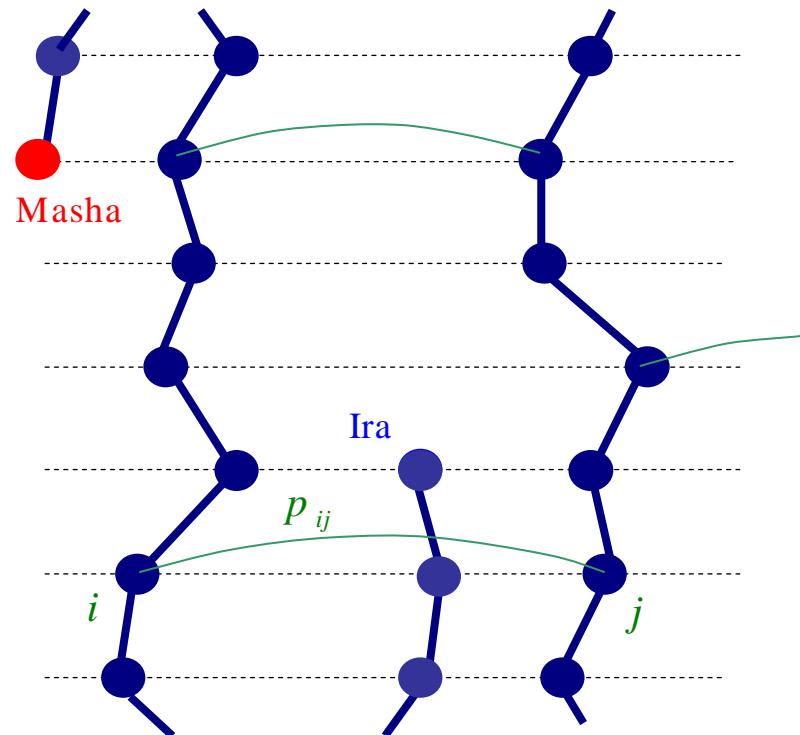
$$Z = \iiint dR_1 \dots dR_P \exp \left\{ - \sum_{i=1}^{P=\beta/\tau} \left(\frac{m(R_{i+1} - R_i)^2}{2\tau} + U(R) \tau \right) \right\}$$

**Path-integrals in continuous space
are “diagrams” of closed loops too!**



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

If $-\tau \sum_{j \neq i}^N U(r_j - r_i) \theta(|r_j - r| - r_c) \ll 1$ and $N \gg 1$ 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

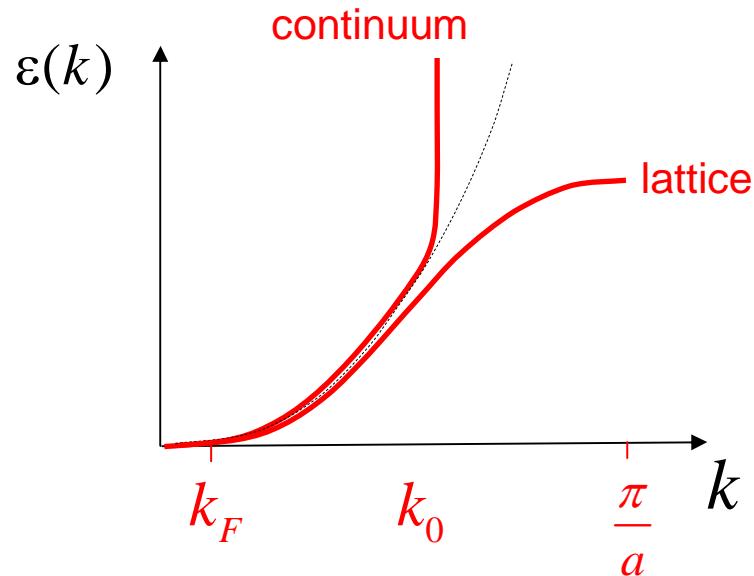
Faster than conventional scheme for $N > 30$, **scalable** (size independent) updates with **exact** account of interactions between all particles

Feynman (space-time) diagrams
for fermions with contact
interaction (attractive) $\bullet = -U$
($n=1$ positive Hubbard model too)

$$H = \sum_{i,\sigma=\uparrow\downarrow} \varepsilon(k_{i\sigma}) + \sum_{i < j} V(r_{i\uparrow} - r_{j\downarrow})$$

$$V(r) = -U \delta(r)$$

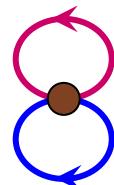
regularize ultra-violet divergences in $\int d^3k \frac{|V(k)|^2}{\varepsilon(k)}$ using appropriate $\varepsilon(k)$



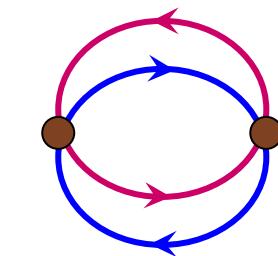
$V(r) = -U \delta(r)$ is crucial

Auxiliary fields, discrete basis set,
and time discretization are avoided !

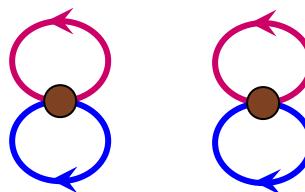
Feynman (space-time) diagrams for the partition function Z



$-U$



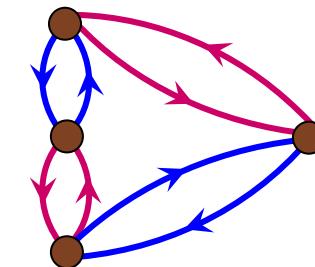
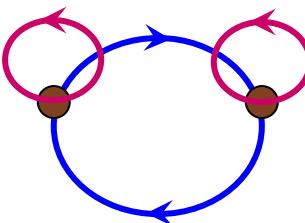
$(-U)^2$



$G_{\uparrow}(r_i - r_j, \tau_i - \tau_j)$

$G_{\uparrow}(r_i - r_j, \tau_i - \tau_j)$

$(-U)^3$

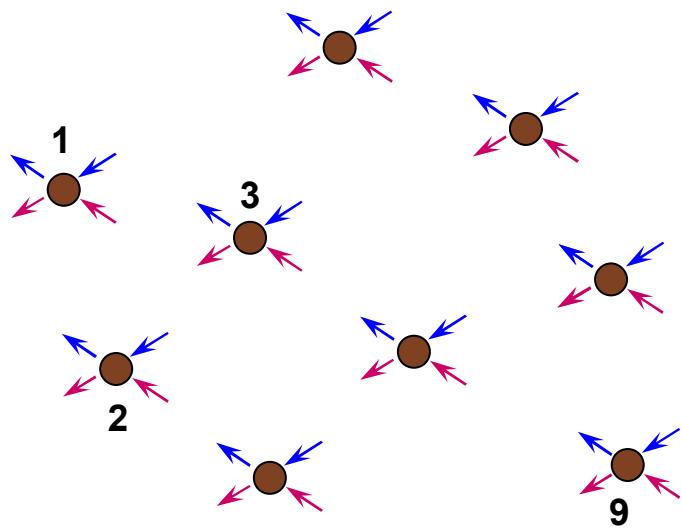


$(-U)^4$

too many to draw all $(p!)^2$ topologies ...

but easy to sum all of them! [about $(5000!)^2$]

The sum of all $(p!)^2$ diagrams for a given vertex configuration $(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2; \dots; \mathbf{r}_p, \tau_p)$ is a determinant squared



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

$$Z = \sum_{p=0}^{\infty} \int \dots \int (\vec{dr} d\tau)^p (-U)^p \det^2 G(\vec{x}_i, \vec{x}_j)$$

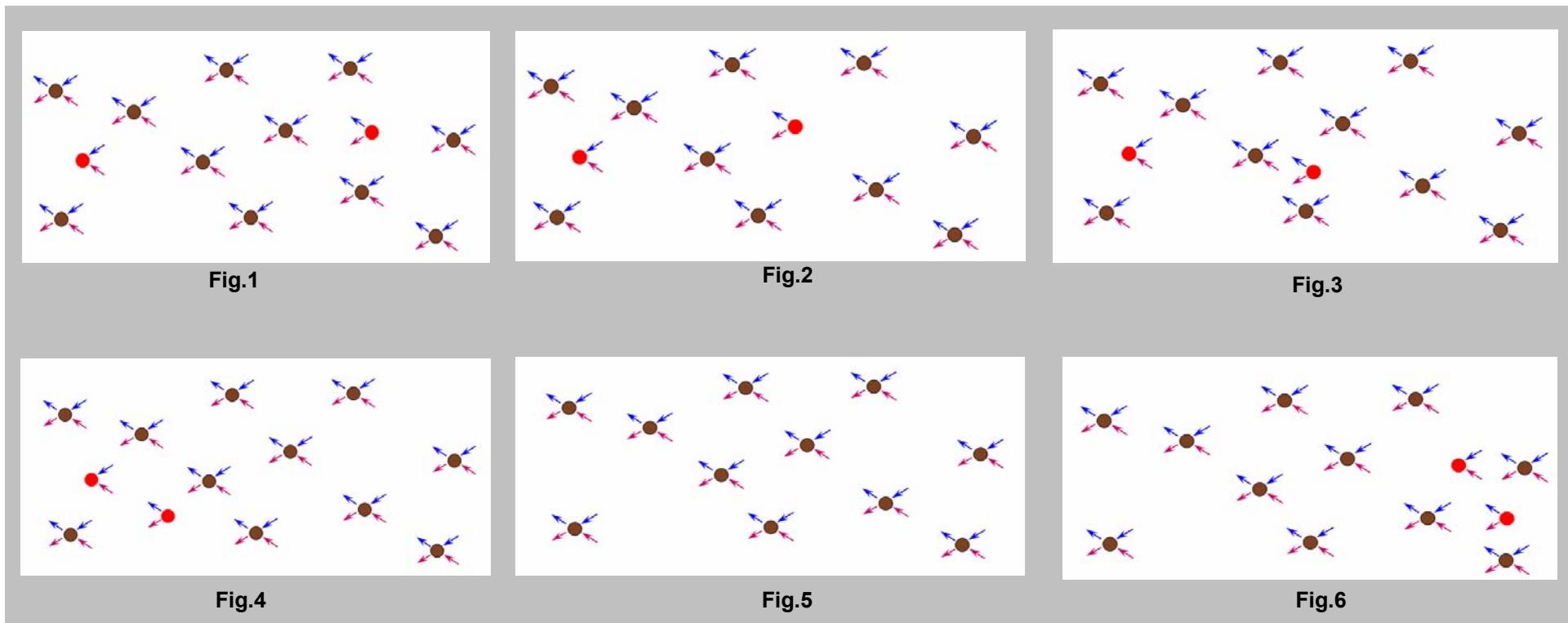
Rubtsov (2003).
Burovski, NP, and Svistunov (2003).

Worm algorithm = extended configuration space of $K \cup Z$

$$K(\mathbf{r}_2 - \mathbf{r}_1, \tau_2 - \tau_1) = \left\langle T_\tau \Psi_{\downarrow}^+(\mathbf{r}_2, \tau_2) \Psi_{\uparrow}^+(\mathbf{r}_2, \tau_2) \Psi_{\uparrow}(\mathbf{r}_1, \tau_1) \Psi_{\downarrow}(\mathbf{r}_1, \tau_1) \right\rangle$$

+ all updates are through the pair operators exclusively

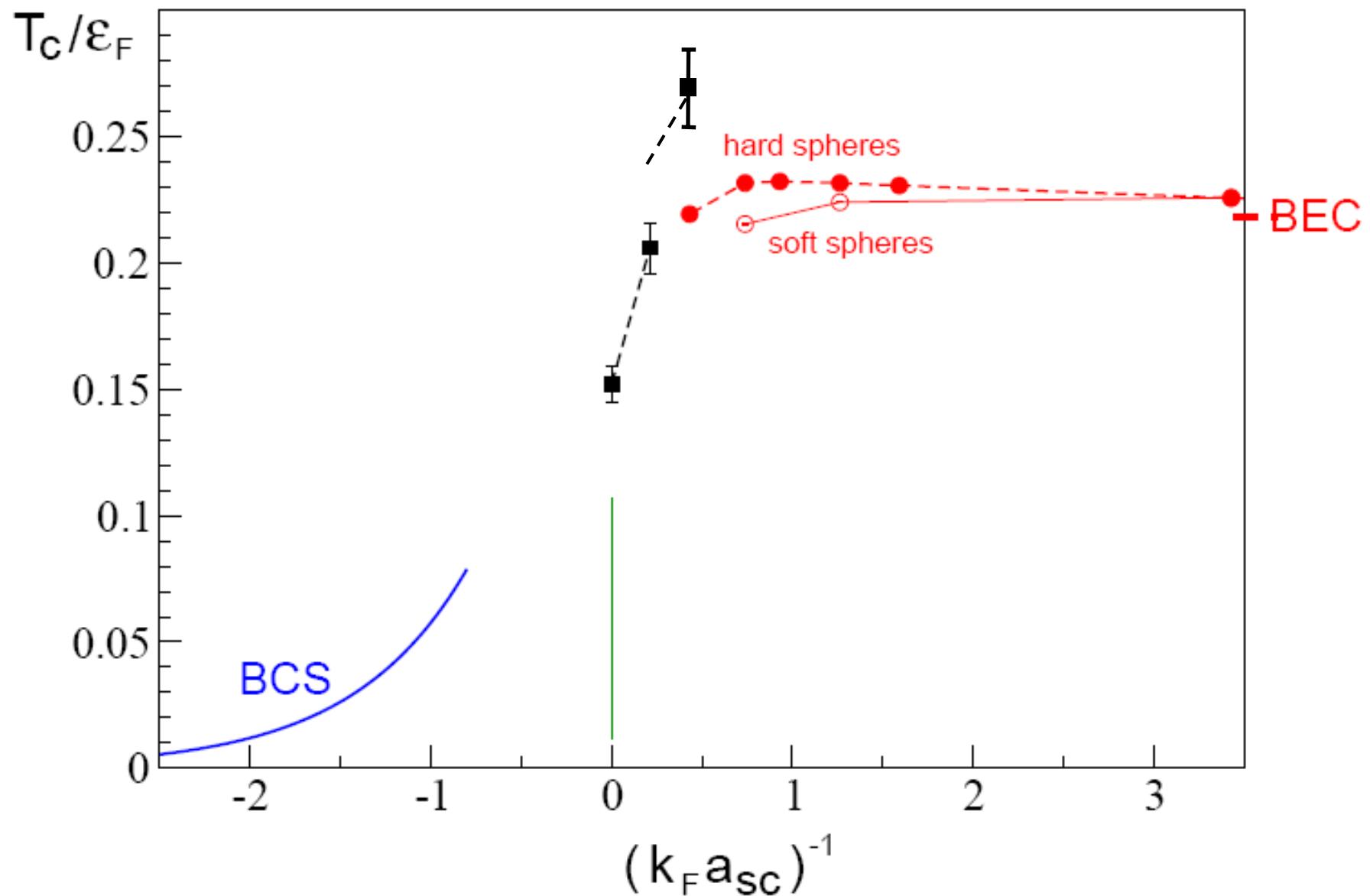
NP, Svistunov, and Tupitsyn '98



$$Q = \frac{1}{V\beta} \int_{-\beta}^{\beta} d\tau \int d\mathbf{r} K(\mathbf{r}, \tau) \sim n_0$$

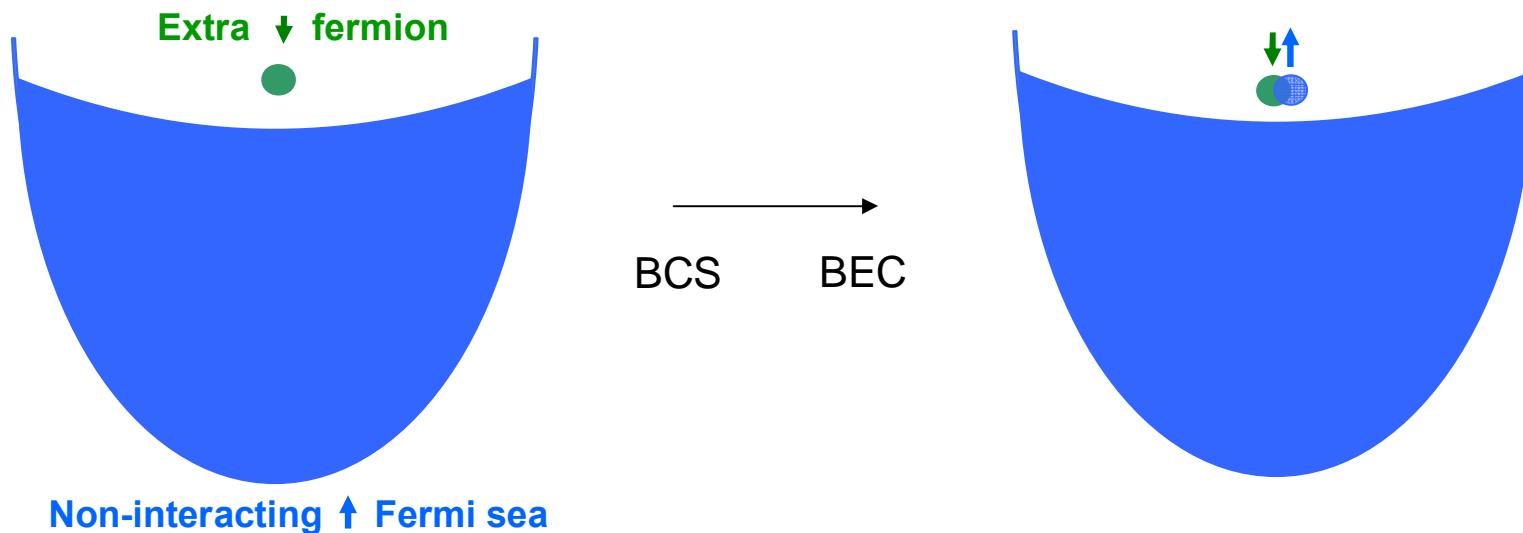
pair condensate density \longrightarrow critical point

BCS-BEC crossover curve.



Resonant Fermions (full polarization)

Fermi-polaron = particle dressed by interactions with the Fermi sea;
orthogonality catastrophe, X-ray singularities, heavy fermions,
quantum diffusion in metals, ions in He-3, etc.



Fermionic quasiparticle
(polaron)

$$E_p(k) = E_p + k^2 / 2m_p$$

+ *quasiparticle residue*

Bosonic quasiparticle
(molecule)

$$E_M(k) = E_M + k^2 / 2m_M$$

+ *quasiparticle residue*

Previous attempts (for polarons):

variational Ψ

variational Ψ , fixed node MC (variational)

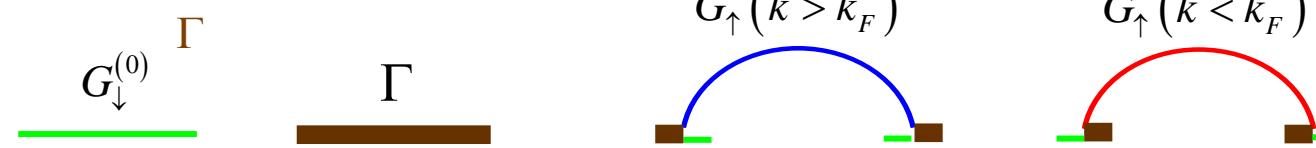
$$\Sigma_1 = \begin{array}{c} G \\ \text{---} \\ \text{---} \end{array} \quad \text{with } E_p < E_{\text{var}}$$

Bulgac,Forbes
PRA 75, 031605 (2007)

Lobo, Recati, Giorgini,
Stringari
PRL 97, 200403 (2006)

Combescot, Recati, Lobo,
Chevy
PRL 98, 180402 (2007)

Graphical notations:

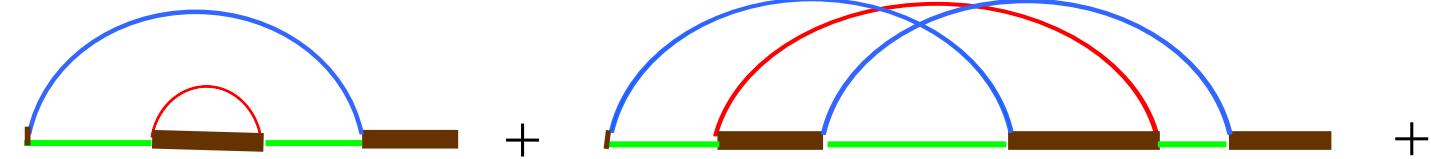


“Exact” solution:

Polaron →



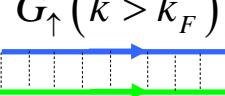
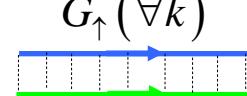
Molecule →



sure, press

Enter

Bold-Line Diagrammatic Monte Carlo for Γ (MC with unknown configuration weight)

Solve for $\Gamma(p, \tau) =$  using known vacuum result $\Gamma_{vac} =$ 

$$\Gamma = \Gamma_{vac} - \text{Diagram with a red semi-circle above a brown line and a green line below it, labeled } G_{\downarrow}^{(0)} \text{ and } G_{\uparrow}(k < k_F)$$

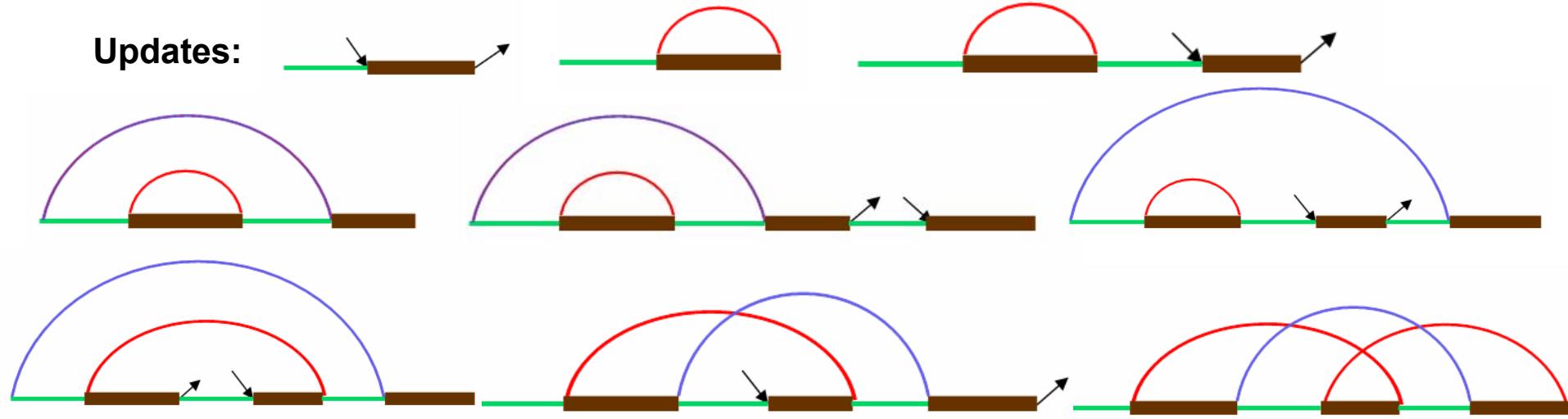
Just two terms on the right-hand-side, but Γ is not known prior to the simulation \rightarrow generate the second diagram from the probability distribution based on the current statistics for Γ :

- far larger (infinite!) convergence radius than for standard iterations
- works when the corresponding series diverge and are sign alternating

For the rest:

$$\Sigma_{mol}$$

- develop an ergodic algorithm sampling diagrams for Σ_{\downarrow} proper self-energy for both polarons and molecules at the same time (an appropriate Worm Algorithm does the job)



- calculate self-energies to higher and higher order (up to 11-th)
- It does **NOT** matter whether the series for self-energy are convergent or divergent! Apply resummation techniques if necessary.
- Implement self-consistent scheme: all diagram in terms of “exact” and , with self-energies produced by the same simulation. Smaller configuration space for diagrams of order m, much better convergence properties (embedded geometrical series are summed up to infinite order exactly).

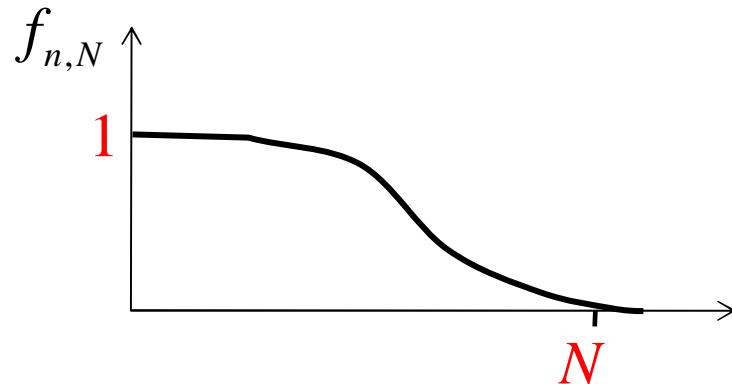
Summation of divergent/asymptotic series:

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

Define a function $f_{n,N}$ which has the following shape, i.e.

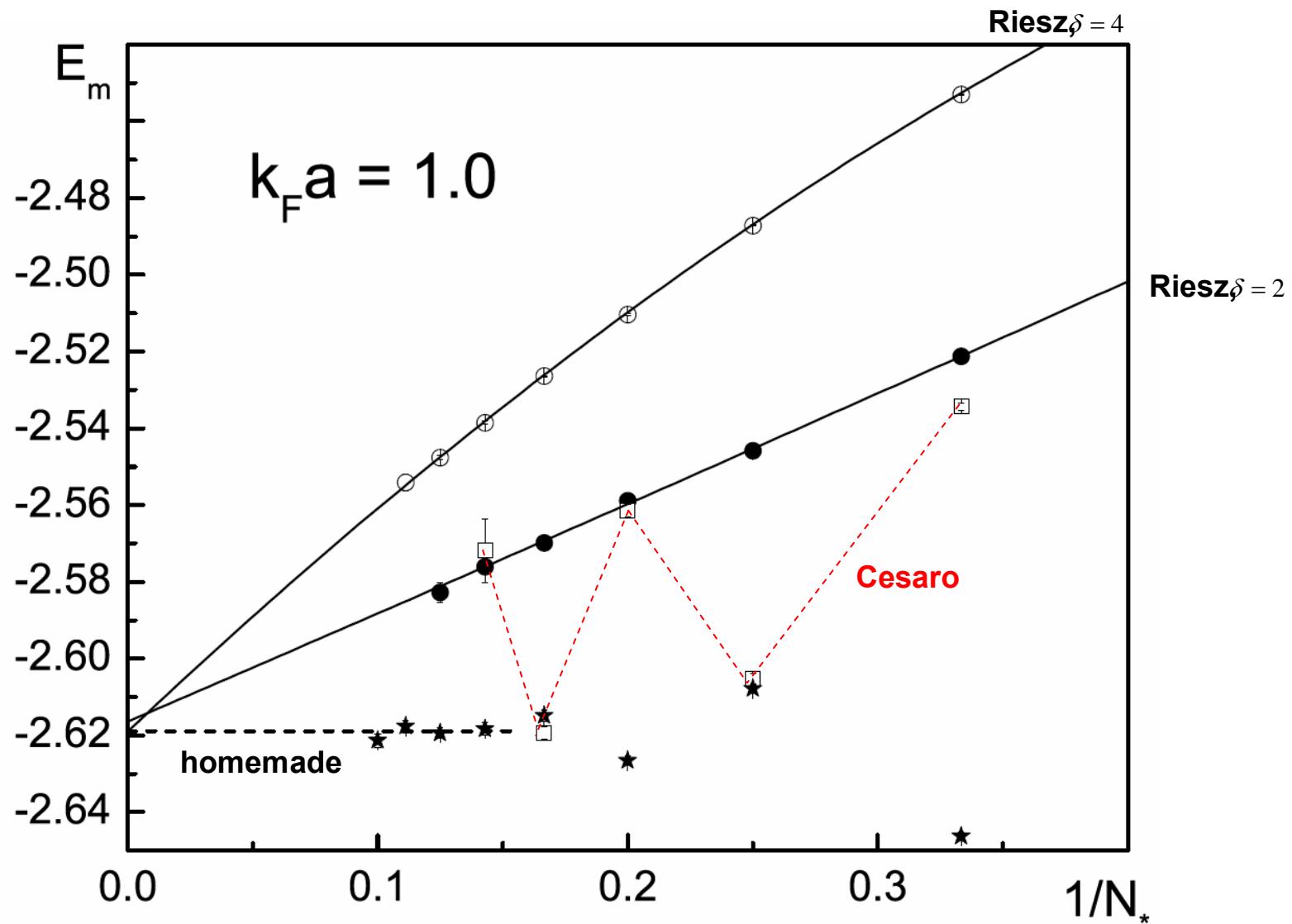
$$f_{n,N} \rightarrow 1 \text{ for } n \ll N$$

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



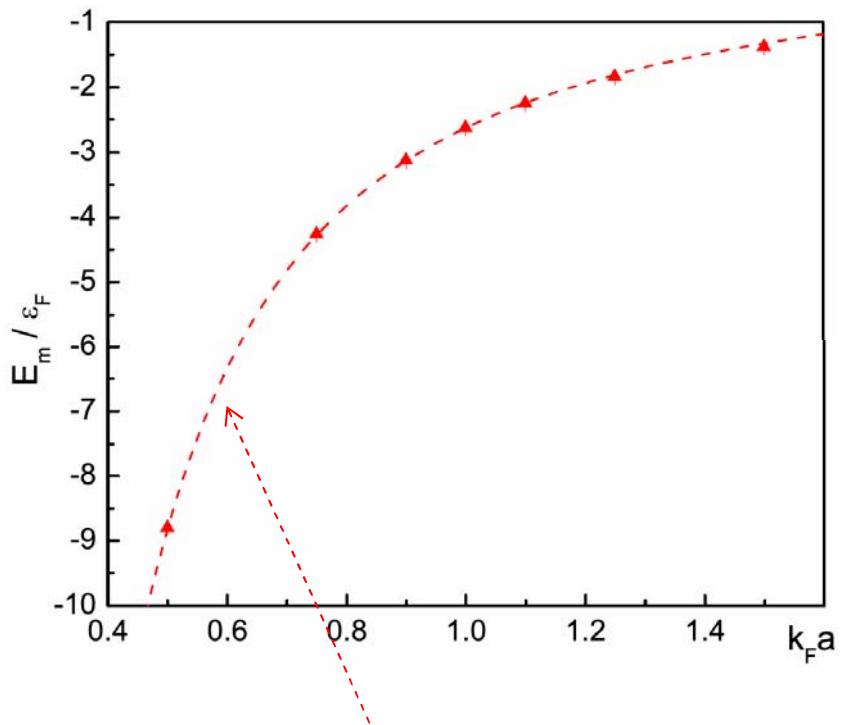
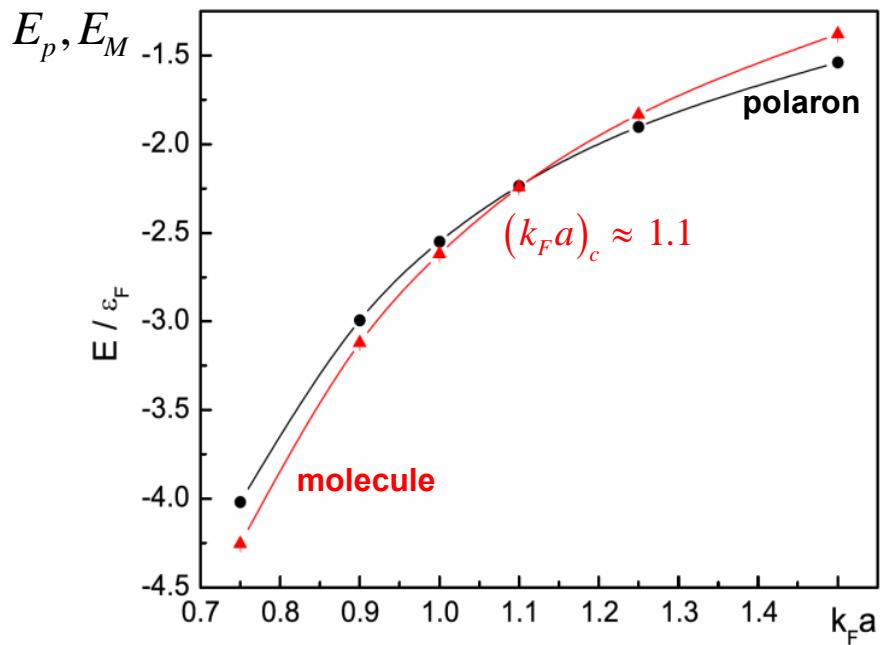
Construct sums $A_N = \sum_{n=0}^{\infty} c_n f_{n,N}$ or partial sums $A_N = \sum_{n=0}^N c_n f_{n,N}$

and extrapolate $\lim_{N \rightarrow \infty} A_N$ to get A



Polaron spectrum from the $G_{\downarrow}(\mathbf{p}, \omega)$ pole: $\omega - p^2 / 2m - \Sigma(\mathbf{p}, \omega) = 0$

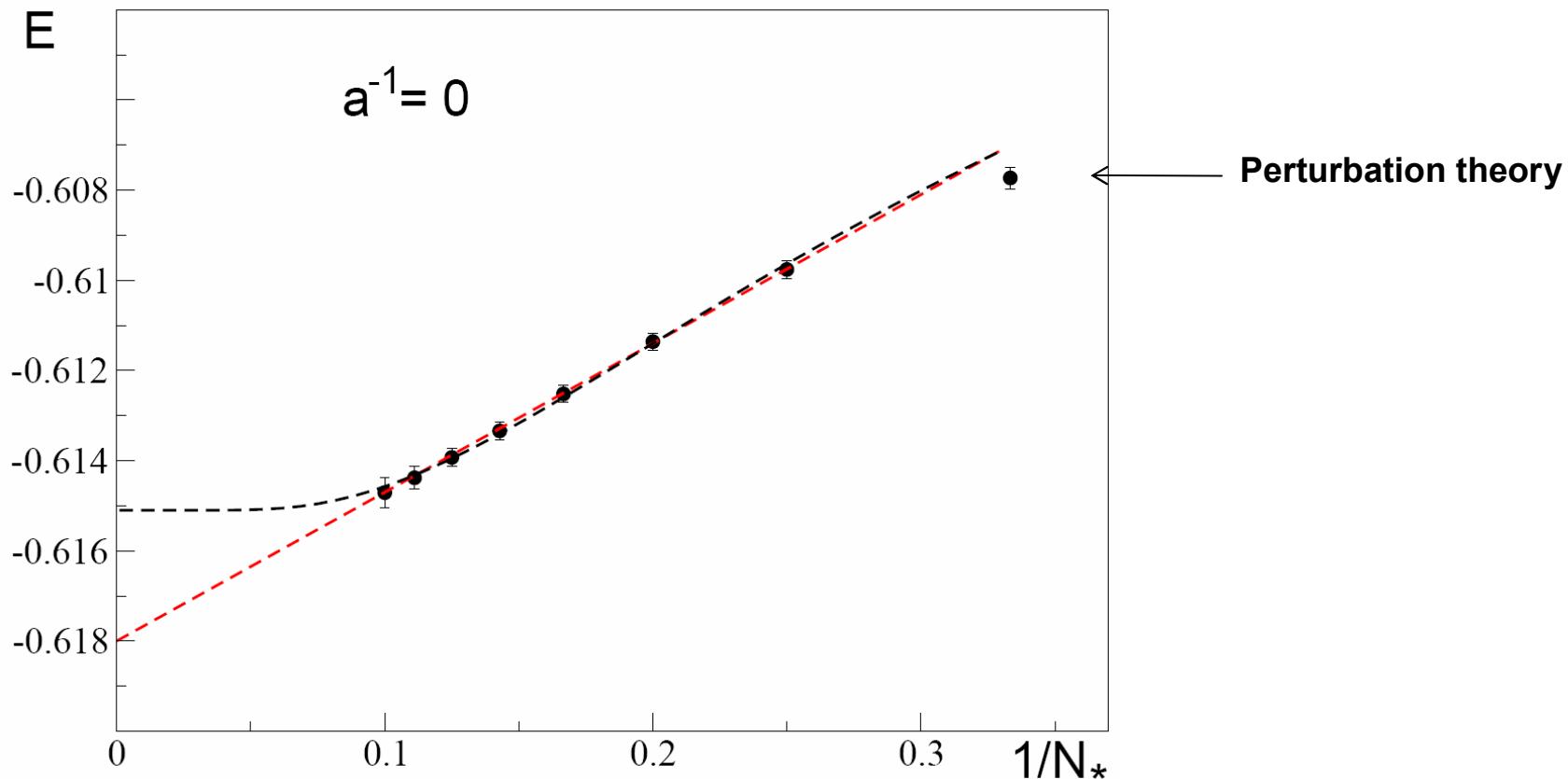
In imaginary time representation: $E - p^2 / 2m - \int_0^{\infty} \Sigma(\mu_{\downarrow}, \mathbf{p}, \tau) e^{(E - \mu_{\downarrow})\tau} d\tau = 0$



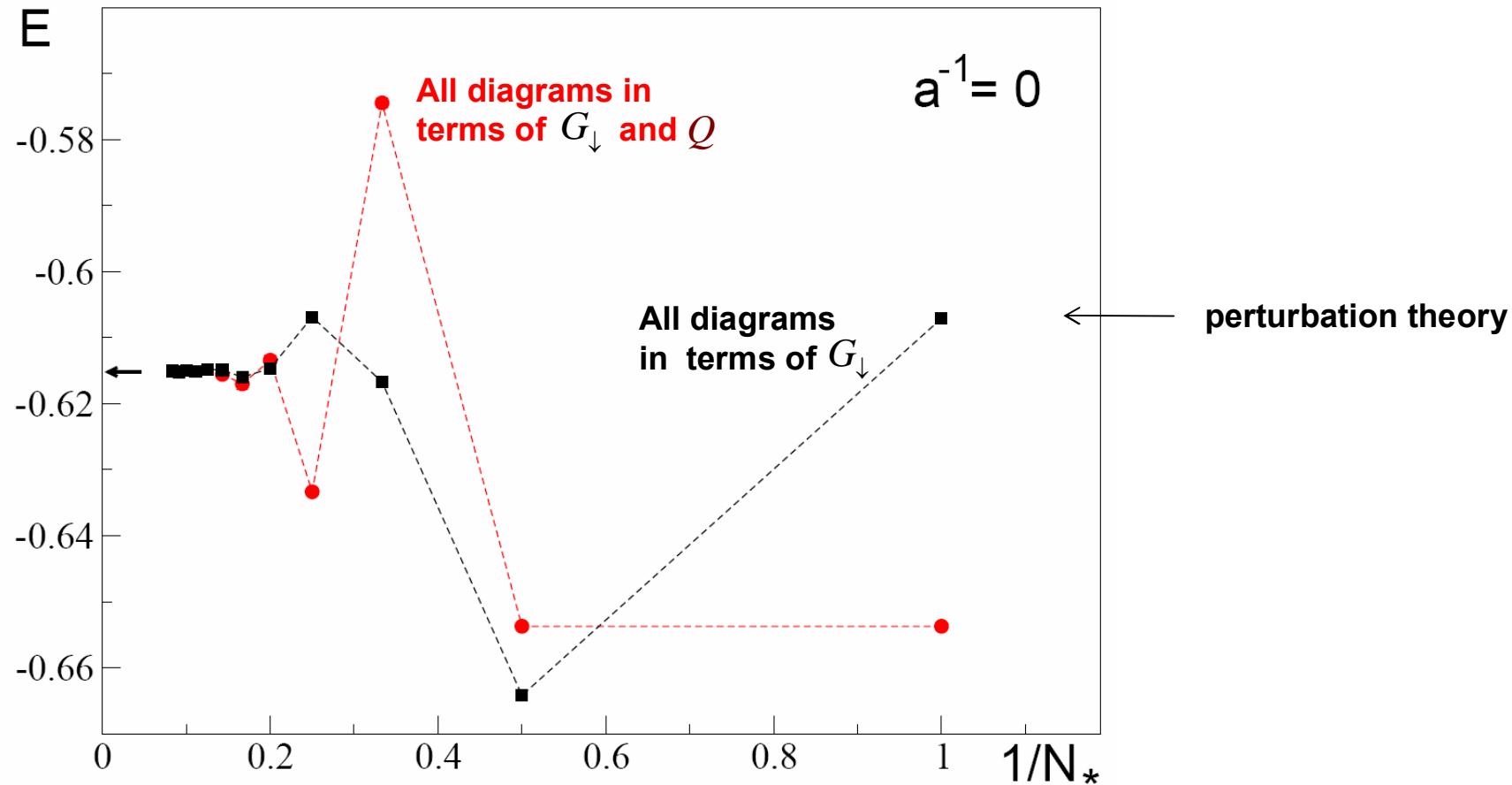
$$E_m = -\frac{1}{ma^2} - \epsilon_F + \frac{2\pi a_M \uparrow}{(2/3)m} n_{\uparrow} \quad (k_F a \ll 1)$$

$$a_M \uparrow = 1.18a \quad \text{Skorniakov, Ter-Martirosian '56}$$

Polaron energy; thin-line diagrams + extrapolation



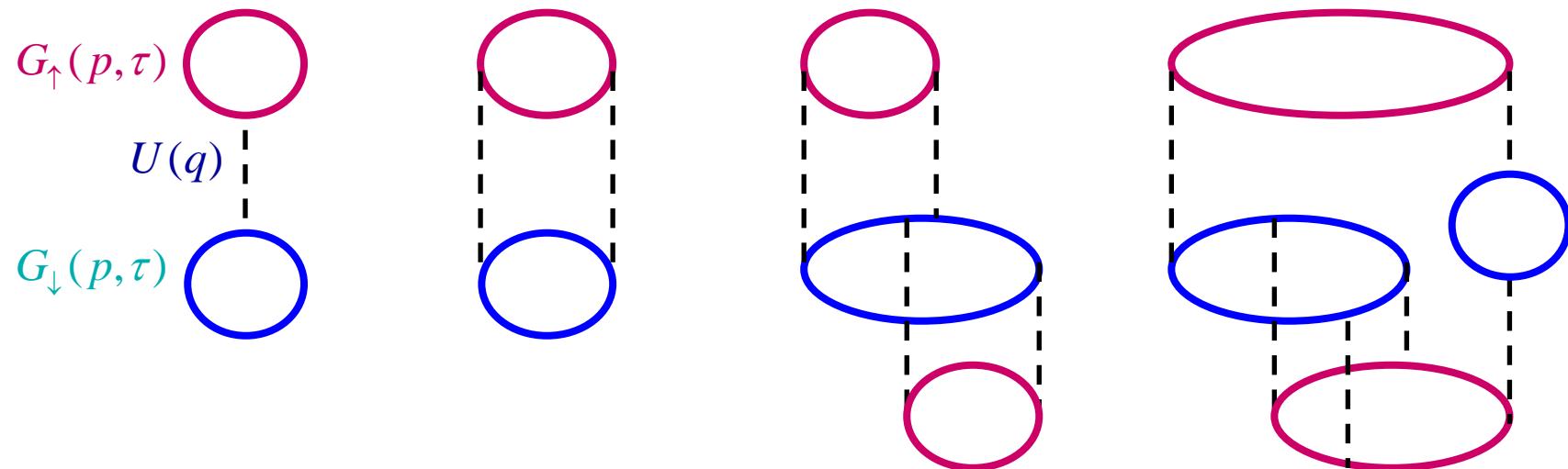
The fate of many “improved calculations” in many-body systems



Before doing it , make sure to ask for the exact answer!

Diagrammatic Monte Carlo in the generic many-body setup

1. Stochastic summation of connected Feynman diagrams for self-energy
(ξ controls the typical diagram order)



2. Self-consistent feed-back in the form of Dyson, T-matrix, RPA, etc. Eqs.

e.g. $\underline{G_{\downarrow}} = \underline{G_{\downarrow}^{(0)}} + \underline{G_{\downarrow}^{(0)}} \Sigma_{\downarrow} G_{\downarrow}$

3. Extrapolation to $\xi \rightarrow \infty$ (asymptotic and divergent series can be dealt with)

Sounds too good to be true ... , but

