Sign Problems and Complex Actions, ECT*, Trento, March 2-6, 2009

Diagrammatic Monte Carlo

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Sign PROBLEM and Sign PROBLEM

Extensive configurational space

$$\text{Complexity} \propto e^{V/V_0}$$

V is the configuration volume

V_0 is the correlation volume

$$V/V_0 \sim 10^2$$

Diagrams (intensive configurational space)

$$\text{Complexity} = C\,(N!)^m$$

$N \lesssim 10$ is the diagram order

$$m \sim 1, \qquad C \sim 1$$

C can be significantly reduced by partial summation

The issue of summability: Can an asymptotic series be regularized?

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

BUT

1. Fermions can be put on a lattice…

2. Bosons can be represented as pairs of fermions…

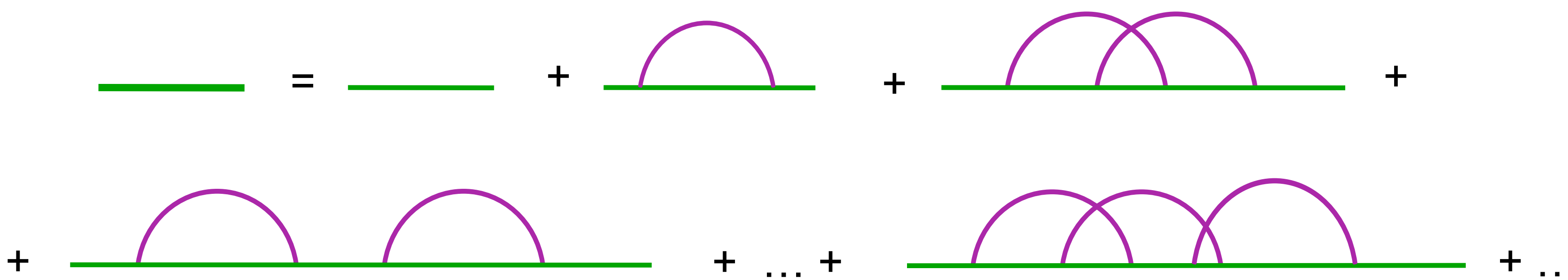
Feynman's Diagrams

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.

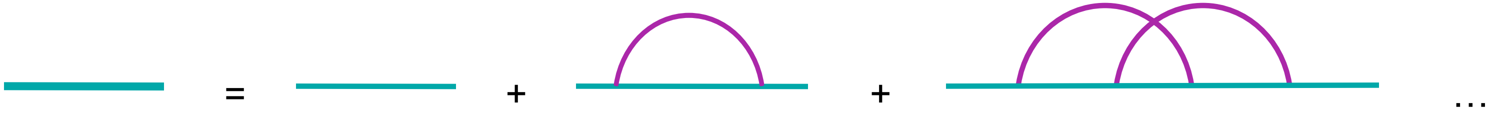
Example:



General principles of Diagrammatic Monte Carlo

Prokof'ev and Svistunov, PRL 81, 2514 (1998)

Take a diagrammatic series, say the one for polaron Green's function,



and interpret it as a partition function for an ensemble of graphical objects (diagrams).
Introduce a Markov process generating ensemble, and calculate corresponding histograms/ averages.

The Markov process is organized in the form of pairs of complementary updates.
In such a pair, A-B, the update A creates a new graphical element with corresponding continuous variables, while the update B removes the element. For example, A creates a new propagator, while B removes it:

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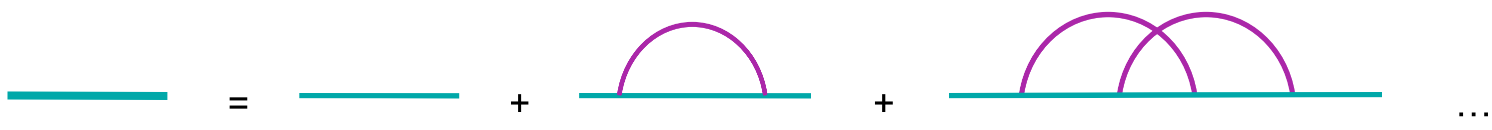

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Balancing diagrammatic Markov process by (generalized) Metropolis-Hastings algorithm

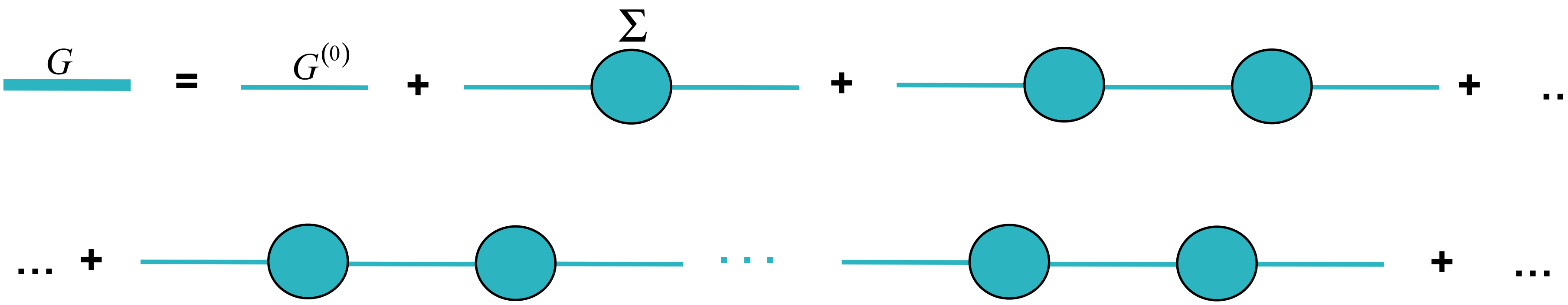
Acceptance ratios for complementary updates A-B

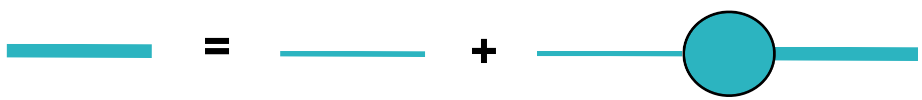
$$R_A\left(\vec{X}\right) = \frac{New\ Diagram}{Old\ Diagram}\,\frac{1}{W\left(\vec{X}\right)}$$

$$R_B\left(\vec{X}\right) = \frac{New\ Diagram}{Old\ Diagram}\,W\left(\vec{X}\right)$$

Arbitrary distribution function for generating particular values of new continuous variables in the update A

Numerical counterpart of analytic bold-line trick: Bold(-line) Diagrammatic Monte Carlo





$$G = G^{(0)} + G^{(0)} \Sigma G$$

Dyson equation

Self-consistent determination of *G*

The Monte Carlo process is *asymptotically* Markovian

Model of Resonant Fermions

(Good for both ultracold atoms and neutron stars!)

No explicit interactions—just the boundary condition:

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

Works whenever $R_0 \ll 1/c$

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

$$|c| \ll n^{1/3} \sim k_F \quad \Rightarrow$$ unitarity regime

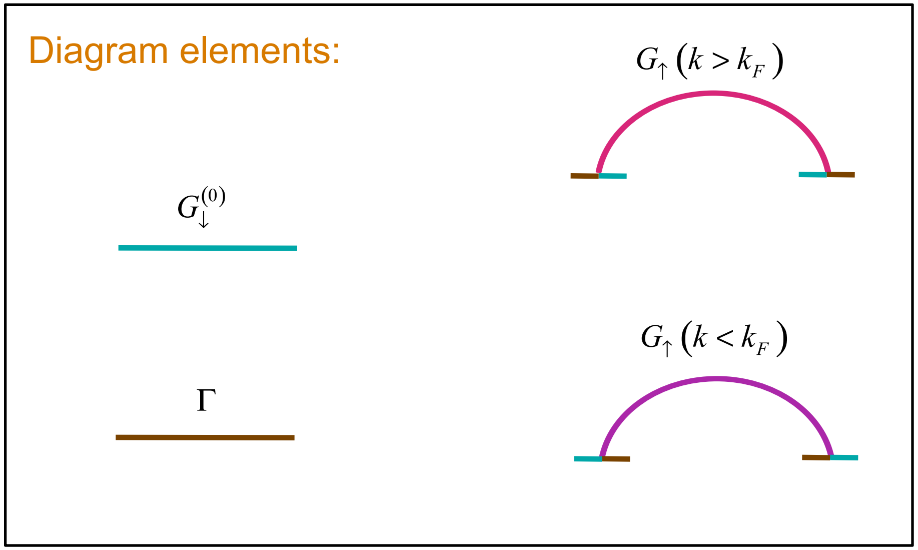
$$-c \gg n^{1/3} \sim k_F \quad \Rightarrow$$ BEC regime

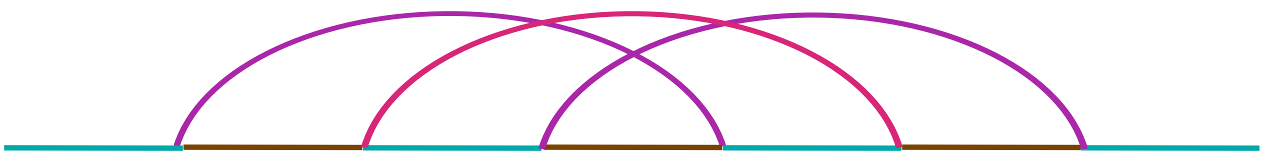
(In two-body problem, the parameter c defines the s-scattering length.)

Resonant Fermipolaron:

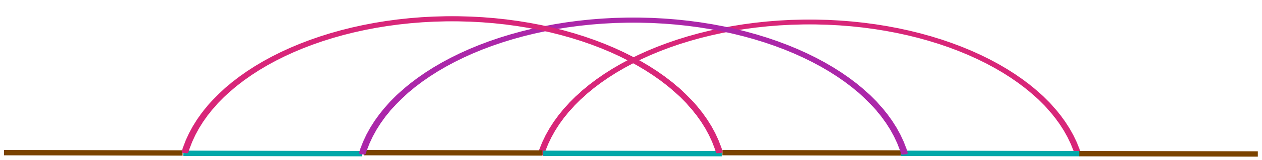
Sign alternating divergent series

Prokof'ev and Svistunov, 2007.



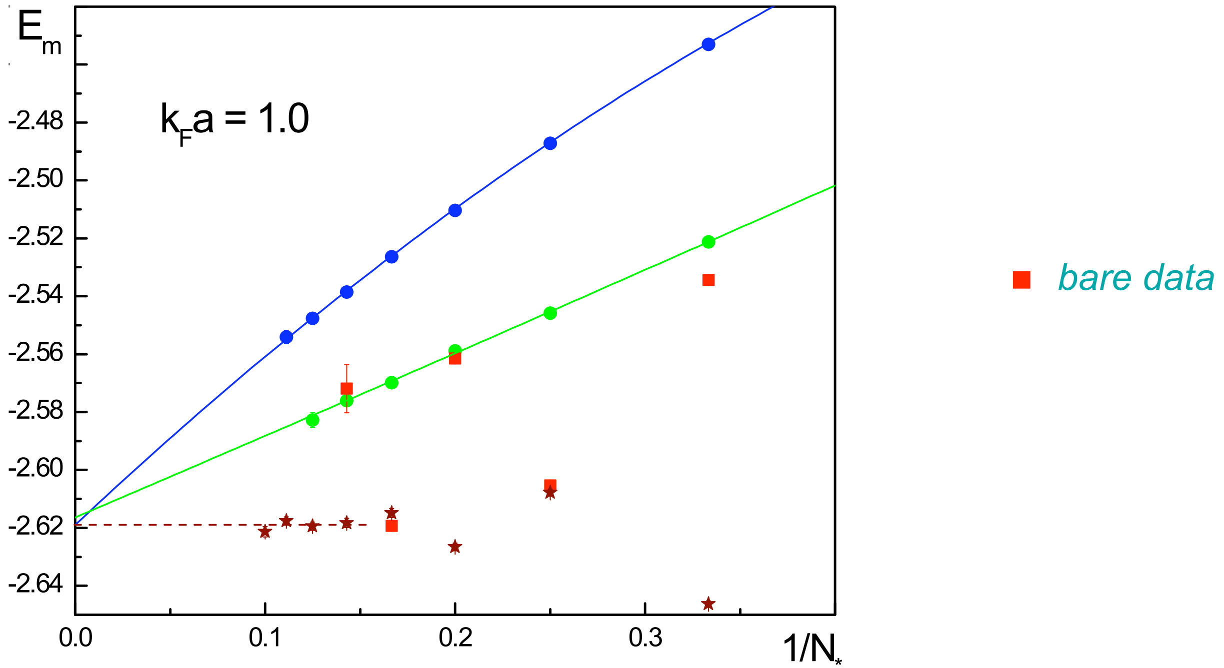


a polaron diagram



a molecule diagram

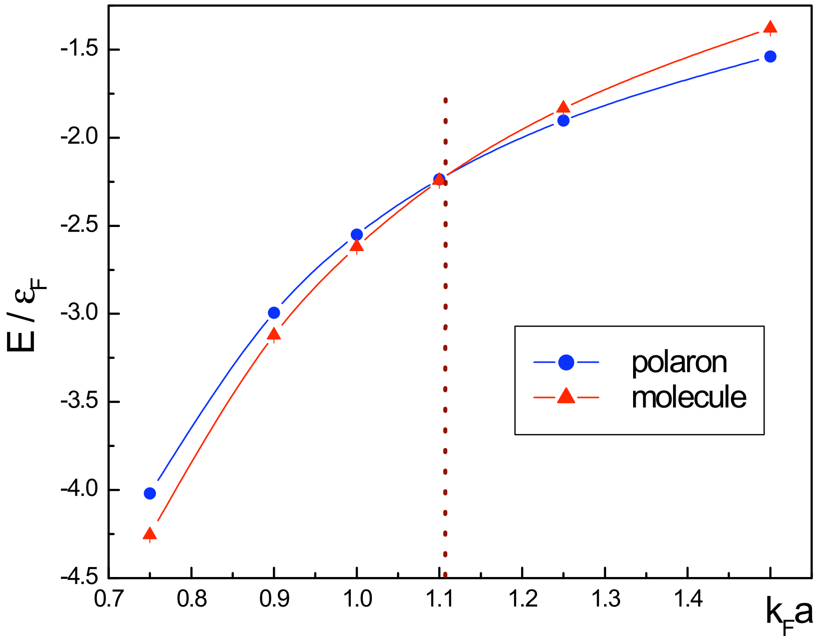
Summability of the divergent series



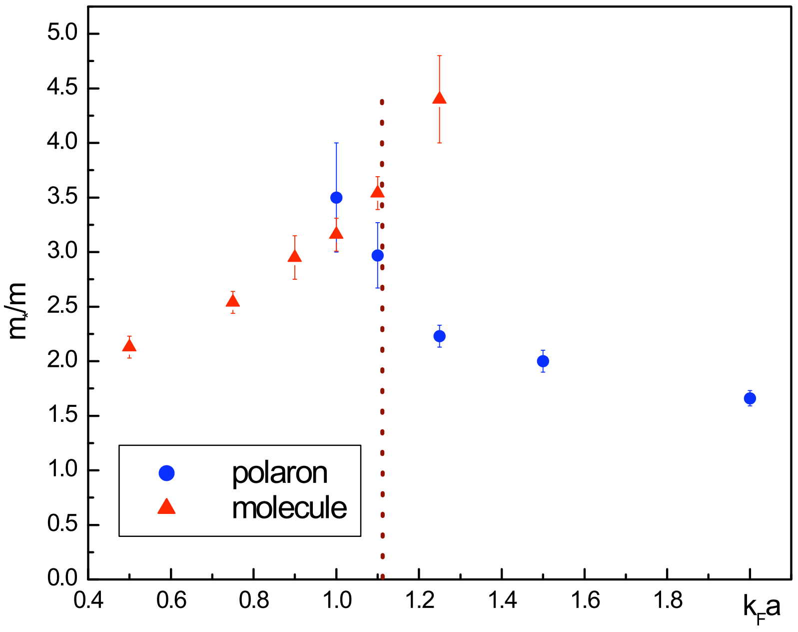
Energy as a function of cutoff parameter for various summation schemes

Answers for fermipolaron

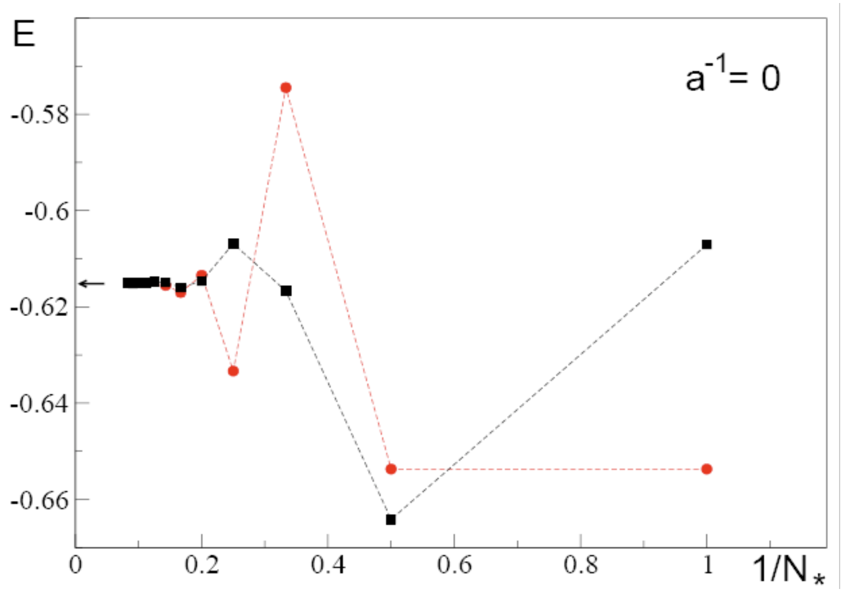
Energy



Effective Mass



Fermipolaron Energy by Bold Diagrammatic Monte Carlo



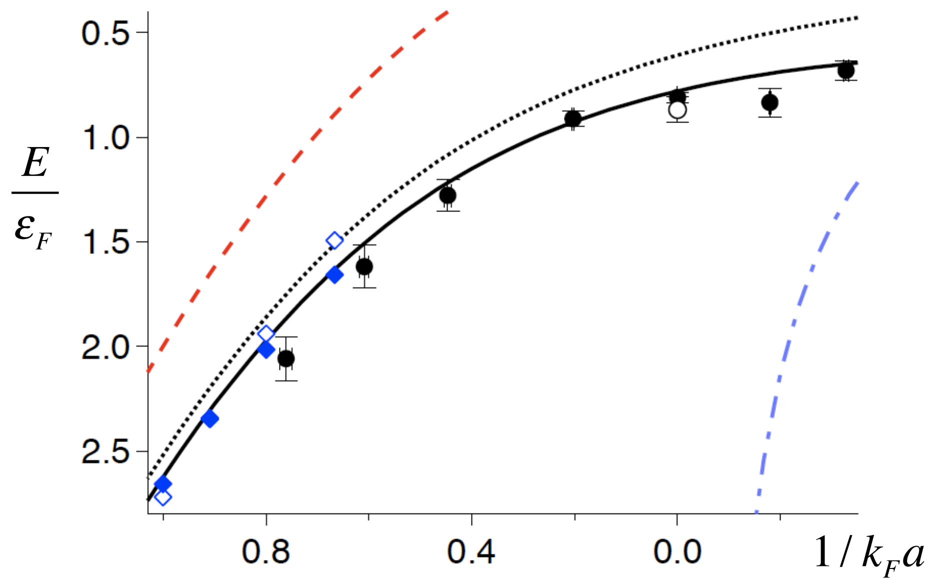
- ■ Polaron lines are bold, molecule lines are not.
- ■ Both polaron and molecule lines are bold.

Prokof'ev and Svistunov, PRB, 2008.

Observation of Fermi Polarons in a Tunable Fermi Liquid of Ultracold Atoms

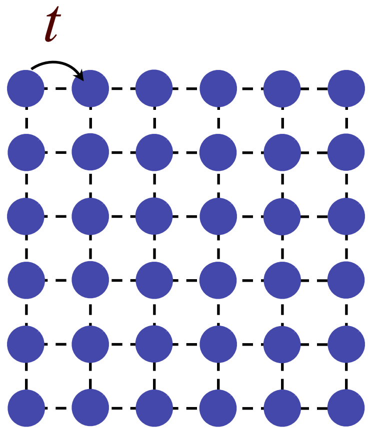
André Schirotzek, Cheng-Hsun Wu, Ariel Sommer, and Martin W. Zwierlein
Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

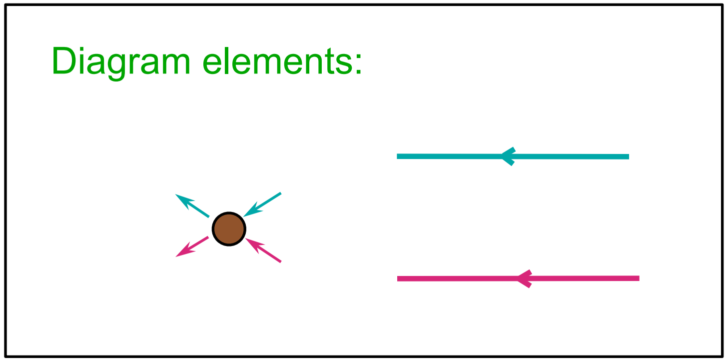
arXiv: 0902.302



Hubbard model

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





Some Results for the Hubbard Model

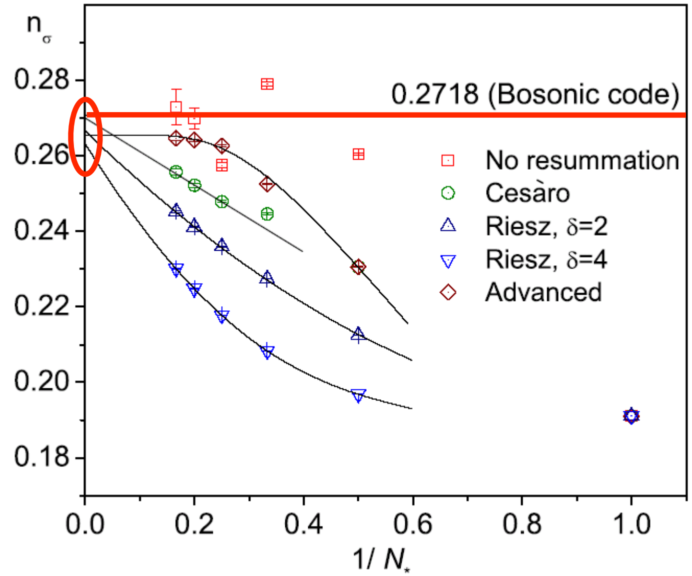
1D

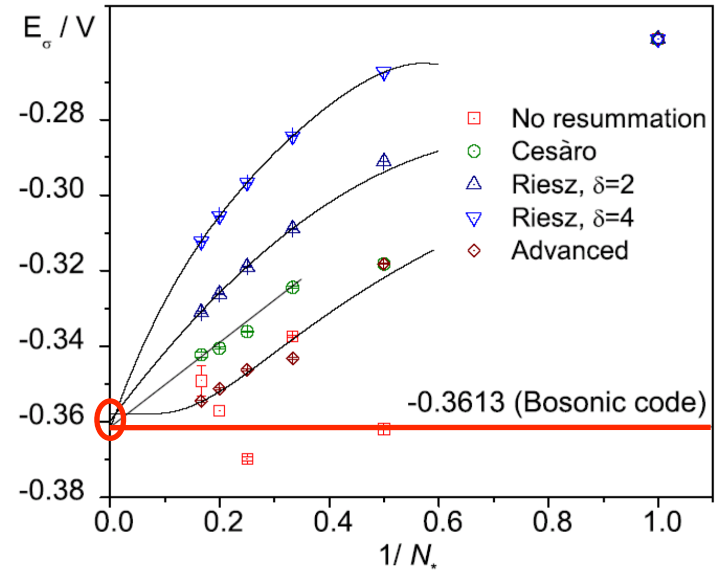
$t = 1.0$

$U = 4.0$

$\mu = -0.5$

$T = 0.3$





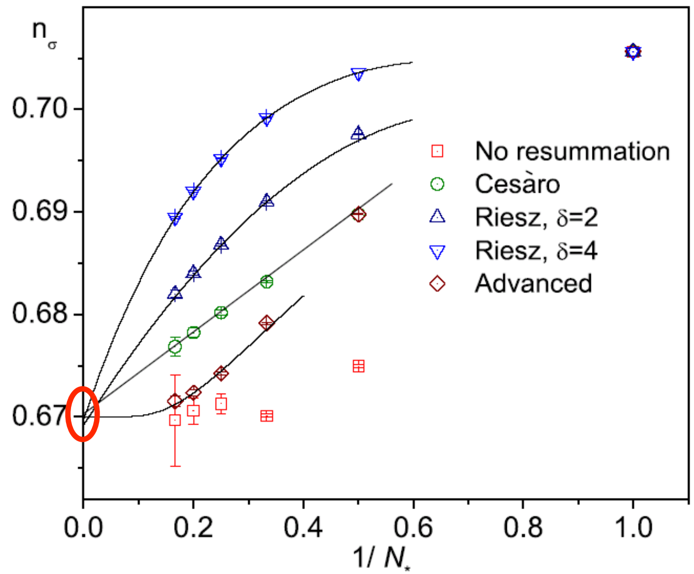
3D

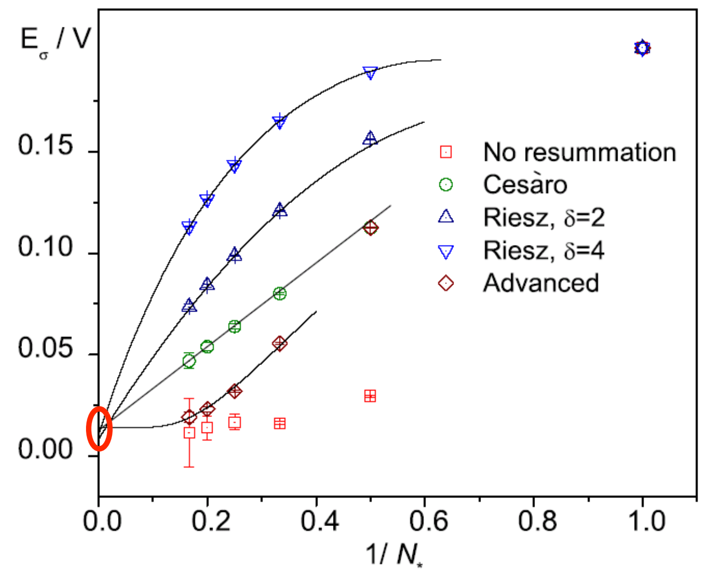
$t = 1.0$

$U = 4.0$

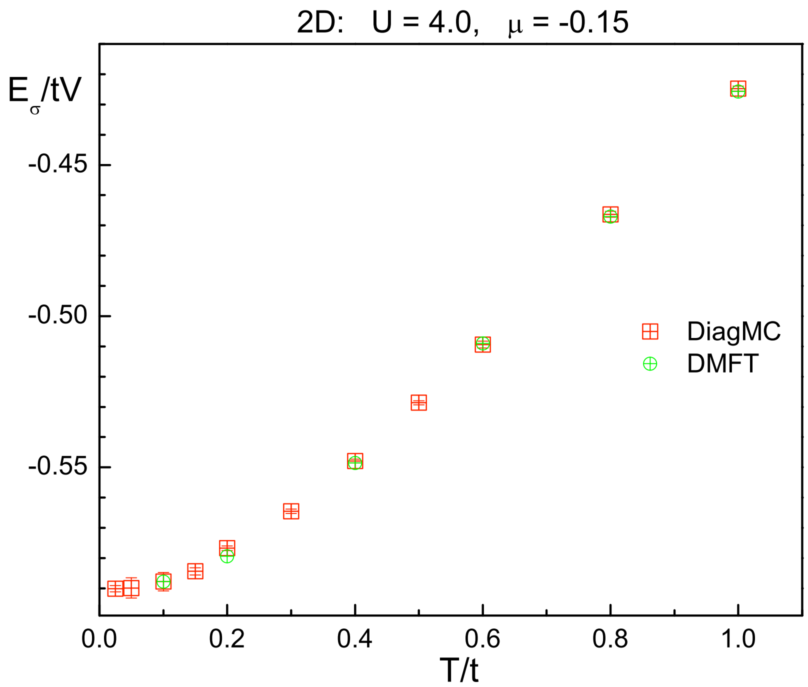
$\mu = 1.5$

$T = 0.5$

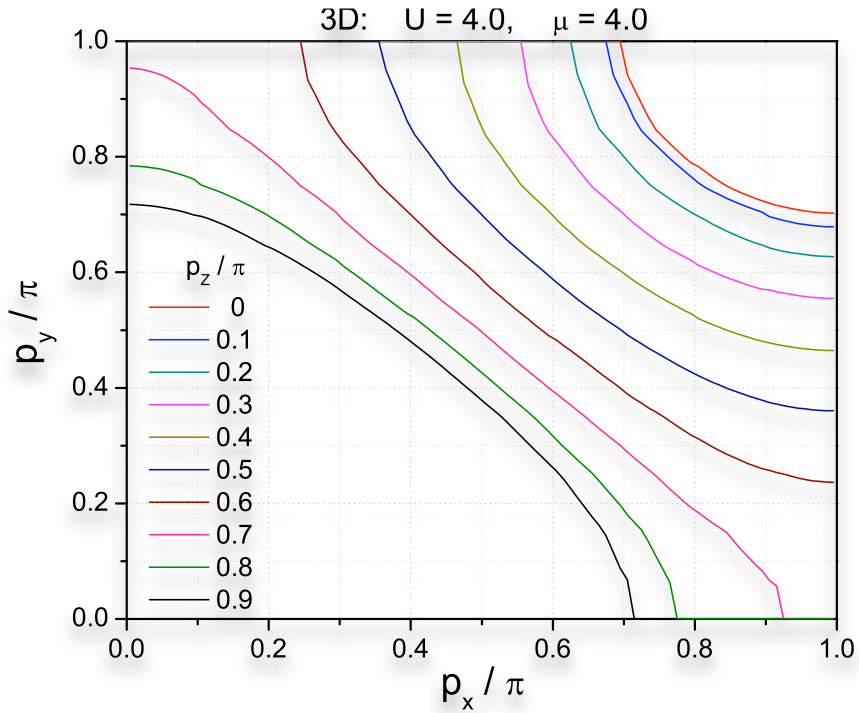




Energy per lattice site



Fermi surface



Resonant Fermions at unitarity: Equation of State