Diagrammatic Monte Carlo for Fermionic and Fermionized Systems:

“Sign Blessing” vs Sign Problem

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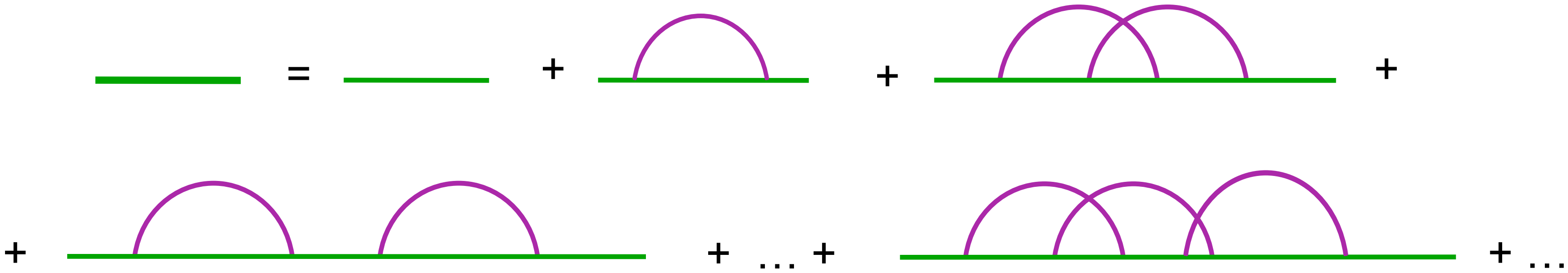
Feynman diagrams

Generic structure of diagrammatic expansions:

$$Q(y) = \sum_{m=0}^{\infty} \sum_{\xi_m} \int D(\xi_m, y, x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m$$

These functions are visualized with diagrams.

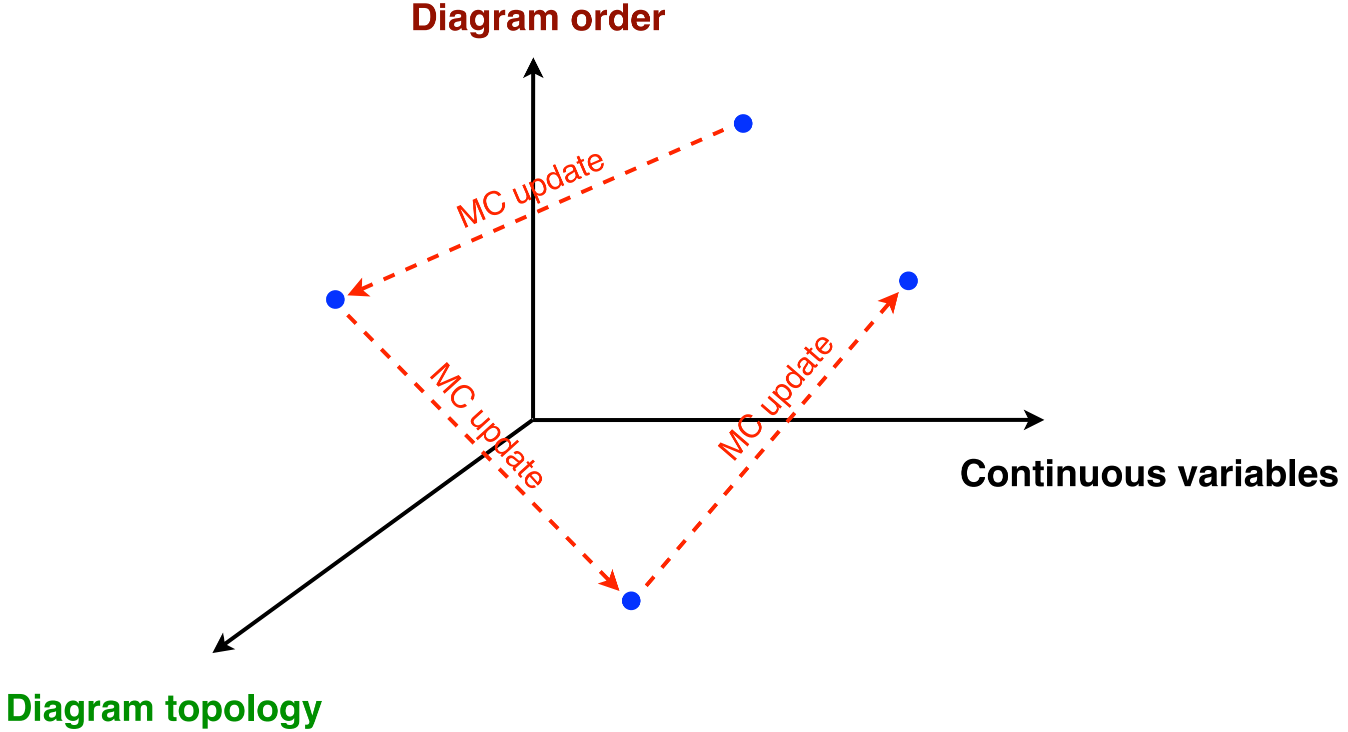
Example:



$Q(y)$ **can be sampled by Monte Carlo**

Diagrammatic MC: Random walk in the diagrammatic space

The space = diagram order + topology + internal/external continuous variables



Not to be confused with the diagram-by-diagram evaluation!

Convergence of the series. Sign blessing

Dyson's collapse as the guiding principle

Dyson's argument (1952): *The perturbative series has* ***zero convergence radius*** *if changing the sign of interaction renders the system pathological.*

A conjecture: ***Finite convergence radius if no Dyson's collapse.***

Pauli principle protects lattice and momentum-truncated fermions from Dyson's collapse.

Resonant Fermions

Hubbard model

Fermionized spin-1/2 on a triangular lattice

Model of Resonant Fermions

(from ultra-cold atoms to neutron stars)

Works whenever $R_0 \ll 1/c$ *, where* R_0 *is the range of interaction.*

No explicit interactions—just the boundary conditions:

$$\forall i,j \quad \text{at} \quad \left|\mathbf{r}_{\uparrow_i} - \mathbf{r}_{\downarrow_j}\right| \to 0: \qquad \Psi\left(\mathbf{r}_{\uparrow 1},\dots,\mathbf{r}_{\uparrow N},\mathbf{r}_{\downarrow 1},\dots,\mathbf{r}_{\downarrow N}\right) \to \frac{A}{\left|\mathbf{r}_{\uparrow_i} - \mathbf{r}_{\downarrow_j}\right|} + B, \qquad \frac{B}{A} = c = \text{const}$$

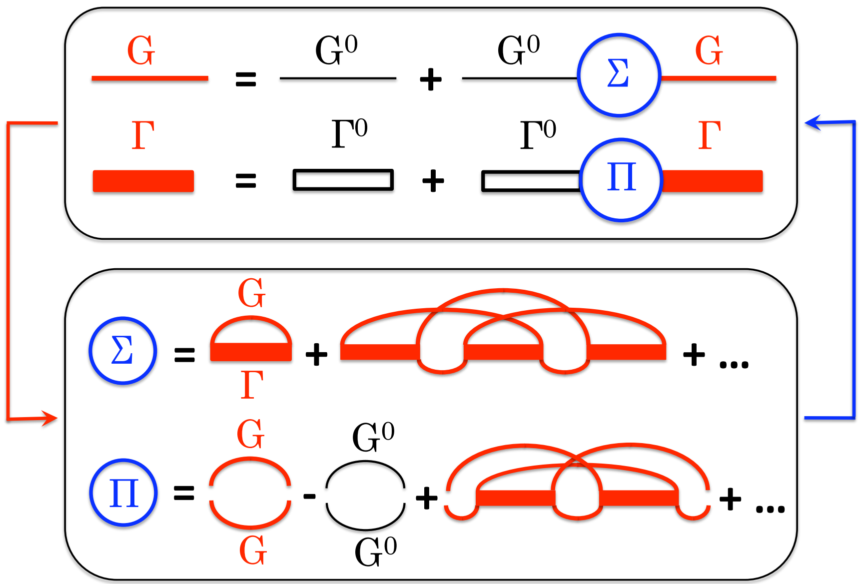
(In the two-body problem, the parameter c defines the s-scattering length: a = -1/c .)

$$c \gg n^{1/3} \sim k_F \quad \Rightarrow$$ BCS regime

$$-c \gg n^{1/3} \sim k_F \quad \Rightarrow$$ BEC regime

$$|c| \sim n^{1/3} \sim k_F \quad \Rightarrow$$ the crossover

$$c = 0 \quad \Rightarrow$$ unitarity point: scale invariance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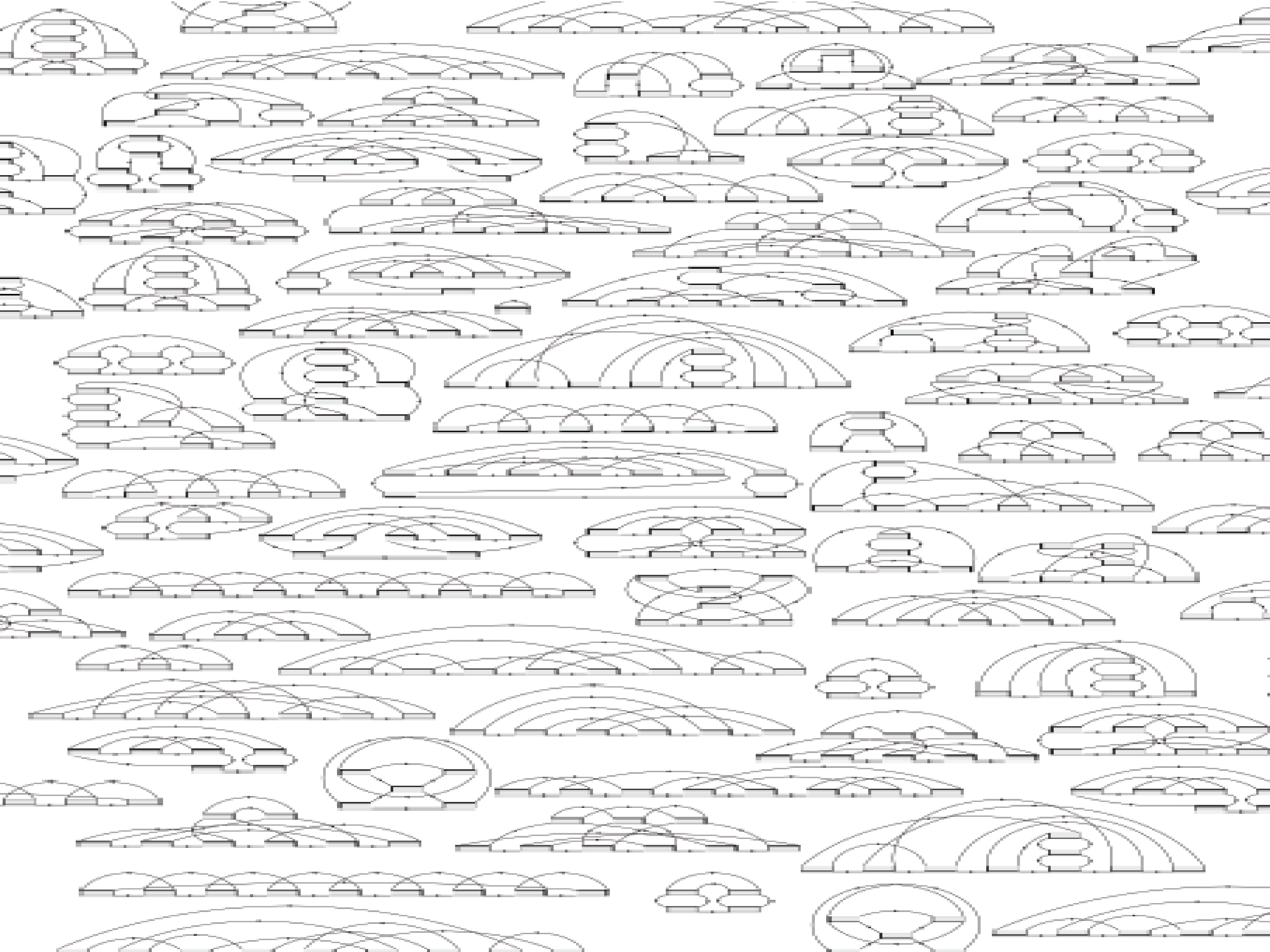
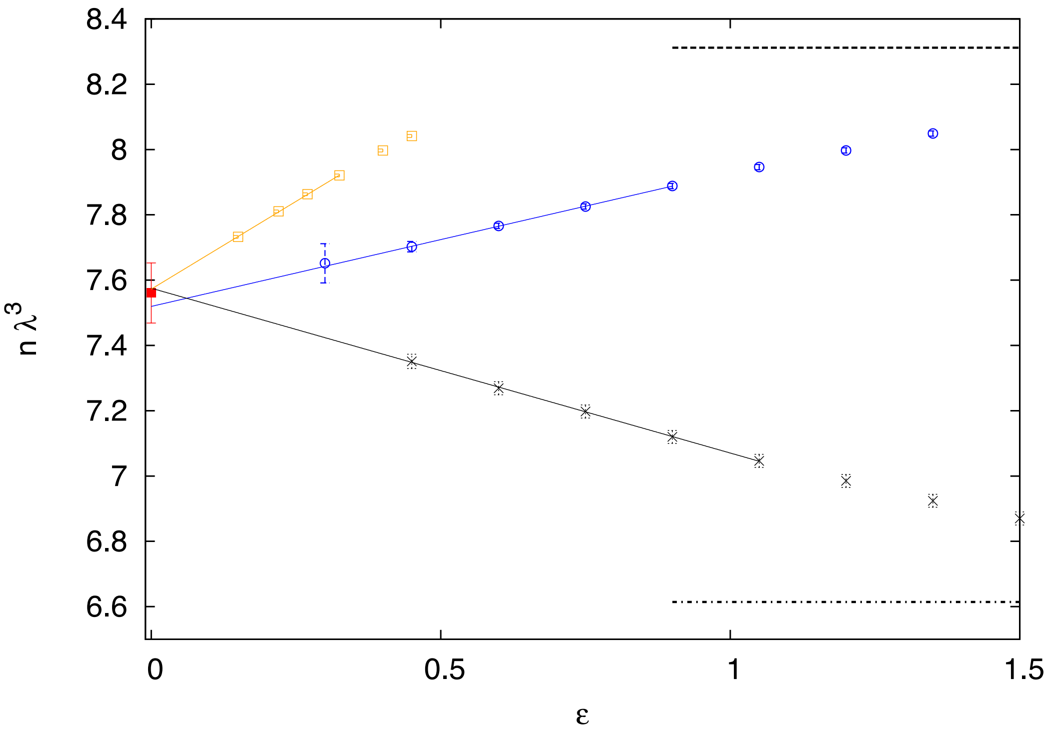
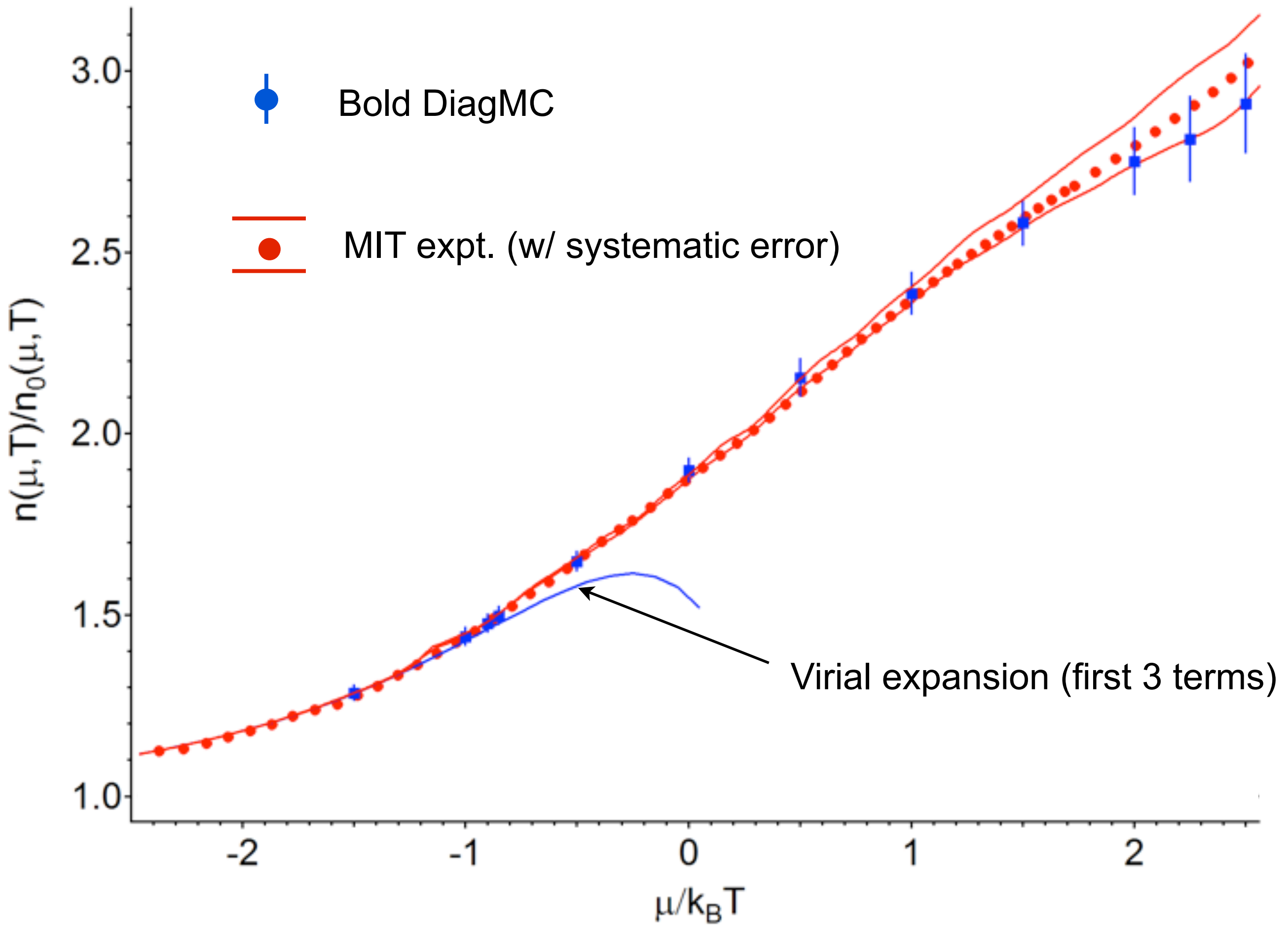


Resummation

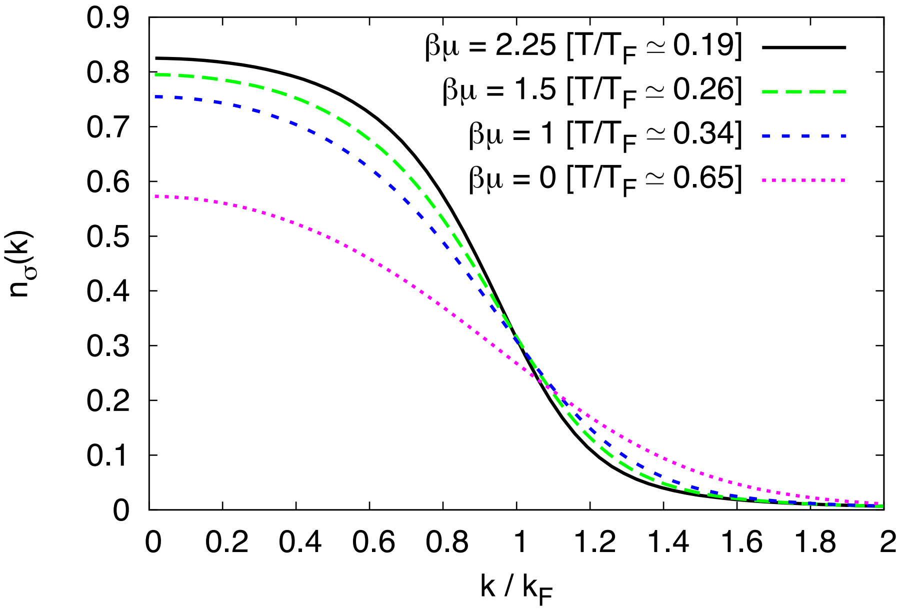


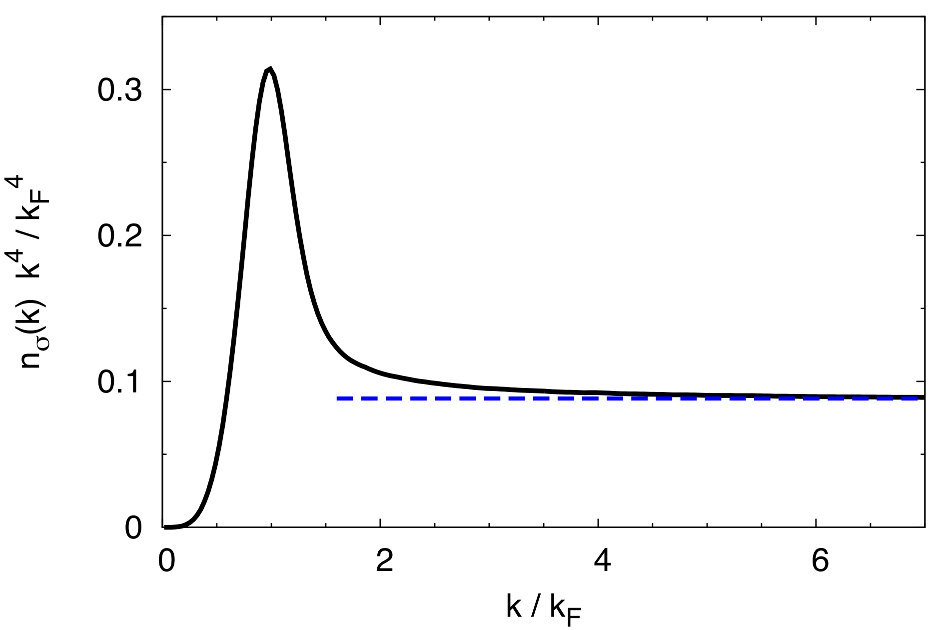
Number density EoS



K. Van Houcke, F. Werner, E. Kozik, N. Prokofev, B. Svistunov, M. Ku, A. Sommer, L. W. Cheuk, A. Schirotzek, and M. W. Zwierlein, Nat. Phys. 8, 366 (2012).

Distribution over momenta



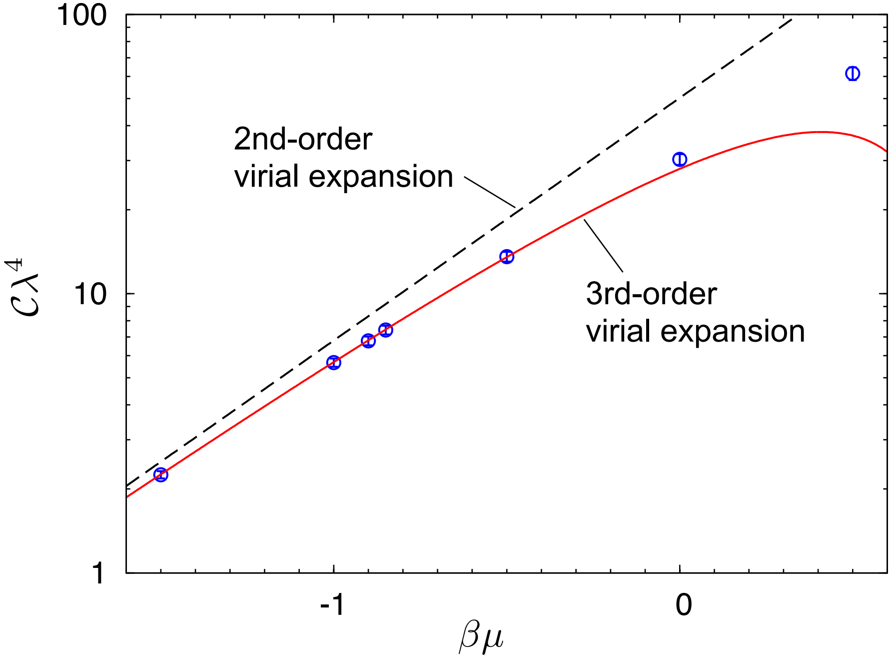


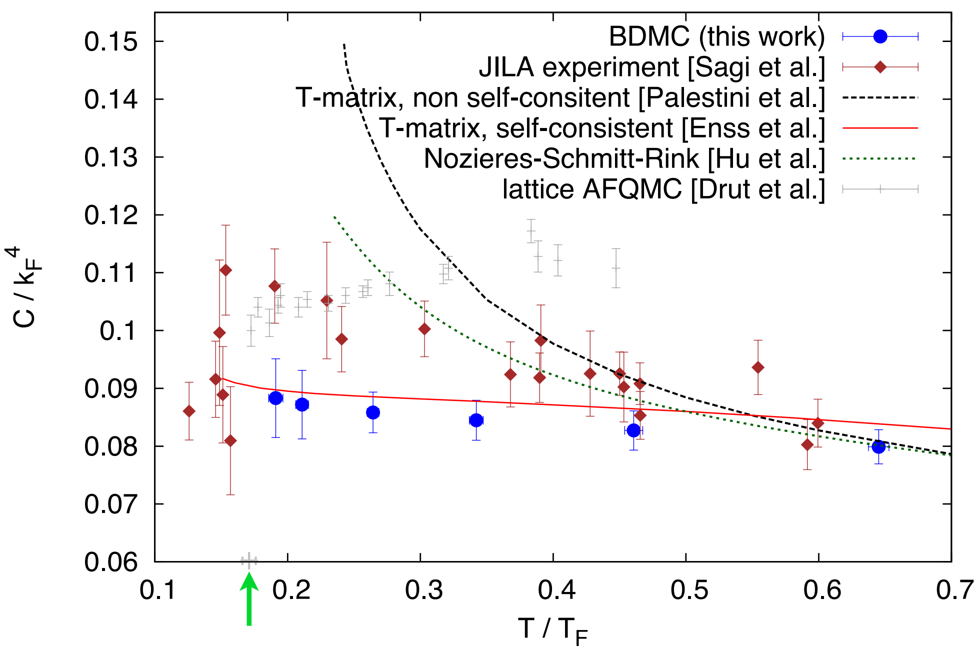
K. Van Houcke, F. Werner, E. Kozik, N. Prokof'ev, and B. Svistunov, arXiv:1303.6245.

Contact parameter

$$\langle \hat{n}_\uparrow(0)\hat{n}_\downarrow(\mathbf{r})\rangle \underset{r\to 0}{\sim} \frac{\mathbf{C}}{(4\pi r)^2}\,, \qquad n_\sigma(\mathbf{k}) \underset{k\to\infty}{\sim} \frac{\mathbf{C}}{k^4}$$

hight-temperature regime





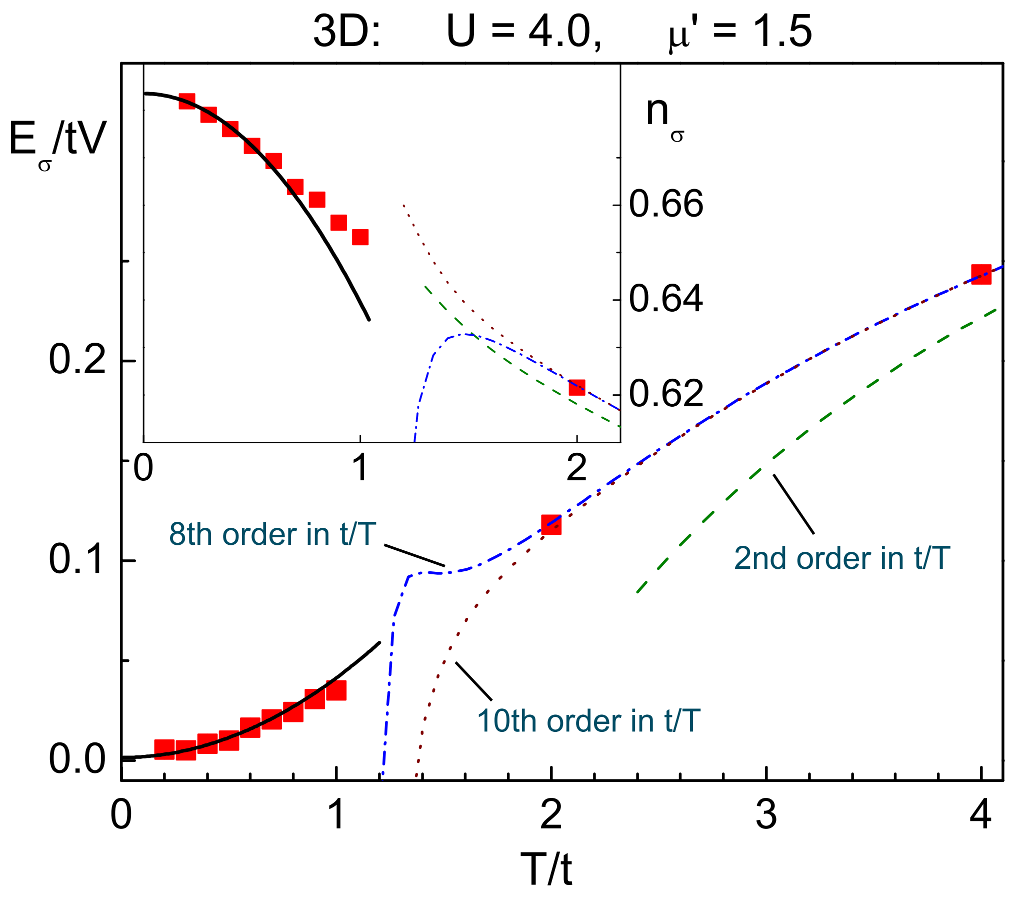
K. Van Houcke, F. Werner, E. Kozik, N. Prokof'ev, and B. Svistunov, arXiv:1303.6245.

Hubbard model

$$H = -t \sum_{\substack{<ij> \\ \sigma=\uparrow,\downarrow}} a^{+}_{\sigma i} a_{\sigma j} + U \sum_{i} n_{\uparrow i} n_{\downarrow i}, \qquad n_{\sigma i} = a^{+}_{\sigma i} a_{\sigma i}$$

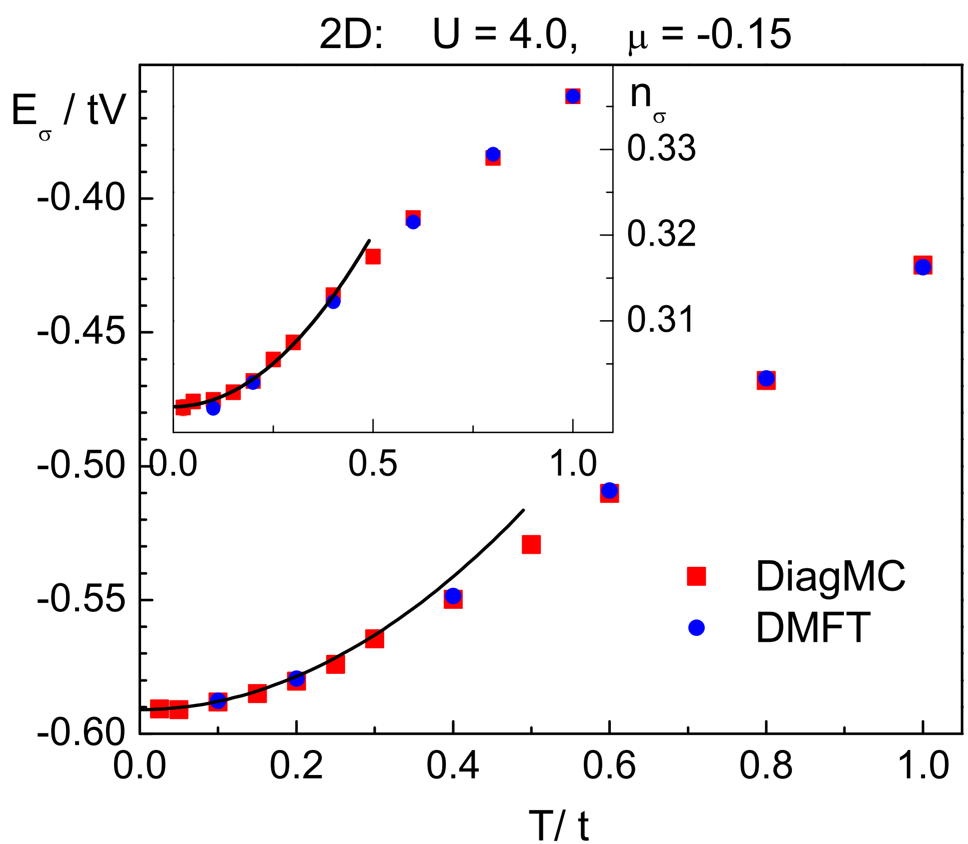
Diagram elements:

DiagMC vs high-temperature series expansion



E. Kozik, K. Van Houcke, E. Gull, L. Pollet, N. Prokof'ev, B. Svistunov, and M. Troyer, EPL **90**, 10004 (2010).

DiagMC vs DMFT

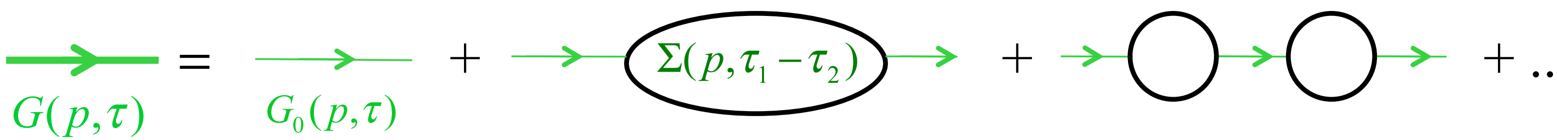


E. Kozik, K. Van Houcke, E. Gull, L. Pollet, N. Prokof'ev, B. Svistunov, and M. Troyer, EPL **90**, 10004 (2010).

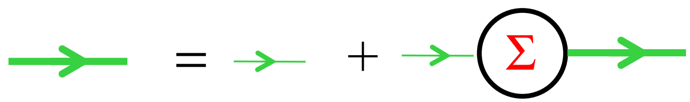
Bold DiagMC for Hubbard Model

Youjin Deng *et al. (in progress)*

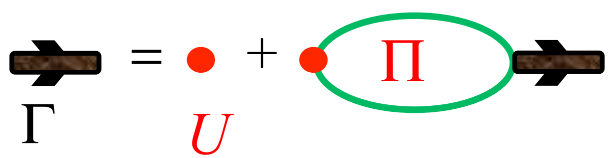
Calculate **irreducible** **diagrams for** Σ **,** Π**, ... to get** G**,** Γ **, ... from Dyson equations**



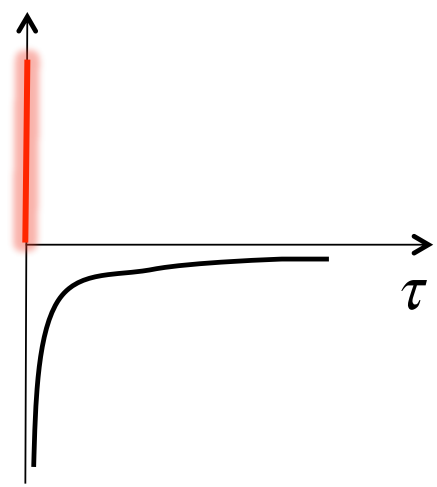
Dyson Equation:



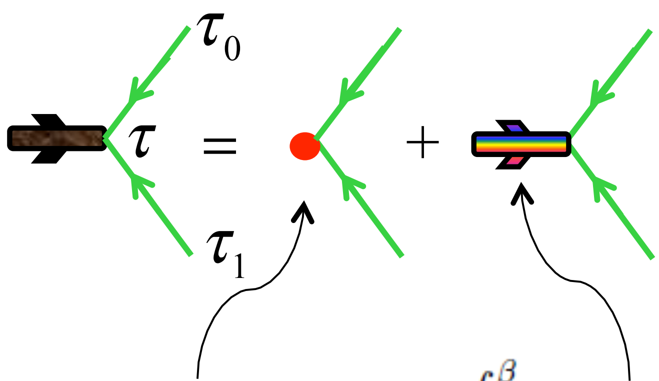
Ladder:
(contact potential)



$$U\delta(t) + \tilde{\Gamma}(t)$$

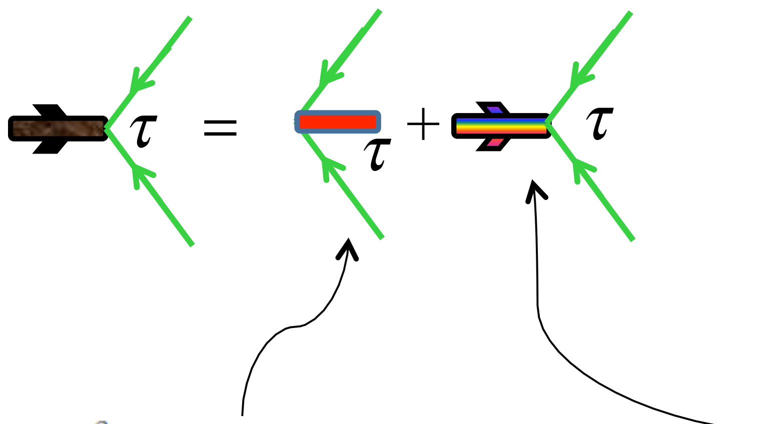


Subtlety of ladder summation in imaginary-time representation



$$A = UG_\uparrow(\tau_0)G_\downarrow(\tau_1) + \int_0^\beta d\tau\ \tilde{\Gamma}(\tau)G_\uparrow(\tau_0-\tau)G_\downarrow(\tau_1-\tau)$$

Define a ``fake" function: $\int_0^\beta d\tau \tilde{\Gamma}_u(\tau) = -U$



$$A \ = \ \int_0^\beta d\tau\ \left[-\tilde{\Gamma}_u(\tau)G_\uparrow(\tau_0)G_\downarrow(\tau_1) + \tilde{\Gamma}(\tau)G_\uparrow(\tau_0-\tau)G_\downarrow(\tau_1-\tau)\right]$$

Pseudo-Bold vs Bold

Presumption of existence of $\Sigma[G]$ may prove wrong!

E. Kozik and A. Georges, 2014

Pseudo-bold expansion is a bare expansion that diagrammatically looks like the bold one: irreducible diagrams only.

(Extra label for the order of expansion of the propagator.)

Popov-Fedotov fermionization trick

Heisenberg model

$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j$$

Dynamical--but not statistical--equivalent

$$H' = J\sum_{\langle ij\rangle} \left(f^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\beta}f_{i\beta}\right)\cdot\left(f^{\dagger}_{j\gamma}\vec{\sigma}_{\gamma\delta}f_{j\delta}\right)$$

Dynamical and statistical equivalent

$$H_{PF} = J\sum_{\langle ij\rangle} \left(f^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\beta}f_{i\beta}\right)\cdot\left(f^{\dagger}_{j\gamma}\vec{\sigma}_{\gamma\delta}f_{j\delta}\right) - \mu\sum_{j\alpha}\left(n_{j\alpha}-1\right), \qquad \mu = i\pi T/2$$

From Popov-Fedotov trick to universal fermionization

N. Prokof'ev and BS, 2011

(i) Treat non-fermionic systems (spins, bosons) as fermions with order-unity coupling.

(ii) The so-called second fermionization: View dublons in the large-U Hubbard model as bosons and then fermionize them. The trick eliminates the large-U problem.

Solution of the form: $$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \mathrm{Tr}\, e^{-\beta \tilde{H}}$$

H is the original Hamiltonian of the system.

$\tilde{H}$ is a ***purely fermionic*** non-Hermitian pseudo-Hamiltonian with ***order-unity couplings***.

Popov-Fedotov case (spin-1/2):

$$\tilde{H} = H + \sum_j H_*^{(j)}, \qquad H_*^{(j)} = \frac{i\pi T}{2}\left[n_{j\uparrow} + n_{j\downarrow} - 1 \right]$$

General principle: *Trace over non-physical states of each site factorizes and nullifies.*

$$H_{\text{intersite}} = \sum_{i \neq j} \sum_{\alpha,\beta,\gamma,\delta} \Lambda^{ij}_{\alpha,\beta,\gamma,\delta} Q^{(i)}_{\alpha\to\beta} Q^{(j)}_{\gamma\to\delta}$$

$$Q^{(i)}_{\alpha\to\beta} = A^{(i)}_{\alpha\to\beta} P^{(i)}_{\alpha}, \qquad Q^{(i)}_{m\to l} = f^{\dagger}_{il} f_{im} \prod_{k\neq m,l} (1 - n_{ik})$$

$A^{(i)}_{\alpha\to\beta}$: changes the state of the *i*-th site

$P^{(i)}_{\alpha}$: corresponding projector

typical example

$$H_*^{(j)} = T\tilde{\mu}\,(\hat{n}_j - 1), \qquad \hat{n}_j = \sum_m n_{jm}$$

Employing projectors onto non-physical states

$$H_*^{(j)} = T \sum_{\bar{\alpha}} \ln(w_{\bar{\alpha}}) P_{\bar{\alpha}}^{(j)}, \qquad \sum_{\bar{\alpha}} w_{\bar{\alpha}} = 0$$

sum over non-physical states

projector onto a particular non-physical state

Employing auxiliary fermionic mode

$$H_*^{(j)} = i\pi T \, P_*^{(j)} \, \tilde{n}_j$$

projector onto non-physical sector

occupation number of the auxiliary fermion

Universal fermionization of spins and bosons; second fermionization.

Advantages:

(i) Feynman diagrammatics with finite convergence radius

(ii) All couplings are order unity (crucial for Diagrammatic Monte Carlo)

Price:

(i) Projected hoppings (many-particle couplings)

(ii) Multi-componentness

On-going projects

Resonant fermions with broken U(1) symmetry

Cooper pairing in Hubbard model at moderate fillings: Fermi liquid+BCS regime

Boldification of the vertex for spins

Dynamic problems for Fermi polaron (by pseudo-bold DiagMC in real time)

Plan for near future

t-J and Hubbard models by second fermionization