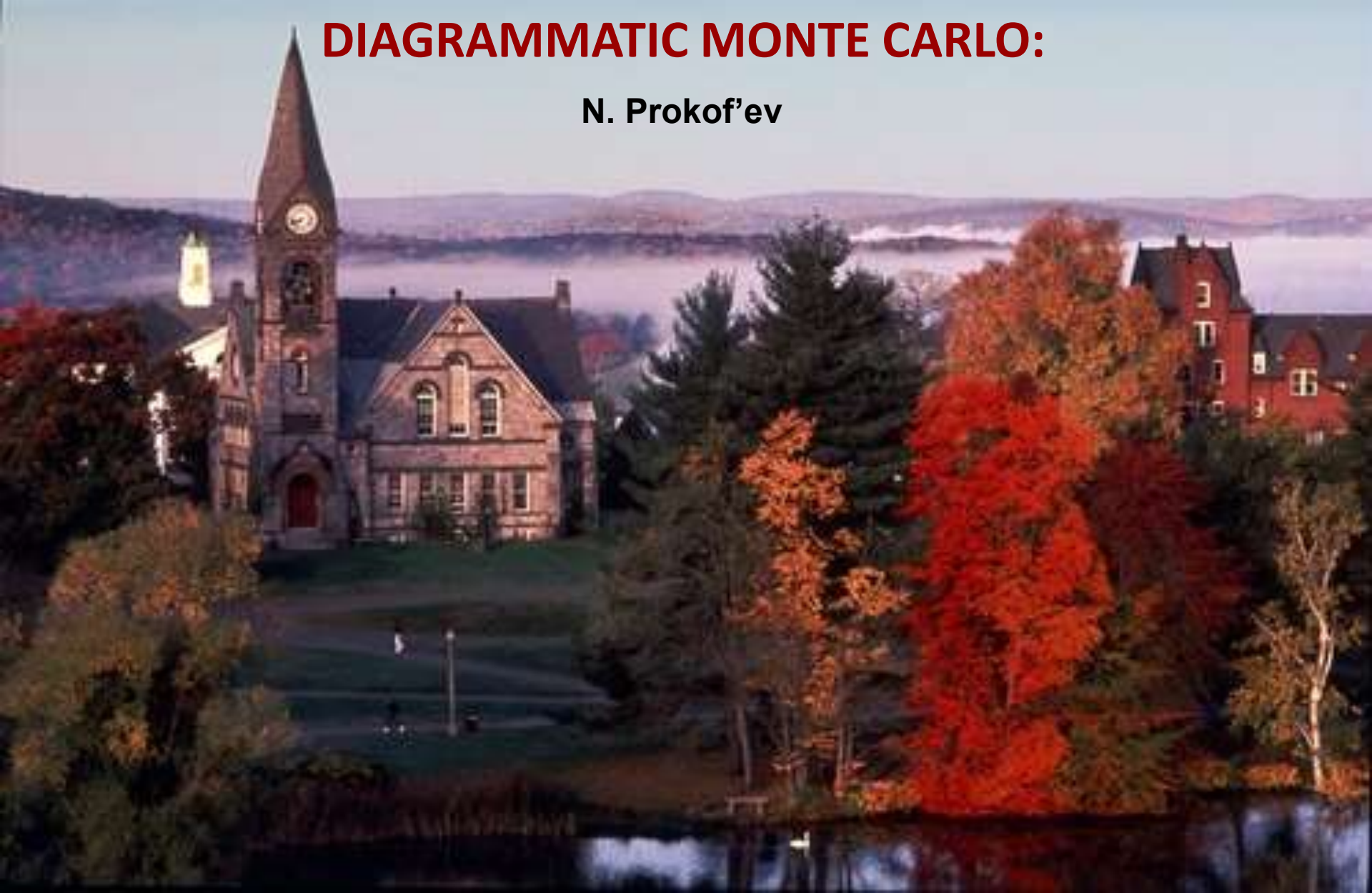
DIAGRAMMATIC MONTE CARLO:

N. Prokof'ev



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Diagrammatic Monte Carlo for connected Feynman diagrams solves the computational complexity problem for fermions*

$$H = \sum_{ka} \varepsilon(k,a) \psi^{\dagger}_{ka} \psi_{ka} + \frac{1}{2} \sum_{rr'abcd} V_{abcd}(r,r') \psi^{\dagger}_{r'd} \psi^{\dagger}_{rc} \psi_{rb} \psi_{r'a} + \ldots$$

Fermionic sign problem? Ask a voltmeter what it thinks about it!

Sign-blessing I: *Feynman diagrammatic expansions converge or can be resummed efficiently only if same order diagrams cancel each other*

Sign-blessing II: *Sum of all con* *roperties of fermionic determinants*
(n! terms in n^3 *tion of all topologies*

***for convergent or subject to resummation series**

Fermions do not have a sign problem

Personal viewpoint (* **f standard thermodynamics):

If it can be measured it can be calculated on classical computers with the same accuracy …

we just don't know yet how exactly in many cases … ☹

Diagrammatic Monte Carlo for connected Feynman diagrams

- How to compute contributions from high-order diagrams without systematic bias

- Why this makes sense to do even for divergent series

Generic Diag.MC case:

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

Integration variables

term order

different terms of of the same order (say, topologies)

Contribution to the answer or weight (with differential measures)

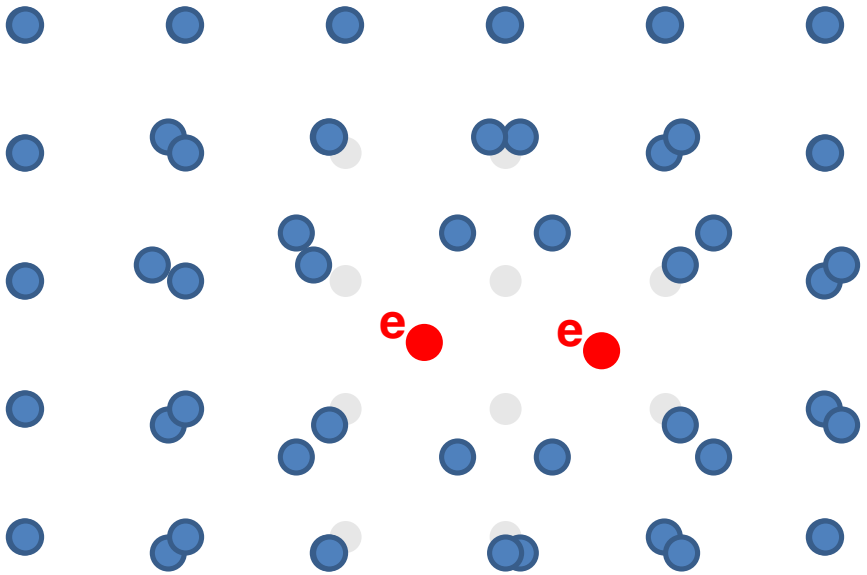
Sums of multi-dimensional integrals are typical for diagrammatic QFT expansions, but can originate from path integrals, impurity solvers, or any other series expansion

Polaron problem:

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

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

Electrons in semiconducting crystals (electron-phonon polarons)



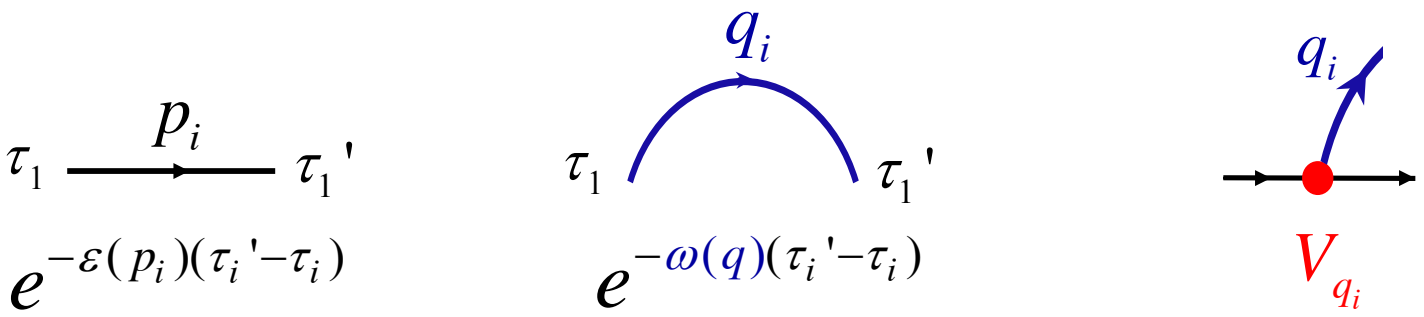
$$H = \sum_p \varepsilon(p) a_p^+ a_p + \quad \textbf{electron}$$

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

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

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

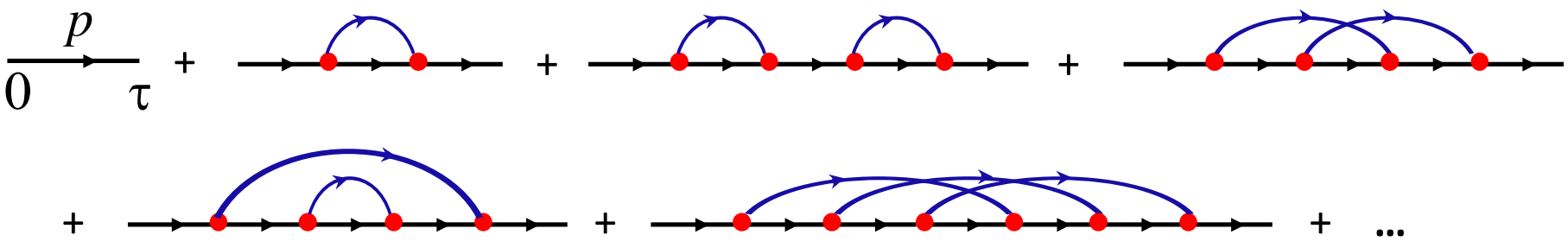
electron **phonons** **el.-ph. interaction**



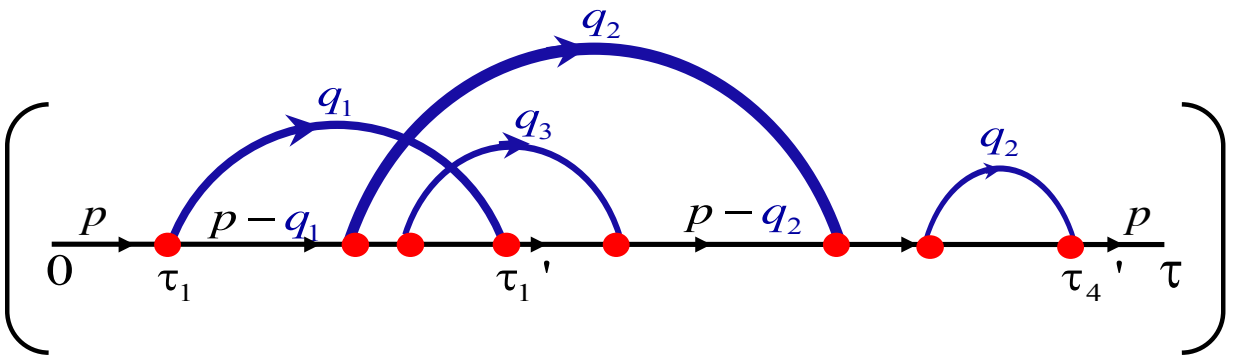
Green function: $G(p,\tau) = \left\langle a_p(\tau) a^\dagger{}_p(0) \right\rangle = \left\langle e^{-\tau H} a_p \; e^{\tau H} \; a^\dagger{}_p \right\rangle$

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

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



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

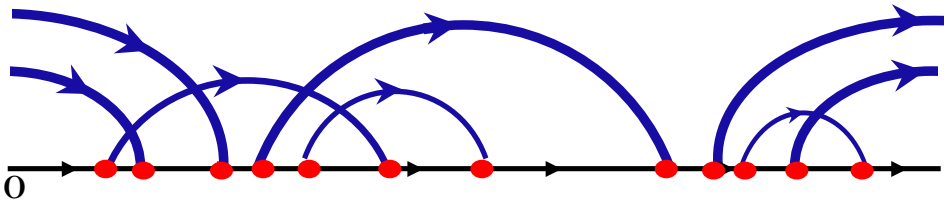


Graph-to-math correspondence:

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

***D* is a product of functions for propagators and vertexes**

Diagrams for:



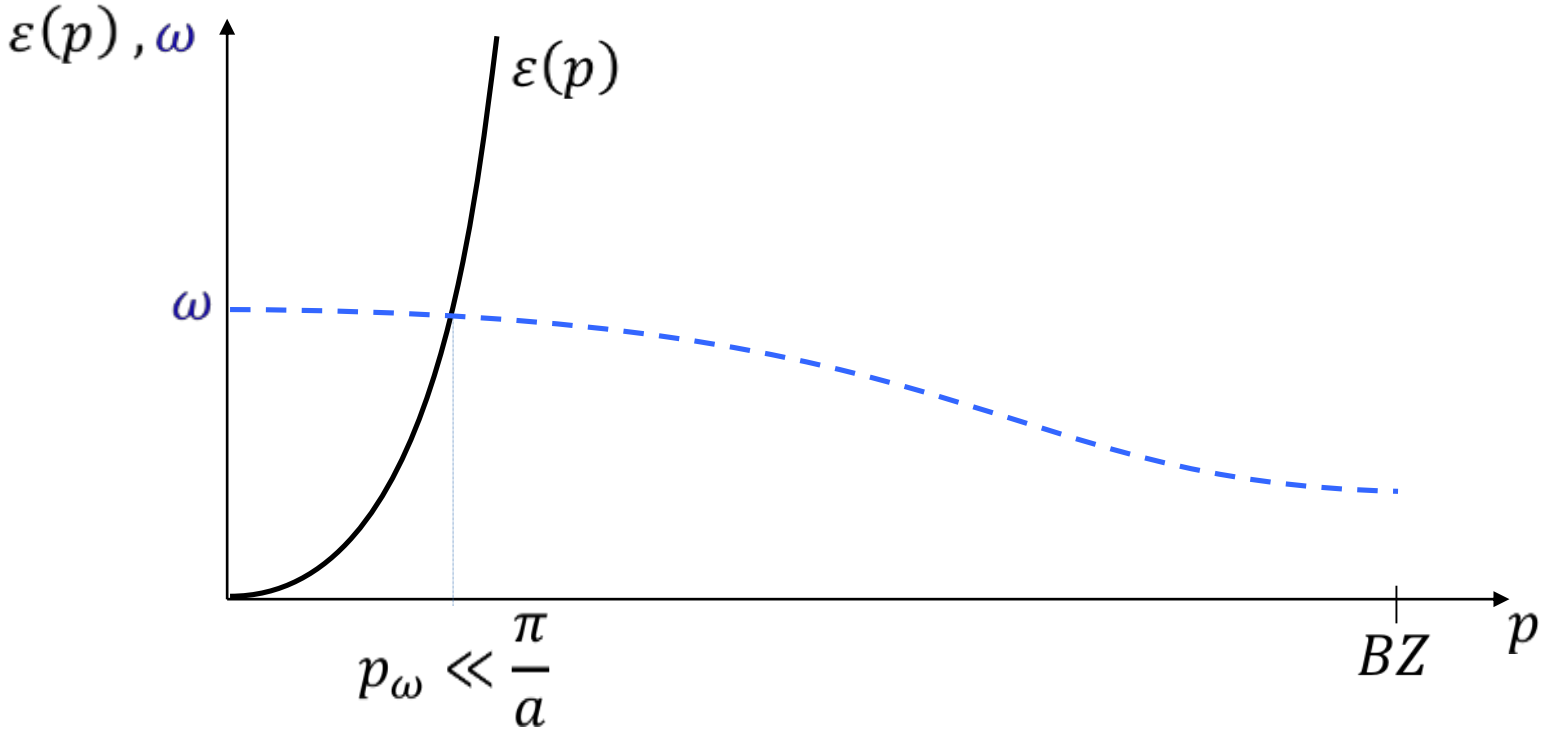
$$\left\langle b_{q_1}(\tau) b_{q_2}(\tau)\; a_{p-q_1-q_2}(\tau)\; a^{\dagger}_{p-q_1-q_2}(0)\; b^{\dagger}_{q_1}(0) b^{\dagger}_{q_2}(0) \right\rangle$$

there are also diagrams for optical conductivity, etc.

MC in the space of Feynman diagrams is an endless fun!

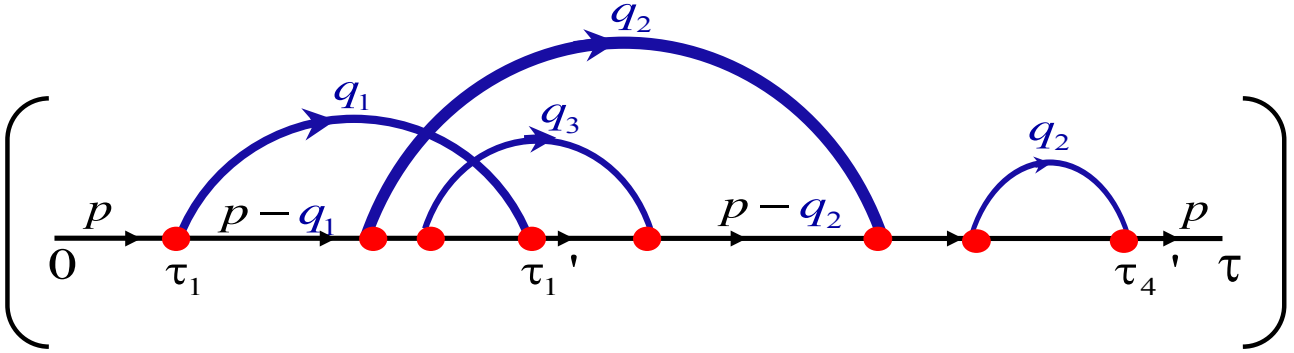
Frohlich polaron = single electron in ionic semiconductor

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



$$\varepsilon(p) = \frac{p^2}{2m}, \qquad \omega(q) = \omega = const, \qquad |V(q)|^2 = \frac{2\sqrt{2}\pi\alpha}{q^2}$$

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



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

***D* is a product of functions for propagators and vertexes**

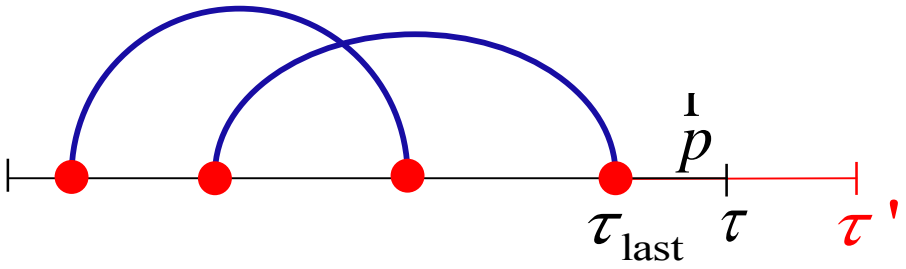
Define $\nu = (n, \xi, \{\vec{x}_i\}; \vec{p}, \tau)$ **as a point in the configuration space**

Sample $G = \sum_{\nu}^{\infty} D_\nu$ **by generating points** ν **from the probability distribution** $\propto |D_\nu|$

Type A
changing existing variables (diagram order is fixed)

Type B
changing diagram order and adding/removing variables

Type A: changing "external" time (the simplest version)



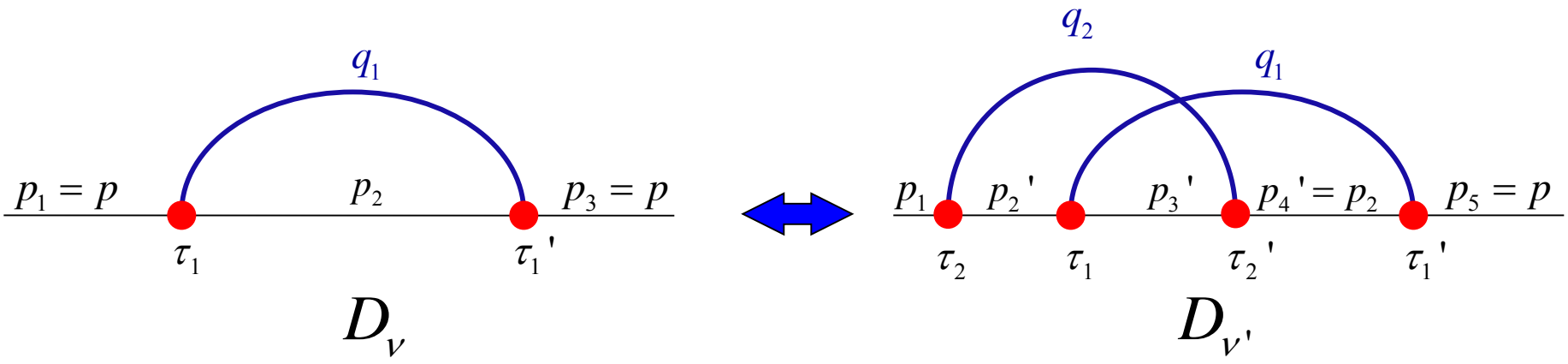
New time: Exponential probability density $\mathcal{P}(\tau';\nu) = \varepsilon(\vec{p})e^{-\varepsilon(\vec{p})(\tau'-\tau_{last})}$

Transformation method: $\tau' = \tau_{last} - ln(r)/\varepsilon(\vec{p})$

Always accepted, $\mathbb{R} = 1$

Type B: changing diagram order (one possible example)

Insert/Delete a phonon line (increasing/decreasing the diagram order by one)



- prob. to call increasing and decreasing updates are $p_{n\to n+1}$ and $p_{n+1\to n}$

- In Insert: Select one of the $2n+1$ electronic intervals at random (let it be interval a of length $\Delta\tau_a$) and seed τ_2 uniformly on this interval; prob. $p = 1/[(2n+1)\Delta\tau_a]$

- Use distribution $\Omega(\tau_2', \vec{q}_2; \nu)$ to seed new variables $\tau_2', \vec{q}_2$

- In Delete: Select any of the n phonon lines at random, prob. $p = 1/n$, and propose to remove it

Type B: changing diagram order (one possible example)

Detailed Balance equation:

$$D_\nu \, p_{n\to n+1}\Omega(\tau_2', \vec{q}_2;\, \nu)\frac{1}{(2n+1)\Delta\tau_a}\, R^{n\to n+1} = D_{\nu'} p_{n+1\to n}\frac{1}{(n+1)}\, R^{n+1\to n}$$

Solution for acceptance ratio in Insert

$$\mathbb{R}^{n\to n+1} = \frac{D_{n+1}(\tau_2\,, \tau_2', \vec{q}_2 \ldots)}{D_n(\ldots)\,\Omega(\tau_2', \vec{q}_2;\, \nu)}\,\frac{p_{n+1\to n}}{p_{n\to n+1}}\,\frac{(2n+1)\Delta\tau_a}{(n+1)}$$

Solution for acceptance ratio in Delete

$$¡^{\,n\to n-1} = \frac{D_{n-1}(\ldots)\Omega(\tau_2', q_2; \nu)}{D_n(\tau_2, \tau_2', q_2, \ldots)}\,\frac{p_{n-1\to n}}{p_{n\to n-1}}\,\frac{n}{(2n-1)\Delta\tau_a}$$

Type B: changing diagram order (one possible example)

Recall that $|V(q)|^2 = \frac{2\sqrt{2}\pi\alpha}{q^2}$

$$\frac{D_{n+1}}{D_n} = |V(q_2)|^2 \, e^{-\omega(\tau_2'-\tau_2)} \, e^{-\Delta E(\tau_2'-\tau_2)} \, \frac{q_2^2 dq_2 d\varphi \sin(\theta)\, d\theta}{(2\pi)^3} \propto$$

$$\propto e^{-\omega(\tau_2'-\tau_2)} \; e^{-\Delta E(\tau_2'-\tau_2)} dq_2 d\varphi d\chi; \quad \textbf{with} \;\; \Delta E = \frac{q_2^2 - 2\langle\vec{p}\rangle\vec{q}_2}{2m}$$

Possible distribution

$$\Omega(\tau_2', \vec{q}_2; \nu) = \frac{d\varphi d\chi}{4\pi} \; \frac{dq_2}{q_0(1+q_2/q_0)^2} \; [\omega(1+q_2/q_0)^2] \, e^{-\omega(1+q_2/q_0)^2(\tau_2'-\tau_2)} =$$

$$\frac{d\varphi d\chi}{4\pi} \, \frac{dq_2}{q_0} \, \omega e^{-\omega(1+q_2/q_0)^2(\tau_2'-\tau_2)} \quad \textbf{with} \quad q_0 = \sqrt{2m\omega}$$

Not perfect, but FAPP "good enough"

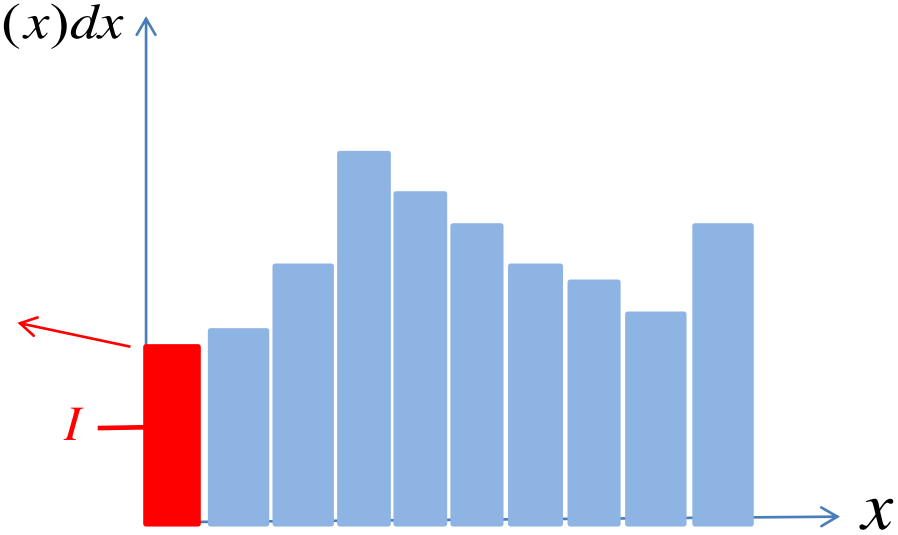
Normalization (not a problem in DiagMC = no sign in denominator ever):

histogram $h_{bin} \propto \int_{bin} f(x)dx$

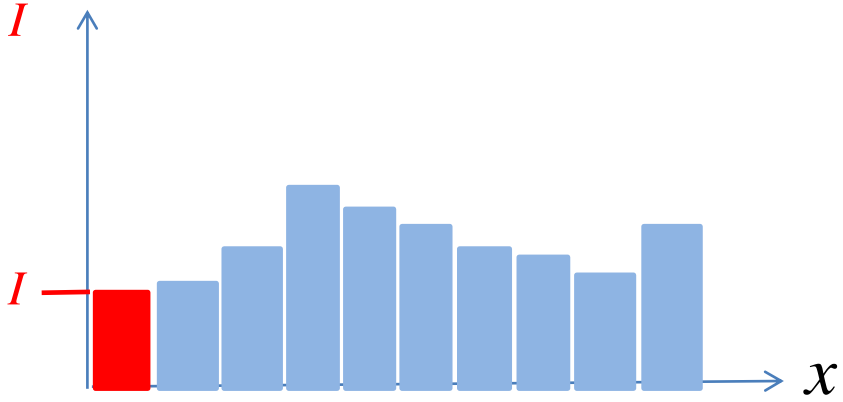
special "bin" where

$$\int_{bin} f(x)dx = I$$

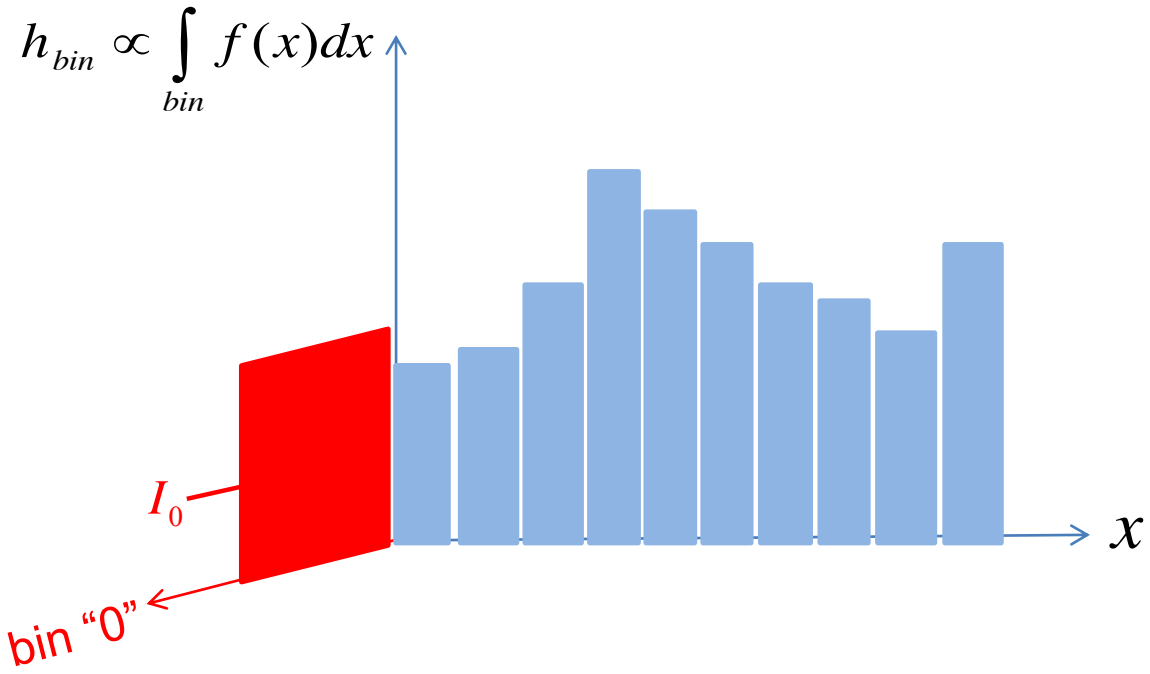
is known exactly

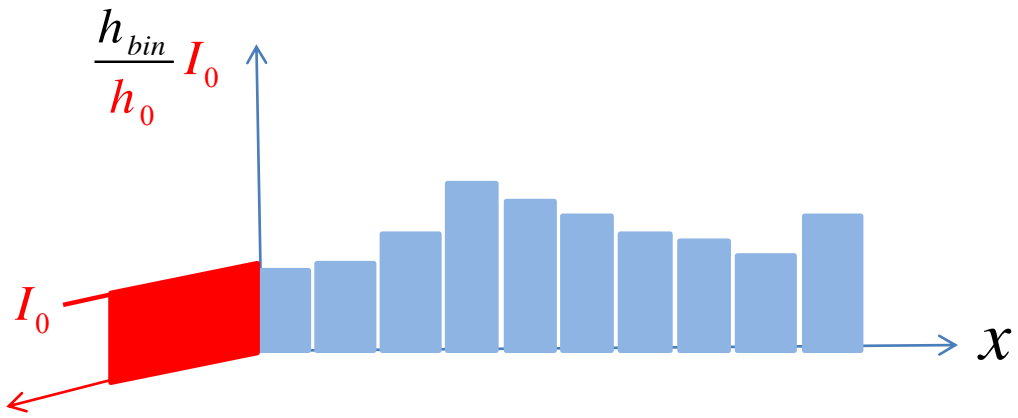


Normalized histogram $\frac{h_{bin}}{h_{sbin}} I$



Normalization using “desined bin”:





Normalization example (statistics is that for G diagrams)

Define "normalization" subspace and compute some physical answer in it

$$G_{norm} = \int_0^{\tau_0} |G_0(p_0, \tau)|\, d\tau = \frac{2m}{p_0^2}\left(1 - e^{-\tau_0 p_0^2/2m}\right)$$

Do it analytically (if possible) or numerically (to high accuracy)

Collect statistics for your answers as usual

$$A_{MC} = A_{MC} + A_v$$

MC estimator for quantity A, say

$1/\Delta_i$ **for** $\tau \in bin_i$ **of size** Δ_i

and record the number of configurations in the normalization subspace

$$Z_{norm} = Z_{norm} + 1 \quad \text{when } \tau \in (0, \tau_0) \ \& \ n = 0$$

Properly normalized physical answer:

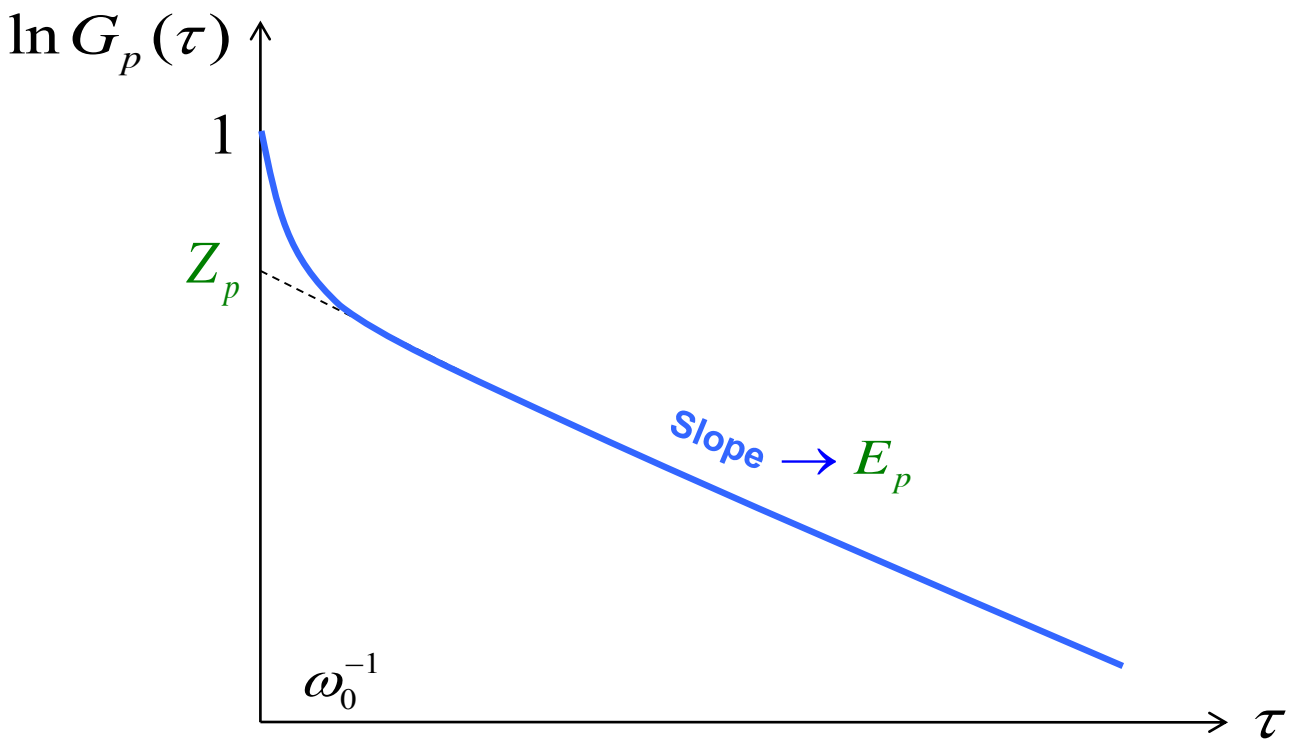
$$A = A_{MC} \frac{G_{norm}}{Z_{norm}}$$

This is it! Collect statistics for $G(p,\tau)$, Monte Carlo estimators for energy, group velocity, effective mass, number and distribution of phonons in the cloud, or some corr. function.

Analyze it. For example: $G(p,\tau\to\infty)\to Z_p e^{-E(p)\tau}$

$Z_p = |C_p|^2$ **probability of getting a bare electron**

Quasiparticle energy



Analyzing data: polaron energy estimator [In the $\tau \to \infty$ limit]

In the limit of large τ we have $E_p = -\frac{dG/d\tau}{G} \equiv \frac{\sum_\nu -dD_\nu/d\tau}{\sum_\nu D_\nu}$; this expression has the standard form of average over an ensemble of G-configurations. For every G-diagram, the dependence on imaginary time is given by (recall "fancy" external time update) $D_\nu \propto \tau^{2n} e^{-E\tau}$ leading to MC polaron energy estimator

$$E_\nu = \tau^{-1}\left[\sum_{i=1}^{2n+1} \varepsilon(\vec{p}_i)\Delta\tau_i + \sum_{j=1}^{n} \omega(\vec{q}_j)\Delta\tau_j - 2n - 2n\right]$$

because $-\frac{dD_\nu}{d\tau} = E_\nu D_\nu$ and $E_p = \frac{\sum_\nu E_\nu D_\nu}{\sum_\nu D_\nu}$. Similarly, one can derive estimators for group velocity an effective mass

$$\vec{v}_\nu = \frac{1}{m\tau}\sum_{i=1}^{2n+1} \vec{p}_i \Delta\tau_i \equiv \qquad \left(\frac{1}{m^*}\right)_\nu = \frac{1}{m} - \frac{\tau}{3}\vec{v}_\nu{}^2$$

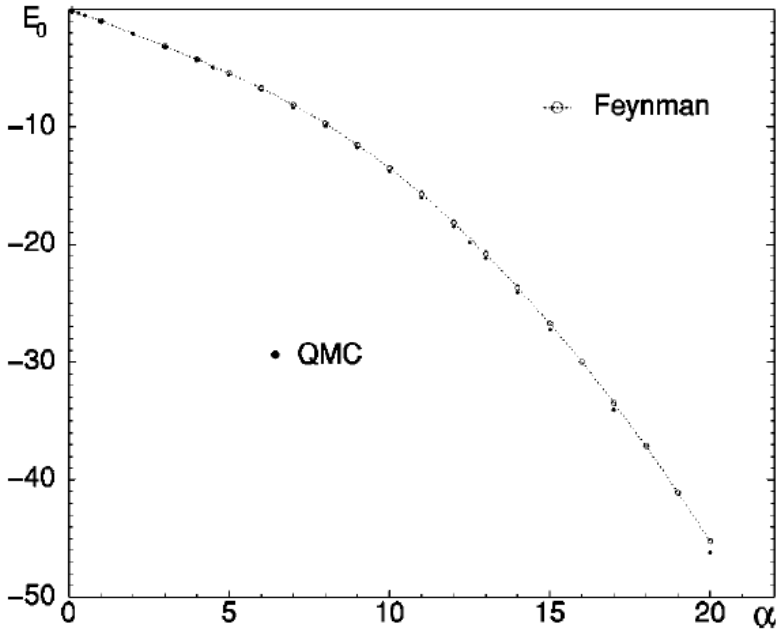


FIG. 4. Bottom of the polaron band E_0 as a function of α. The error bars are much smaller than the point size.

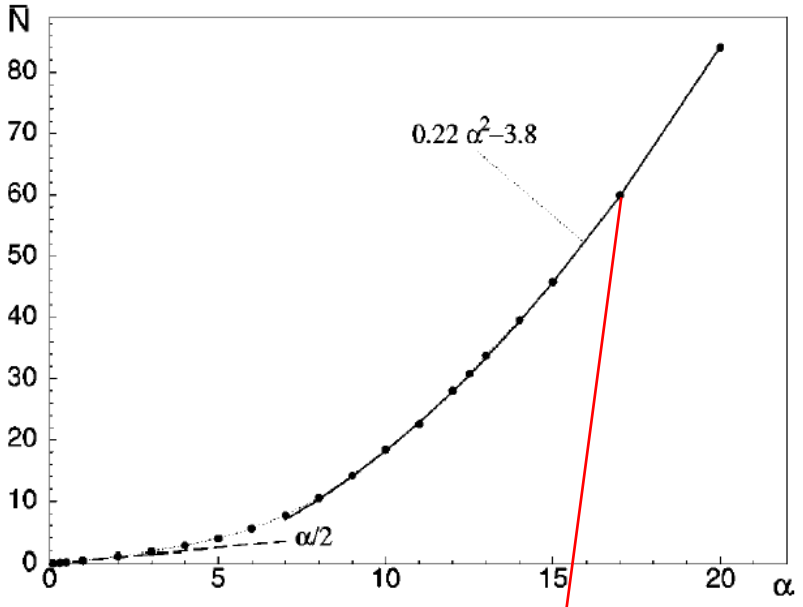
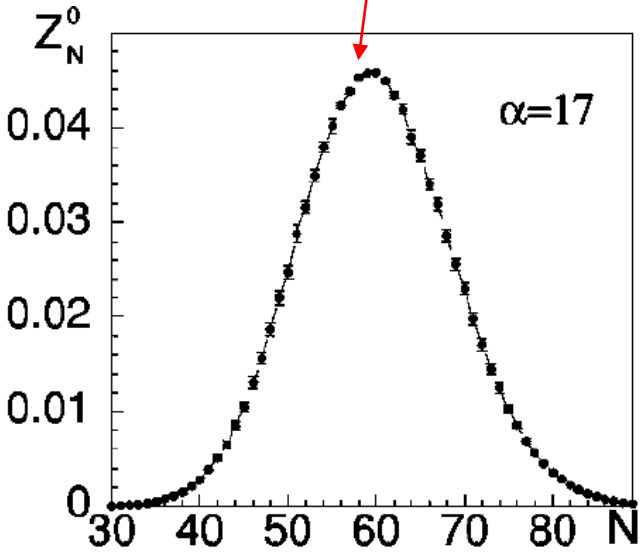


FIG. 8. The average number of phonons in the polaron ground state as a function of α. Filled circles are the MC data (calculated to the relative accuracy better than 10^{-3}), the dashed line is the perturbation theory result (4.1), and the solid line is the parabolic fit for the strong coupling limit.



Not Landau Pekar limit yet: broad superposition of phonon-number states, while

$$m^*(17)/m > 1000$$

A. Mishchenko, B. Svistunov, A. Sakamoto, NP, '98, '00

Many-body case is similar, but the expansion (for fermions) is not sign positive.

This is great!

FSP does not apply to connected Feynman diagrams because

- There is no dependence on the particle number or system volume
  (thermodynamic limit directly)

- Series convergence is only possible for fermions because different diagrams cancel each other = **sign blessing I**

- Fast summation of topologies with the help of determinants = **sign blessing II**

sign blessing I: All by itself the coupling constant U^n can never compensate for the factorial number of diagrams at large diagram order n. If not for the fermionic sign, the series of connected diagrams would always diverge! (similarly to

Computational Complexity Problem (CCP)

[Revelent question: ***How easily can one improve the accuracy of computed answers?*****]**

Let Q and ε be the quantity of interest **in the thermodynamic limit (TL)** and its desired relative accuracy $\varepsilon = \left|\delta Q / Q\right|$, respectively.

The numerical scheme is said to have CCP if the CPU time, t_Q ***, required to compute*** Q ***with accuracy*** ε ***diverges faster than any polynomial function of*** $\varepsilon^{-1} \to \infty$.

The problem is considered to be solved if $\ln t_Q \propto \ln \varepsilon^{-1}$.

Why thermodynamic limit? Because in finite size systems with $N = L^d$ particles the ultimate scaling of $t_Q(N)$ (if it can be reached in practice) is always subject to CLT with $t_Q(N) \propto \varepsilon^{-2}$

CCP and Diagrammatic MC

DiagMC has no sign problem, but what about CCP?

Define approximation $Q_n = \sum_{j=0}^{n} b_j g^j$ **(truncated sum)**

For convergent series $\left|\left(Q - Q_{n-1}\right)/Q\right| \propto g^n$ **with** $g < 1$**, and accuracy** ε **is reached at**

$$n_\varepsilon \propto \ln \varepsilon / \ln g$$

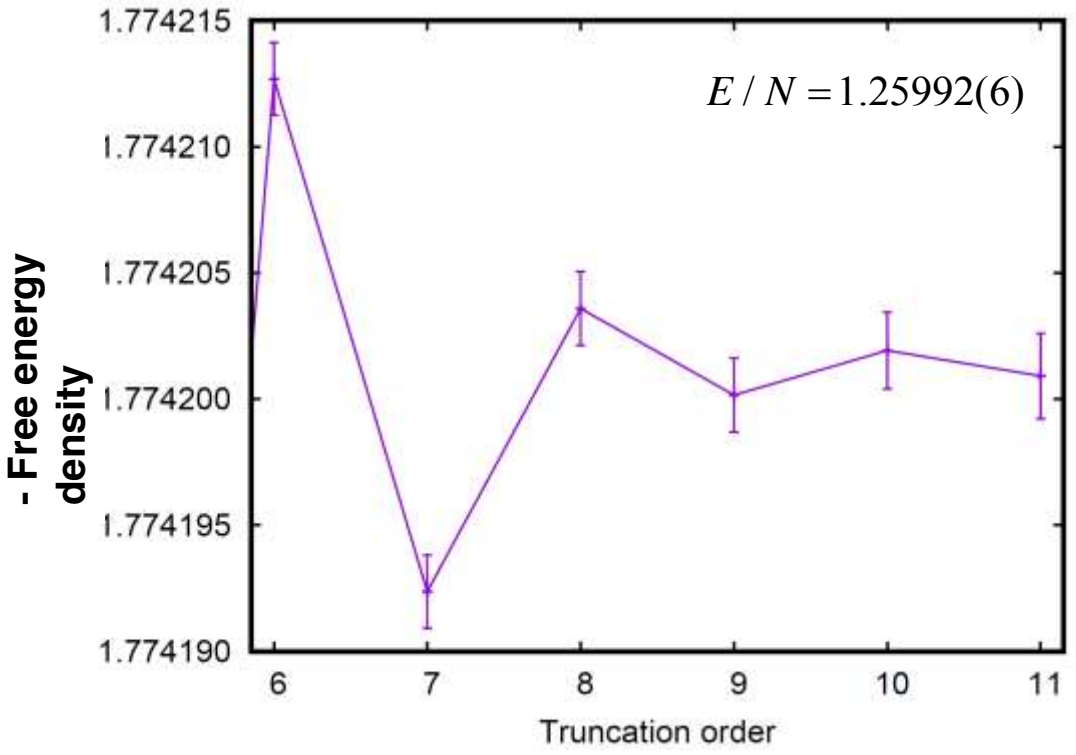
For fermions, all order-n contributions can be computed in time [R. Rossi PRL'17**]**

$$\tau_Q(n) \propto e^{\#n}$$ **(sign-blessing II)**

and the CCP is solved!

$$\boxed{\ln t_Q \propto n_\varepsilon \propto \ln \varepsilon^{-1}}$$

When series converge: 2D Fermi-Hubbard model at $U/t = 2,\ \ T/t = 0.125,\ \ n = 0.87500(2)$



R. Rossi, PRL '17

Six to five digit (depending on quantity) accuracy for a finite-T answer!

Sign alternating contributions

Sample or sum?

(Diagrammatic series for fermions converge, despite having about n! of them at order n, only because they cancel each other)

Consider $Z = \sum_{i=1}^{M} D_i \, Sign_i$ with $M \gg 1$ and relatively uniform distribution of weights and signs such that the net result is $Z \sim 1$. We assume that $t_{CPU} > M$, but is very long.

Need to know Z with accuracy $\varepsilon = \frac{\delta Z}{Z} < 1$

Sample

in M operations (one random "sweep" over the configuration space) the MC estimate will be $\delta Z \sim Z\sqrt{M} \gg Z$

By CLT the error will subsequently decrease as $\varepsilon \sim \sqrt{M}\,\sqrt{M/t_{CPU}}$. To get $\boldsymbol{\varepsilon} = \frac{\delta Z}{Z} < 1$ one needs

$$t_{CPU} > M^2$$

Sum

$$t_{CPU} = M$$

exact answer !

Definitely sum!

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

in to $$A(\vec{y}) = \sum_{n=0}^{\infty} \iiint d\vec{x}_2 \,\mathrm{K}\, d\vec{x}_n \; \tilde{D}_n\left(\vec{x}_1, \vec{x}_2, \mathrm{K}\; \vec{x}_n; \vec{y}\right)$$

with $$\tilde{D}_n\left(\vec{x}_1, \vec{x}_2, \mathrm{K}\; \vec{x}_n; \vec{y}\right) = \sum_{\xi} D_n\left(\vec{x}_1, \vec{x}_2, \mathrm{K}\; \vec{x}_n, \xi; \vec{y}\right)$$

All topologies are summed up efficiently to account for significant sign cancellations

- Codes become very easy to develop - change n and shuffle x_i
- Configuration weights are expensive to compute, but efficiency is radically improved
- Will global updates help? Likely yes

Spending CPU on performing "smart" global updates

Local or Global updates?

The key advantage of local updates is in $\mathbb{R}\sim 1$)

Let $D_v = D(x_1, \ldots, x_n) = \left| \sum_{\xi=1}^{M} D(x_1, \ldots, x_n; \xi) \right|$ with $M \gg 1$. Then, making local updates $x_s \to x_s'$ is not optimal because getting an uncorrelated set $\{x_i'\}$ will require $L \gg n$ updates

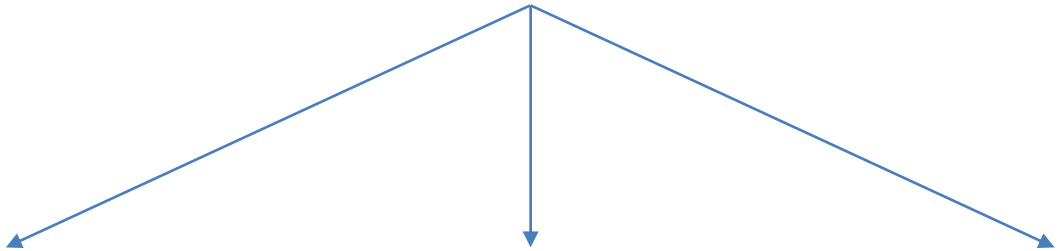
``Learn" how to propose global updates $\{x_i\} \to \{x_i'\}$

with acceptance ratio $\mathbb{R}\sim 1$

``Heat bath" idea + ``machine-learning" algorithms to approximate

$D(\{x_i'\}) / D(\{x_i\})$ with easy-to-compute $\exp\{-H(\{x_i'\}) + H(\{x_i\})$

When bare series do NOT converge



Do MF/HF/RPA/GW/NCA and publish

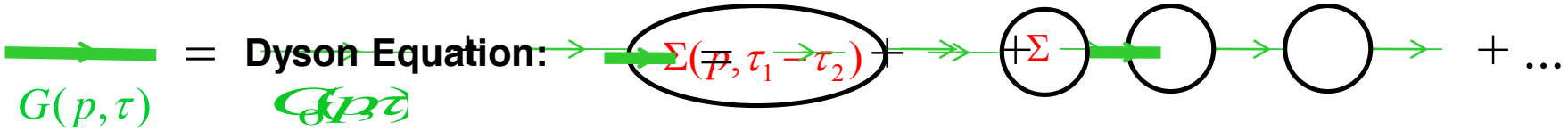
Change research topic

Keep fighting at your own peril and solve unsolvable (may be)!

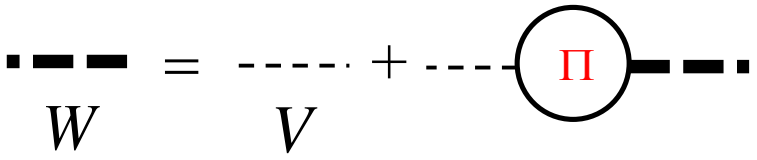
Bold (self-consistent) Diagrammatic Monte Carlo

Diagrammatic technique admits partial summations and self-consistent formulations

No need to compute all diagrams for G and W:

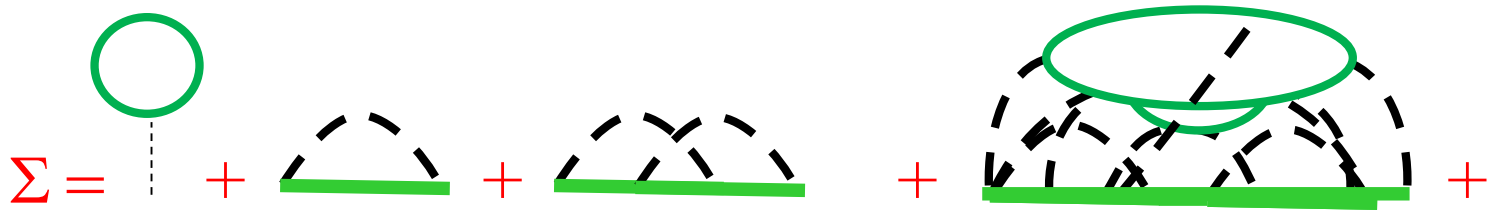


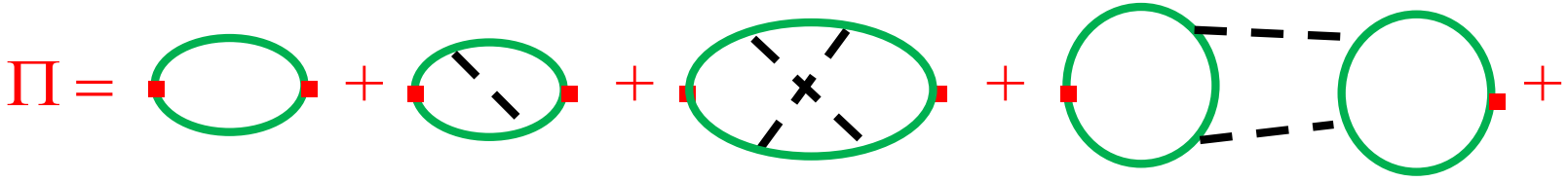
Screening:



Calculate irreducible diagrams for Σ, Π, … to get G, W, …. from Dyson equations

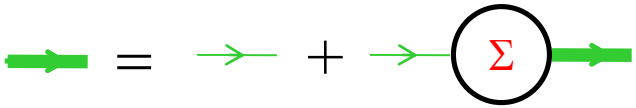
One possible scheme: G^2W- expansion



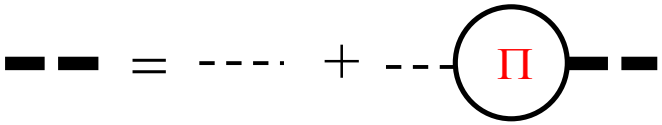


In terms of "exact" propagators

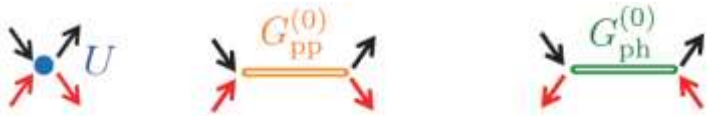
Dyson Equation:

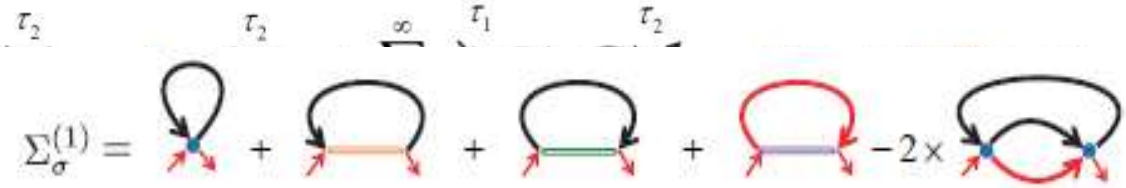


Screening:



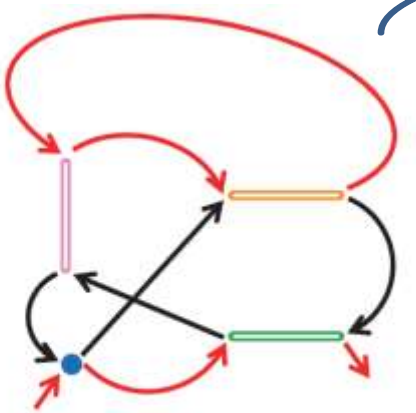
Hubbard model: Build diagrams using four propagators:
(contact potential)





Diagrammatic elements

The only triple-couting (at the lowest order)

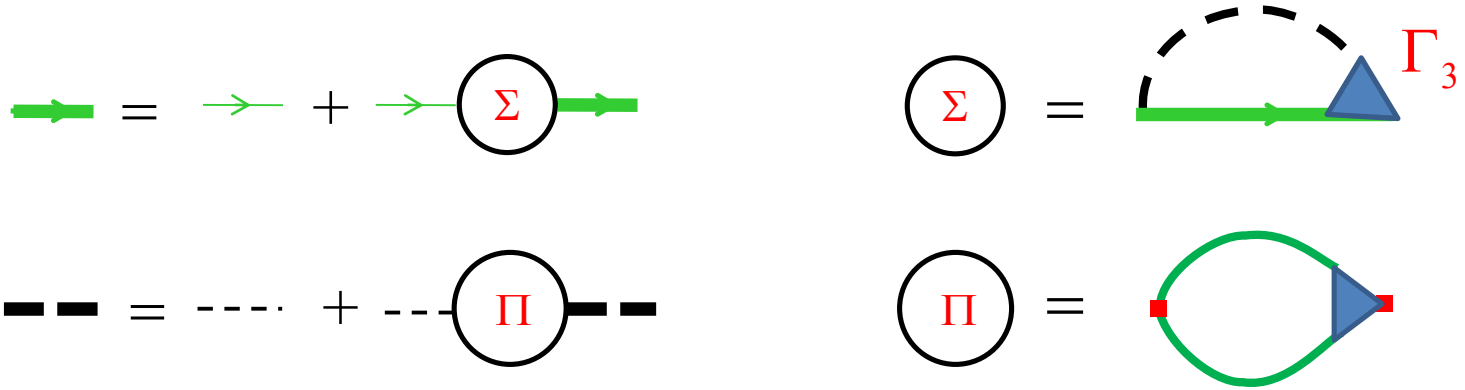


An example of a Σ diagram

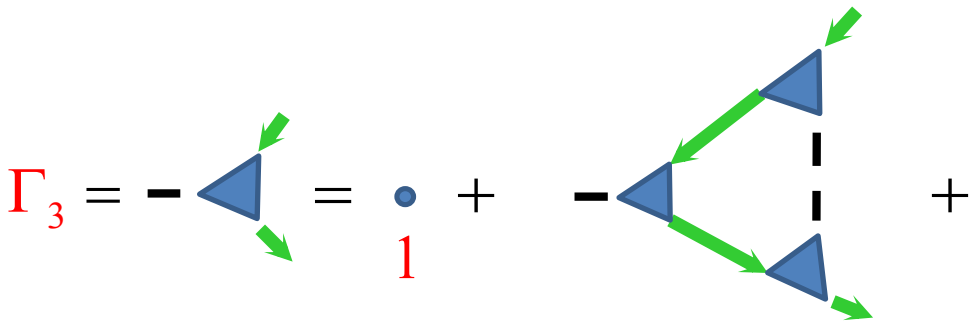
$$G_\sigma = \frac{G^{(0)}_\sigma}{1 - G^{(0)}_\sigma \Sigma_\sigma}, \qquad W = \frac{U}{1 - U\Pi} - U,$$

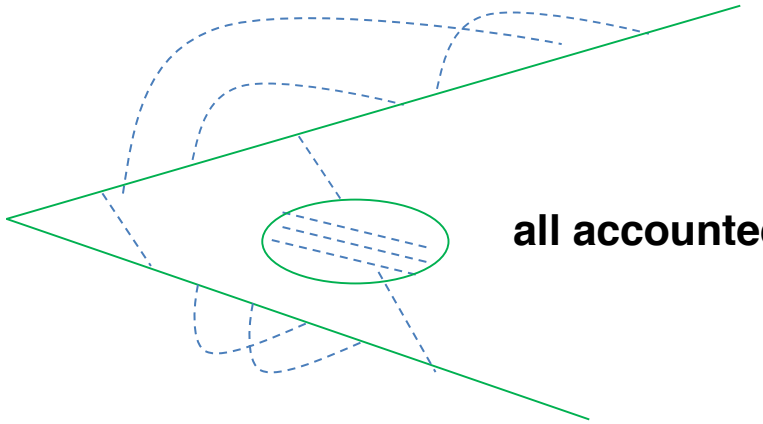
$$G_{pp} = \frac{U}{1 - U\Sigma_{pp}} - U, \qquad G_{ph} = \frac{U}{1 - U\Sigma_{ph}} - U$$

Fully dressed skeleton graphs (Heidin):

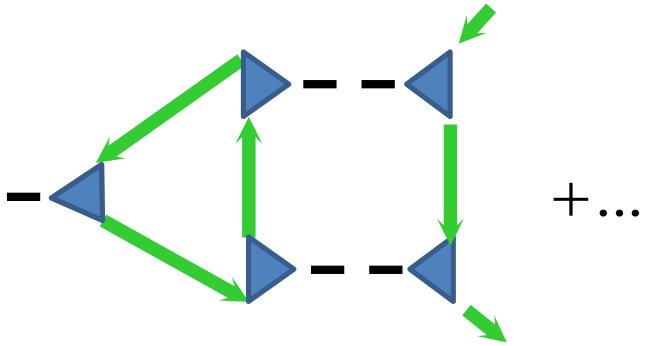


Irreducible 3-point vertex:





all accounted for already!



Bare or "dressed" series or skeleton sequences?

Pros. for bare:

- Taylor series → theory of analytic functions & resummation techniques
  [work outside of convergence radius]

- F_{line} in diagrams are analytic; no self-consistent loops

Pros. for dressed/skeleton:

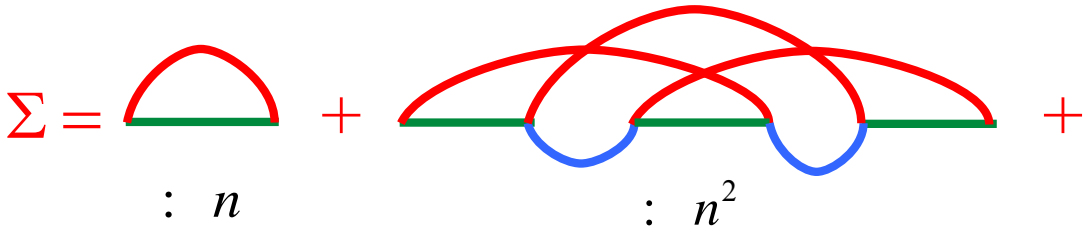
- Same graphs as in bare, just a much smaller set → # of irreducible graphs at order n is smaller by a factor of about 1/n for each "dressed" channel: G vs G_0 , W vs V
  One can simulate higher orders faster

- F_{line} are readily available from tables → as fast and easy, as intrinsic

- Bare series for long-range interactions are ill-defined, e.g. for $V_C(q) = 4\pi e^2 / q^2$ the 2d-order bubble diagram involves $\int d^3q V_C^2(q) \to \infty$. Need to screen, or sum up all bubble chains.

Pros. for dressed/skeleton:

- Different expansion parameter: consider a dilute gas with large *V*. Define a pair propagator $\Gamma = V + V(GG)\Gamma$ based on ladder diagrams, and arrive at the techniques where expension is in powers of density, not *V* .



Con. for skeleton (despite having well defined Luttinger-Ward functional):

- Skeleton sequence for divergent bare series will converge to the wrong answer!

Solution for this Con.

- dress lines only partially by low-order bare or skeleton graphs
- do Taylor series for the rest using an auxiliary parameter ξ

Shifted action tools

Original setup: $S = \bar{\psi} G_0^{-1} \psi + S_{\text{int}}\left[\bar{\psi}, \psi\right] \rightarrow \bar{\psi} G_0^{-1} \psi + \xi S_{\text{int}}\left[\bar{\psi}, \psi\right]$

Bare series produce Taylor series in ξ and the physical answer corresponds to $\xi = 1$

Introduce $S_\xi\left(\Lambda\right) = \bar{\psi} G_\Lambda^{-1} \psi + \sum_{k=1}^{K} \xi^k \bar{\psi} \Lambda_k \psi + \xi S_{\text{int}}\left[\bar{\psi}, \psi\right]$

Unphysical, in general, with formally arbitrary set of functions Λ_k, but if we demand

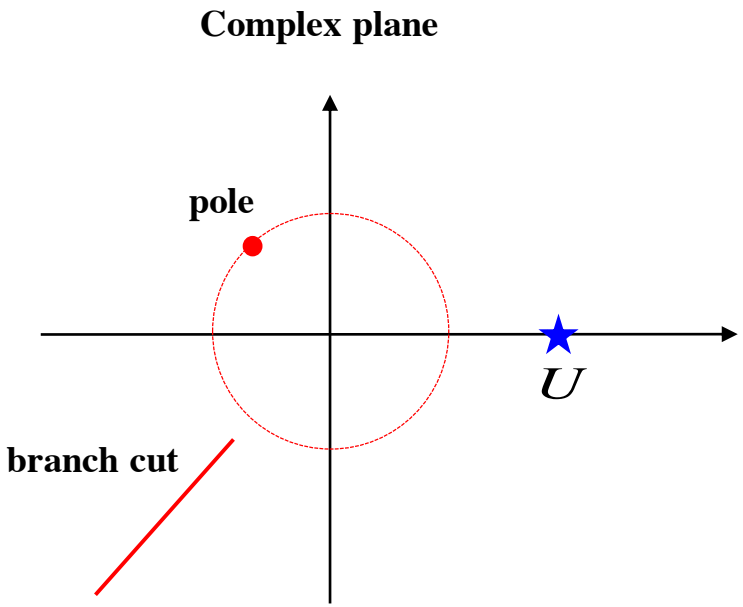
$$G_0^{-1} = G_\Lambda^{-1} + \sum_{k=1}^{K} \Lambda_k$$

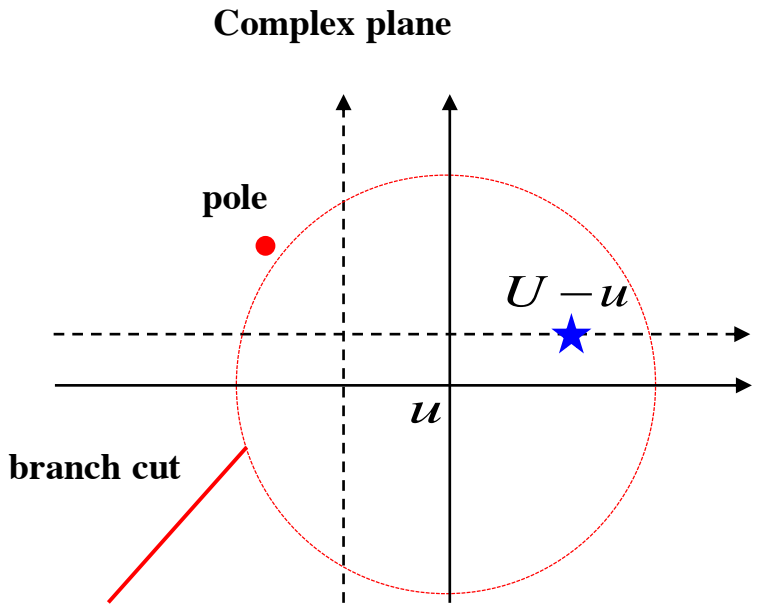
then at $\xi = 1$ we will recover the physical action identically $S_{\xi=1}\left(\Lambda\right) = S$. Proceed with Taylor series expansion in ξ but it's a different series because of counter-terms $\left\{\Lambda_k\right\}$

- **If Λ_n are based on $\Sigma_n[V, G_0]$ diagrams, then we expand on top of partially dressed G**
- **If Λ_n are based on $\Sigma_n[V, G_\Lambda]$ diagrams, then we deal with skeleton dressing**
- **This setup can be generalized (with the help of Hubbard-Stratanovich transformation) to partial or skeleton dressing of interactions, ladders, etc.**

When series diverge or convergence is slow

Recall

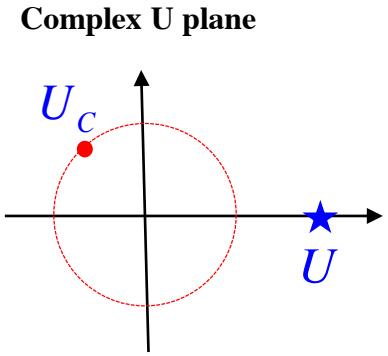




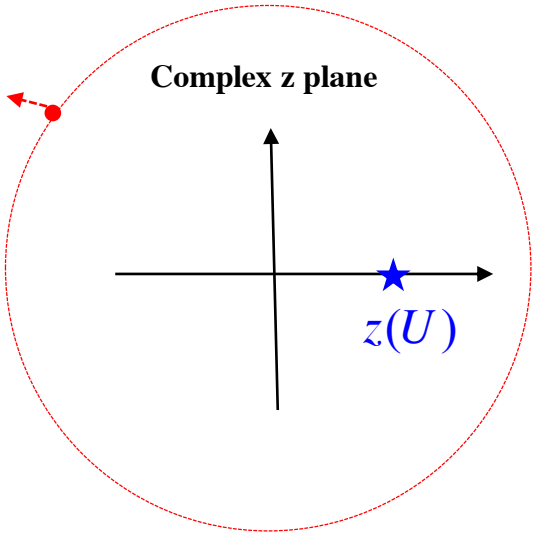
This is just a cartoon analogy, in shifted action we change the "origin of expansion" in the functional space, and $\xi = 0$ may not be even physical

When series diverge or convergence is slow

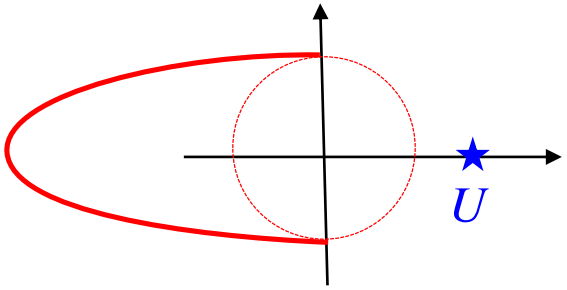
Conformal mapping:



$$z = \frac{U}{U - U_C}$$

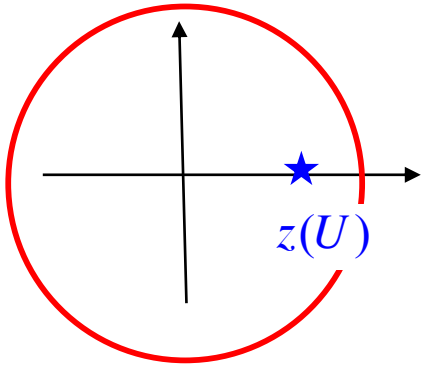


Generalization = Pade $z = \dfrac{P_k(U)}{P_m(U)}$



$$z = \frac{{}_pF_q(a,b,c,U)}{{}_sF_t(a',b',c',U)}$$

Hypergeometric functions



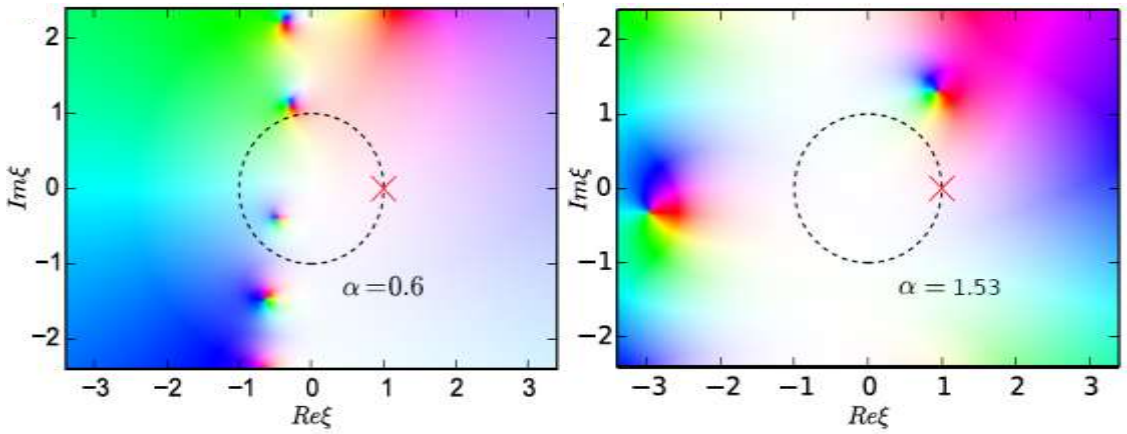
Borel, conformal Borel, never-heard-of-method …

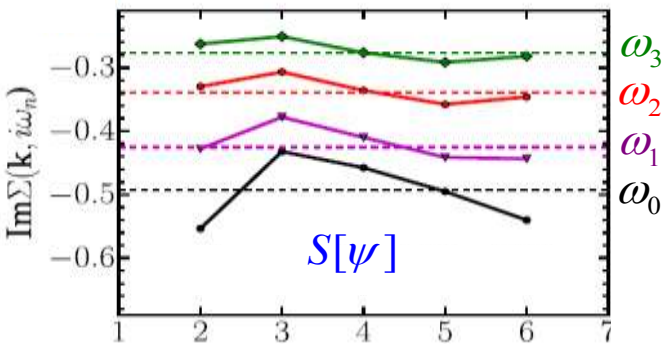
When series diverge or convergence is slow: 2D Fermi-Hubbard model

$S_\xi[\psi, \alpha = \xi]$ (optimize for best convergence in the atomic limit)

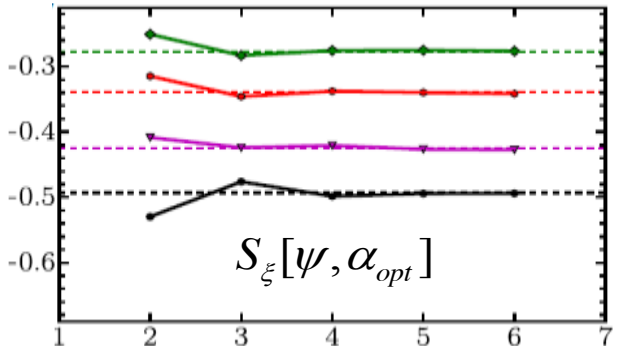
$S[\psi]$

Divergent series





Expansion order



Expansion order

W. Wu, M. Ferrero, A. Georges, E.Kozik, arXiv:1608.08402

When convergence radius is zero & series are asymptotic (unitary ultra-cold Fermi gas)

Quantitative understanding of series divergent behavior

$$Z(g)=\sum_{n=0}^{\infty} g^n z_n \quad \Rightarrow \quad z_n=\oint_C \frac{dg}{2\pi i}\frac{Z(g)}{g^{n+1}}=\oint_C \frac{dg}{2\pi i} e^{-(n+1)\ln g+\ln Z(g)} \quad \Rightarrow$$

saddle-point in g method for large exp.

$$Z(g)=\int D\psi\, e^{-S_0[\psi]-gS_{\text{int}}[\psi]} \quad \Rightarrow \quad z_n=\oint_C \frac{dg}{2\pi i}\int D\psi\, e^{-S_0[\psi]-gS_{\text{int}}[\psi]-(n+1)\ln g} \quad \Rightarrow$$

saddle-point in g and bosonic field Φ (after Hubbard-Stratanovich transformation) for large exponent

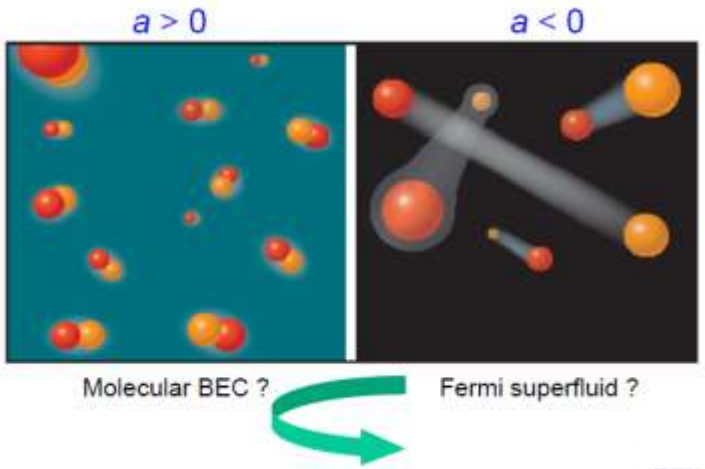
L. N. Lipatov, Sov. Phys. JETP **45**, 216 (1977)]

- **Can be generalized for partially summed and skeleton series**
- **Suggests efficient resummation technique & uniqueness of Z(g)**
- **"designer" conformal Borel transforms series from asymptotic**
- **to convergent!**

R. Rossi, K. van Houcke, F. Werner '19

When the convergence radius is zero: unitary Fermi gas

Fermions with strong "zero"-range potential leading to large s-wave scattering length a_S



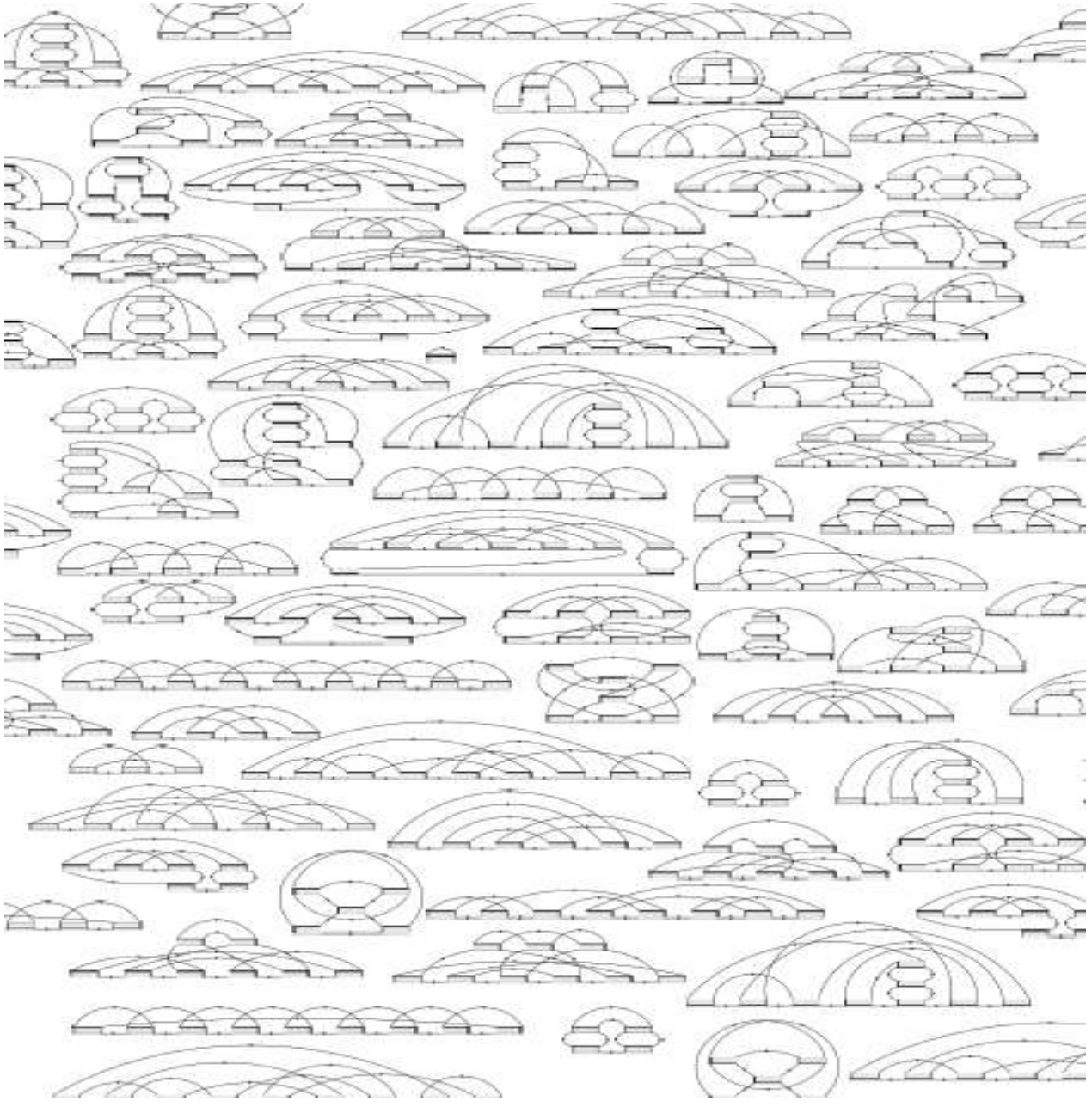
Unitary limit: $k_F a_S \to \infty$

In this case k_F **and** ε_F **are**

the only length/energy scales

Skeleton diagrammatic series are asymptotic with leading divergence $(n!)^{1/5}$**,**
but are subject to the series resummation technique

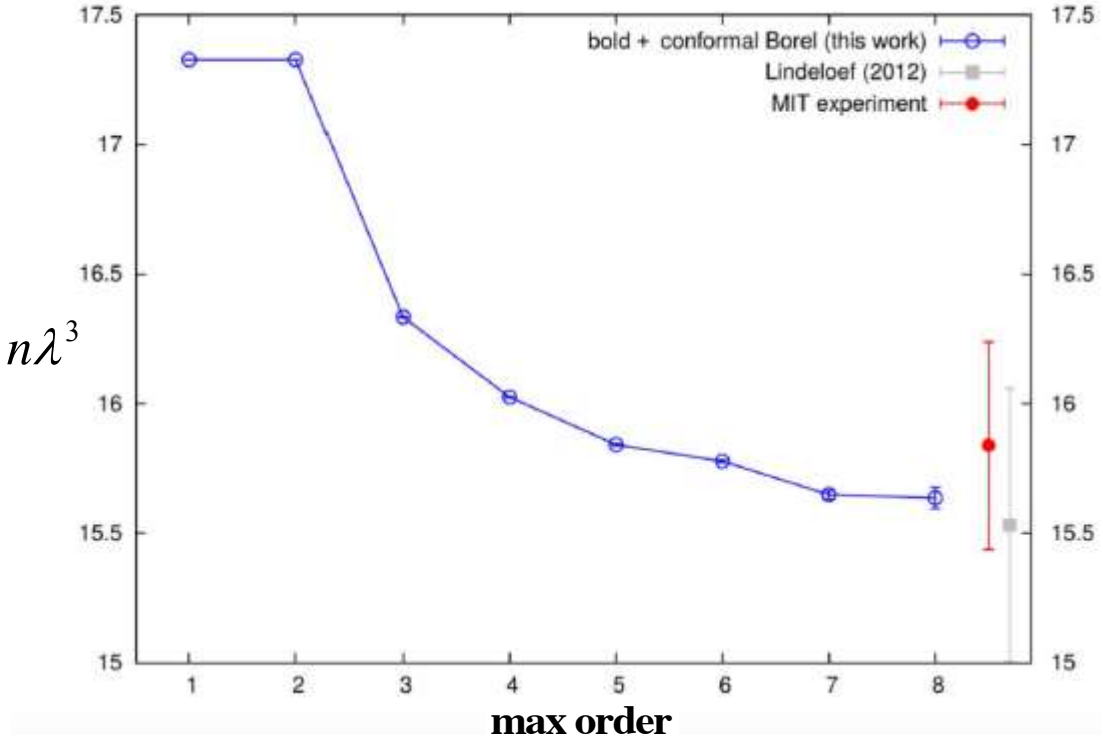
Real thing, not a cartoon!



tiny 10^{-6} fraction

Equation of state for the unitary Fermi gas

$T / E_F = 0.2$ (superfluid transition is at $T_C / E_F = 0.16$



R. Rossi, F. Werner, K. van Houcke (private comm. '16)

If you can

- **compute enough orders (say n~10; billions of skeleton graphs) and**

- **know what to do with them**

then any interacting Fermi system can be solved accurately

Conclusions:

1. For convergent and subject to re-summation series, Diag.MC solves the computational complexity problem ($t \propto \varepsilon^{-c}$) → correlated fermionic systems can be addressed with systematically improvable accuracy. What we lack mostly, is understanding of the model analytic properties in the complex plane.

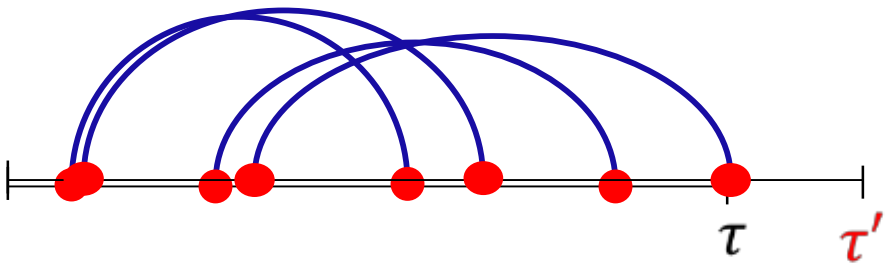
2. If item 1 above is understood, then the possibilities are unlimited !

- **Hubbard model (need better formulations near half-filling → second fermionization, dual fermions, parquet, …**
- **Resonant fermions (develop DiagMC for superfluid states, explore polarized gases, move away from unitarity, …)**
- **frustrated magnets (unique method for the cooperative paramagnet regime (can do pyrochlore), but need to explore alternative formulations for T<<J, develop SU(N) schemes, …)**
- **interacting topological materials (ready to explore stability bounds and phase diagrams)**

- Real materials? In progress (Simons Collaboration on the Many Electron Problem)

Type A: changing "external" time (another, more fancy, version)

Notice that $D \propto \tau^{2n} e^{-E\tau}$ where $E = \tau^{-1}\left[\sum_{i=1}^{2n+1} \varepsilon(\vec{p}_i)\Delta\tau_i + \sum_{j=1}^{n} \omega(\vec{q}_j)\Delta\tau_j\right]$



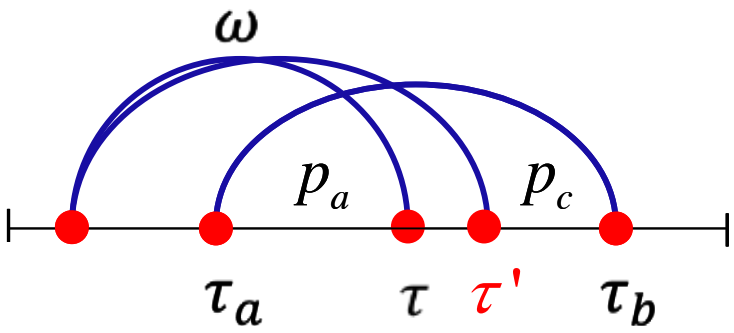
$\mathcal{P} = (E\tau)^{2n} e^{-E\tau} E$ but generating random numbers for large n is not easy.

Instead, use Gaussian $\mathcal{P} = e^{-(E\tau-2n)^2/4n}\, E/\sqrt{4\pi n}$ (reject negative τ)

Acceptance ratio

$$\mathbb{R} = exp\left\{2n \ln\left(\frac{\tau'}{\tau}\right) - E(\tau' - \tau) + \frac{(E\tau\prime-2n)^2-(E\tau-2n)^2}{4n}\right\} \approx 1 \quad \text{for} \quad n \gg 1$$

Type A: changing internal time



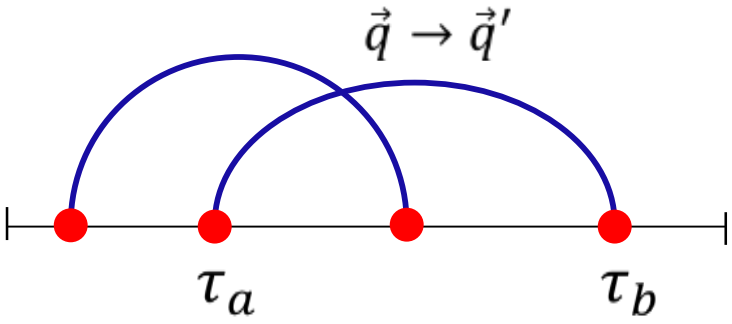
1. Select any electron interval except the last one at random

2. Use $P(\nu;\tau') = \dfrac{Ee^{-E(\tau_c'-\tau_a)}}{1-e^{-E(\tau_b-\tau_a)}}$ **with** $E = \dfrac{p_a^2}{2M} - \dfrac{p_c^2}{2M} \pm \Omega$ **to seed new variable**

$$\tau' = \tau_a - \ln\left[1 - r\left(1 - e^{-E(\tau_b-\tau_a)}\right)\right] / E$$

Always accepted, $\mathbb{R} = 1$

Type A: changing internal momentum angle



$$|\vec{q}| = |\vec{q}'|$$

1. **Select any phonon line out of *n* interval at random**

2. **Use simple exponential in $cos(\theta)$ distribution $\mathcal{P}(\tau'; \nu) \propto exp\{Acos(\theta)\}$ to seed new polar angle θ and use $\varphi = 2\pi\, rndm()$ to seed a new azimutal angle (both relative to a fixed vector $\langle \vec{p} \rangle = (\tau_b - \tau_a)^{-1} \int_{\tau_a}^{\tau_b} \vec{p}\,(\tau)\, d\tau + \vec{q}$.**

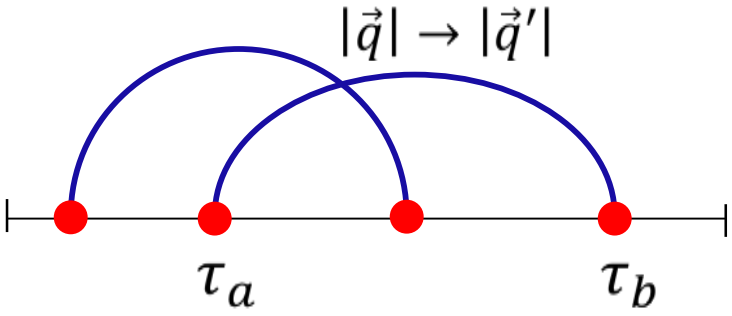
This setup follows from the diagram weight related to the updated interval

$$E = \frac{1}{2m}\left[\int_{\tau_a}^{\tau_b} (\vec{p}(\tau) + \vec{q} - \vec{q}')^2\, d\tau\right] = \boldsymbol{const} + \frac{(\tau_b - \tau_a)}{m}\langle \vec{p} \rangle \vec{q}'$$

Momenta for $q=0$

Always accepted, $\mathbb{R} = 1$

Type A: changing internal momentum modulus



$$\frac{\vec{q}}{|\vec{q}|} = \frac{\vec{q}'}{|\vec{q}'|}$$

1. Select any phonon line out of *n* interval at random

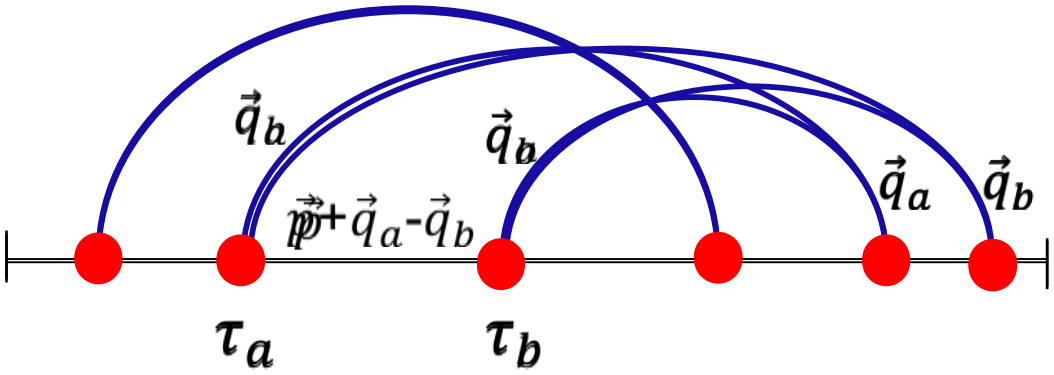
2. Use Gaussian distribution $\mathcal{P}(\tau'; \nu) \propto exp\left\{-\frac{(q\prime - q_0)^2}{s^2}\right\}$ to seed new modulus of momentum transfeer $\boldsymbol{q'}$. Again, this follows from the diagram weight related to the updated interval $E = \frac{1}{2m}\left[\int_{\tau_a}^{\tau_b} (\vec{p}(\tau) + \vec{q} - \vec{q}')^2 \, d\tau\right] = \boldsymbol{const} + \frac{(\tau_b - \tau_a)}{2m}(q' - q_0)^2$

where $q_0 = \langle\vec{p}\rangle\vec{q}/\mathrm{q}$.

For unlimited Gaussian, we simply reject negative values of q' to make sure that q' is always positive we need to use the error function. Either way

Always accepted, $\mathbb{R} = 1$

Type A: changing local "topology"



1. Select any electron interval except the first and last one at random

2. Propose to swap its interaction vertexes places (electron momentum changes from $\vec{p}$ to $\vec{p}' = \vec{p} + \vec{q}_a - \vec{q}_b$)

Acceptance ratio

$$\mathbb{R} = exp\{-(\tau_b - \tau_a)[\varepsilon(\vec{\boldsymbol{p}}') - \varepsilon(\vec{\boldsymbol{p}}) \pm \omega_a \pm \omega_b]\}$$