Diagrammatic Monte Carlo. Homotopic Expansions

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The Future of Neutron Rich Matter: From Neutron Skins to Neutron Stars

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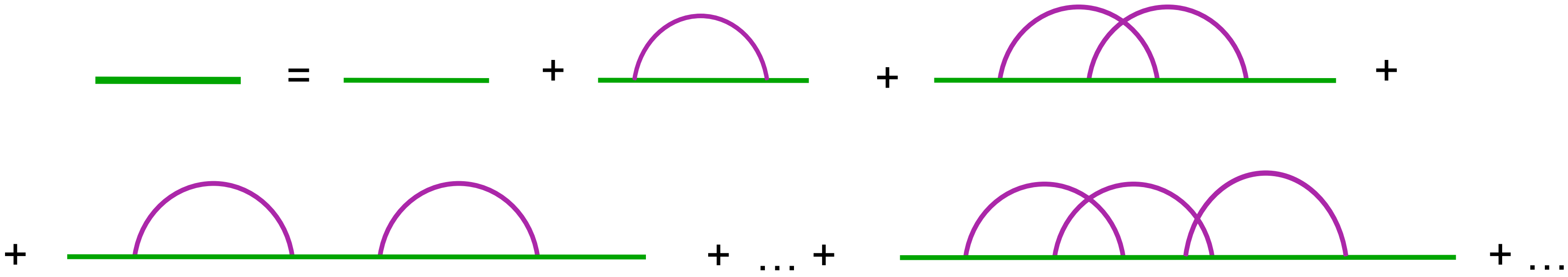
Feynman diagrams

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:

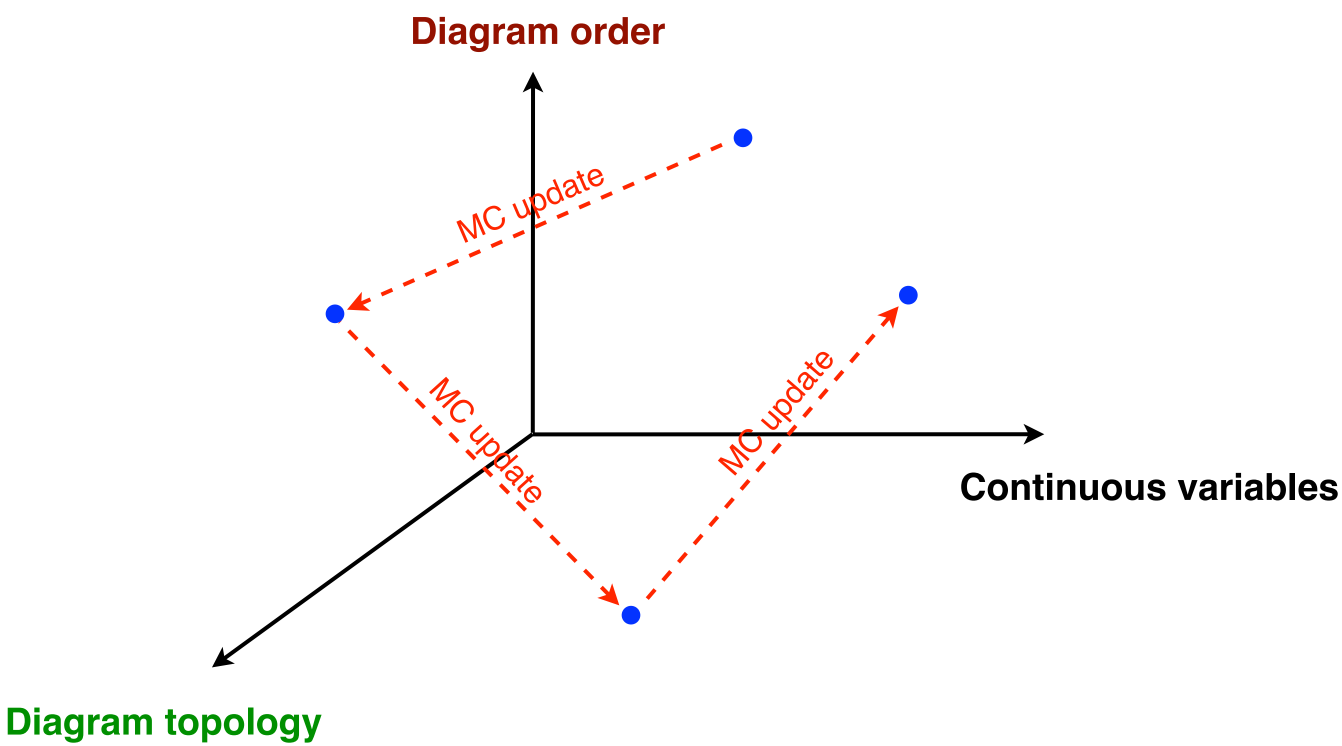


$Q(y)$ ***can be sampled by Monte Carlo***

Diagrammatic MC: Random walk in the diagrammatic space

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

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



Convergence of the series. Fermionic sign blessing

Q. How can a series with *factorially* growing number of diagrams within a given order converge?

A. *Fermionic sign blessing*: Factorially accurate cancellation of different diagrams within a given order.

But why should we expect the miracle of the fermionic sign blessing ?...

Dyson's collapse as the guiding principle

Dyson's argument (1952): *A 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.

Computational complexity of diagrammatic Monte Carlo

Rossi, Prokof'ev, Svistunov, Van Houcke, and Werner, EPL 118, 10004 (2017)

$t(\varepsilon)$ the computational time needed to achieve the relative accuracy ε

$t(\varepsilon) \sim \varepsilon^{-\#\ln(\ln \varepsilon^{-1})}$ with standard DiagMC: ***quasi-polynomial***

$t(\varepsilon) \sim \varepsilon^{-\alpha}$ with Rossi's determinant trick: ***polynomial***

Rossi, PRL, 119, 045701 (2017)

Model of Resonant Fermions

from ultra-cold atoms to (dilute) neutron matter

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

No explicit interactions—just the boundary conditions:

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

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

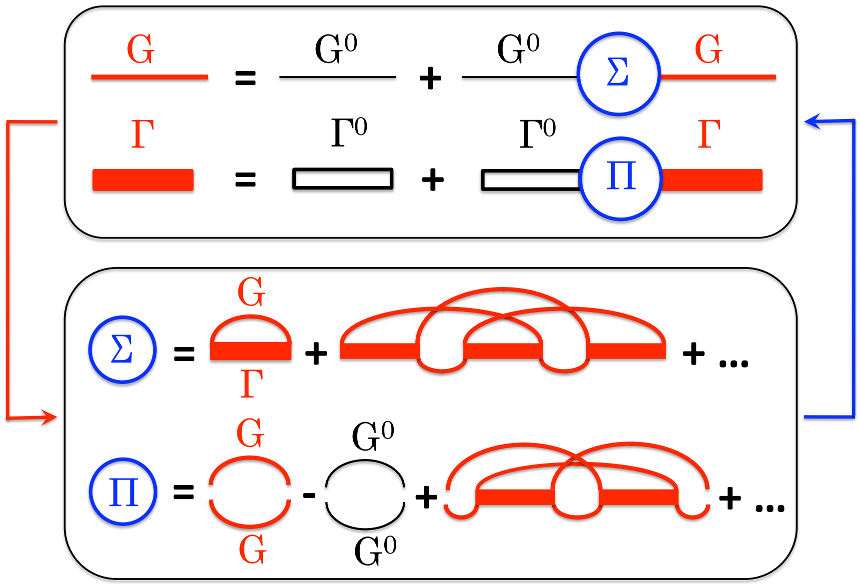
$$c \gg n^{1/3} \sim k_F \quad \Rightarrow$$ BCS regime

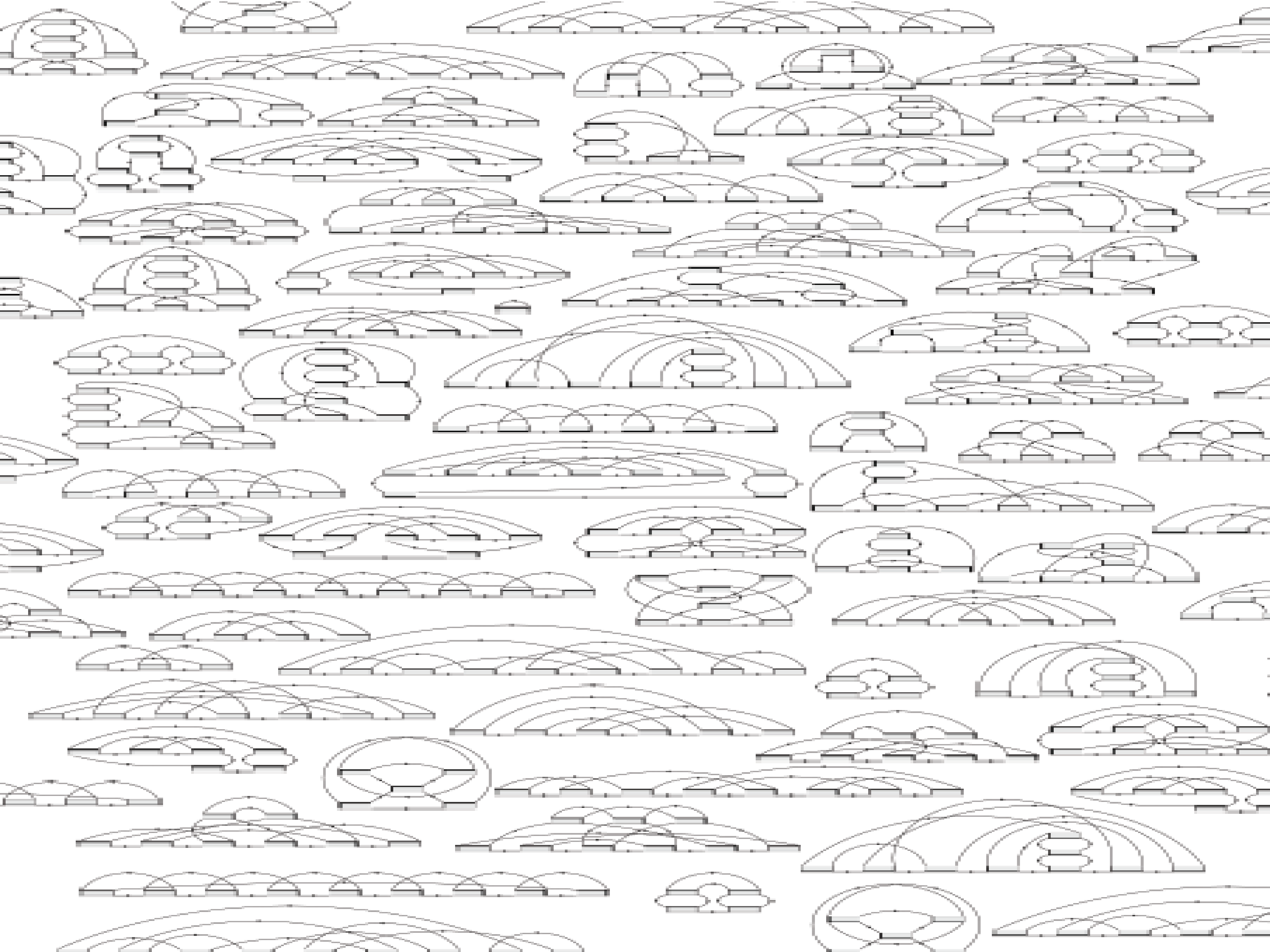
$$-c \gg n^{1/3} \sim k_F \quad \Rightarrow$$ BEC regime

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

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

Bold Diag MC protocol





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nature physics

Feynman diagrams versus Fermi-gas Feynman emulator

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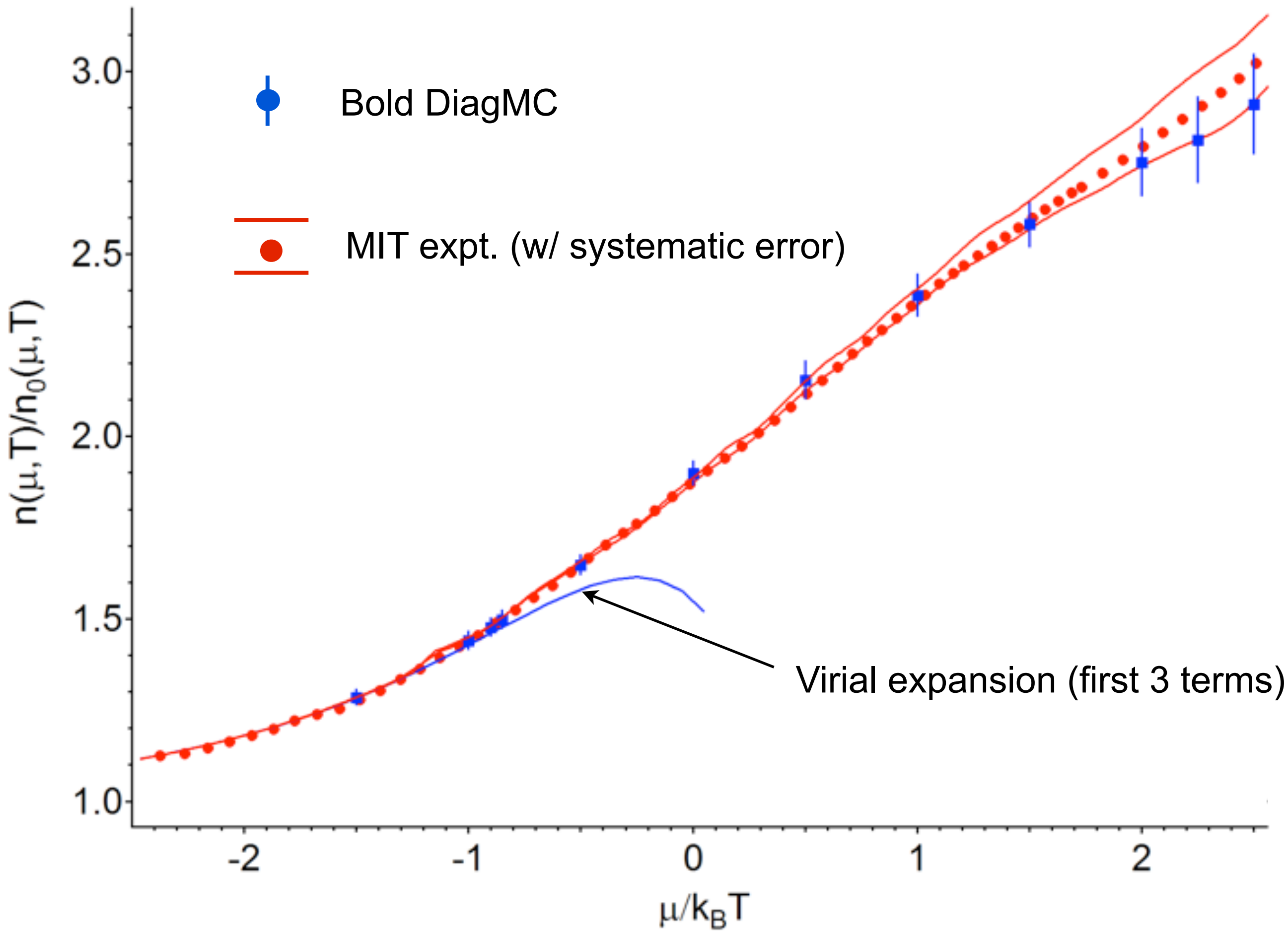
Precise understanding of strongly interacting fermions, from electrons in modern materials to nuclear matter, presents a major goal in modern physics. However, the theoretical description of interacting Fermi systems is usually plagued by the intricate quantum statistics at play. Here we present a cross-validation between a new theoretical approach, bold diagrammatic Monte Carlo[1-3], and precision experiments on ultracold atoms. Specifically, we compute and measure, with unprecedented precision, the normal-state equation of state of the unitary gas, a prototypical example of a strongly correlated fermionic system[4-6]. Excellent agreement demonstrates that a series of Feynman diagrams can be controllably resummed in a non-perturbative regime using bold diagrammatic Monte Carlo.

In his seminal 1981 lecture[7], Richard Feynman argued that an arbitrary quantum system cannot be efficiently simulated with a classical universal computer, because generally, quantum statistics can only be imitated with a classical theory if probabilities are replaced with negative (or complex) weighting factors. For the majority of many-particle models this indeed leads to the so-called sign problem, which has remained an insurmountable obstacle. According to Feynman, the only way out is to employ computers made out of quantum-mechanical elements[7]. The recent experimental breakthroughs in cooling, probing and controlling strongly interacting quantum gases prompted a challenging effort to use this new form of quantum matter to realize Feynman's emulators of fundamental microscopic models[7,8]. Somewhat ironically, Feynman's arguments, which led him to the idea of emulators, may be defied by a theoretical method that he himself devised, namely Feynman diagrams. This technique organizes the calculation of a given physical quantity as a series of diagrams representing all the possible ways particles can propagate and interact (for example, ref. 9). For the many-body problem, this with zero-range interactions at infinite scattering length[4-6]. This system offers the unique possibility to stringently test our theory against a quantum emulator realized here with trapped ultracold ^{6}Li atoms at a broad Feshbach resonance[4-6]. This experimental validation is indispensable for our theory, based on resummation of a possibly divergent series: although the physical answer is shown to be independent of the applied resummation technique—suggesting that the procedure is adequate—its mathematical validity remains to be proven. In essence, nature provides the 'proof'. This presents the first—although long-anticipated—compelling example of how ultracold atoms can guide new microscopic theories for strongly interacting quantum matter.

At unitarity, the disappearance of an interaction-imposed length scale leads to scale invariance. This property renders the model relevant for other physical systems such as neutron matter. It also makes the balanced (that is, spin-unpolarized) unitary gas ideally suited for the experimental high-precision determination of the equation of state (EOS) described below. Finally, it implies the absence of a small parameter, making the problem notoriously difficult to solve.

In traditional Monte Carlo approaches, which simulate a finite piece of matter, the sign problem causes an exponential increase of the computing time with system size and inverse temperature. In contrast, BDMC simulates a mathematical answer in the thermodynamic limit. This radically changes the role of the fermionic sign. Diagrammatic contributions are sign-alternating with order, topology and values of internal variables. Because the number of graphs grows factorially with diagram order, a near-cancellation between these contributions is actually necessary for the series to be resummable by techniques requiring a finite radius of convergence. We find that this 'sign blessing' indeed takes place.

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).

PHYSICAL REVIEW LETTERS **121,** 130405 (2018)

Resummation of Diagrammatic Series with Zero Convergence Radius for Strongly Correlated Fermions

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We demonstrate that a summing up series of Feynman diagrams can yield unbiased accurate results for strongly correlated fermions even when the convergence radius vanishes. We consider the unitary Fermi gas, a model of nonrelativistic fermions in three-dimensional continuous space. Diagrams are built from partially dressed or fully dressed propagators of single particles and pairs. The series is resummed by a conformal-Borel transformation that incorporates the large-order behavior and the analytic structure in the Borel plane, which are found by the instanton approach. We report highly accurate numerical results for the equation of state in the normal unpolarized regime, and reconcile experimental data with the theoretically conjectured fourth virial coefficient.

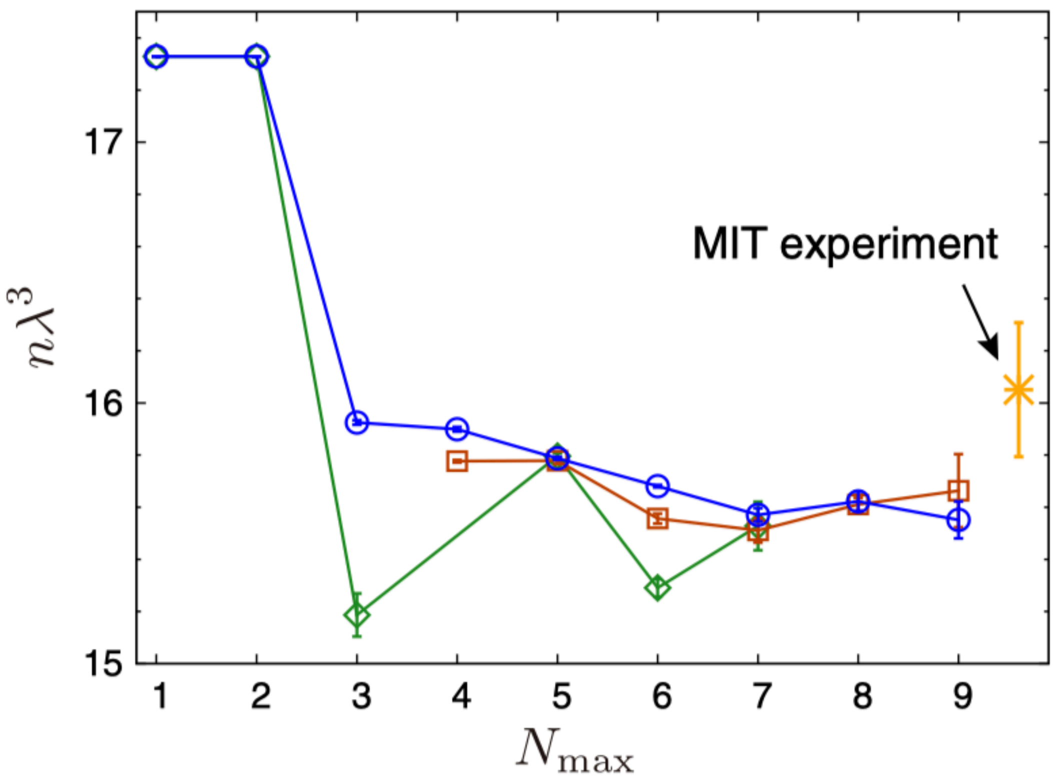

FIG. 4. Density vs maximal diagram order at $\beta\mu = 2$ ($T/T_F \approx 0.2$). The bold diagrammatic series is resummed by three variants of the conformal-Borel transformation (see text).

R. Rossi, T. Ohgoe, K. Van Houcke, and F. Werner, PRL **121**, 130405 (2018)

Non-Fermi-liquid behavior of unitary Fermi gas

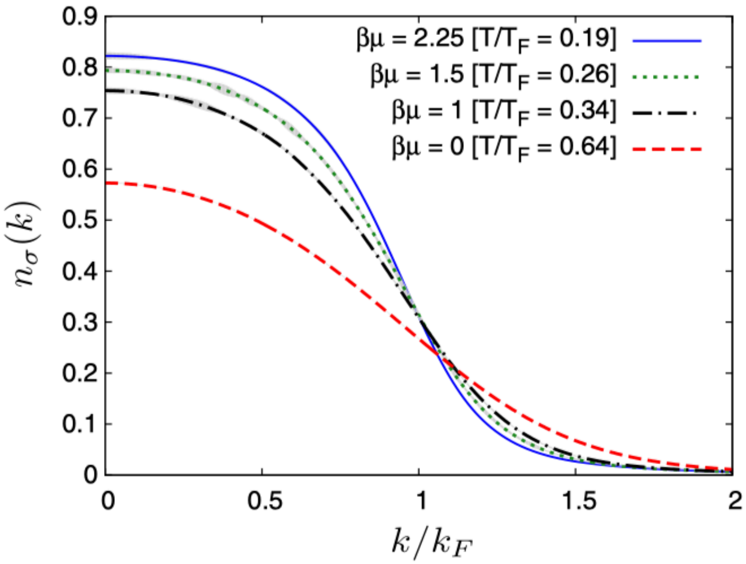

FIG. 5. BDMC data for the momentum distribution at various temperatures. Error bars are represented by the gray error bands.

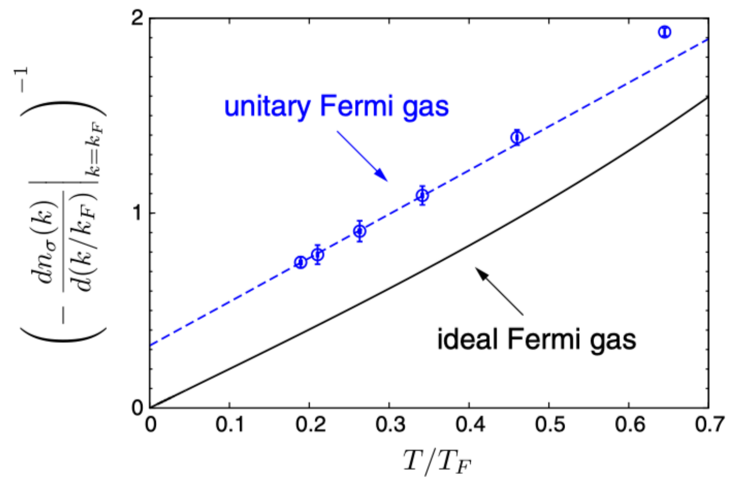

FIG. 6. Inverse slope of the momentum distribution at the Fermi momentum vs temperature. For a Fermi liquid this quantity linearly tends to zero for $T/T_F \to 0$ (see solid line). In contrast, a linear extrapolation of our data for the unitary Fermi gas (dashed line) does not go through the origin.

R. Rossi, T. Ohgoe, E. Kozik, N. Prokof'ev, B. Svistunov, K. Van Houcke, and F. Werner, PRL **121**, 130406 (2018)

Homotopic action

PHYSICAL REVIEW LETTERS **126,** 257001 (2021)

Homotopic Action: A Pathway to Convergent Diagrammatic Theories

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The major obstacle preventing Feynman diagrammatic expansions from accurately solving many-fermion systems in strongly correlated regimes is the series slow convergence or divergence problem. Several techniques have been proposed to address this issue: series resummation by conformal mapping, changing the nature of the starting point of the expansion by shifted action tools, and applying the homotopy analysis method to the Dyson-Schwinger equation. They emerge as dissimilar mathematical procedures aimed at different aspects of the problem. The proposed homotopic action offers a universal and systematic framework for unifying the existing—and generating new—methods and ideas to formulate a physical system in terms of a convergent diagrammatic series. It eliminates the need for resummation, allows one to introduce effective interactions, enables a controlled ultraviolet regularization of continuous-space theories, and reduces the intrinsic polynomial complexity of the diagrammatic Monte Carlo method. We illustrate this approach by an application to the Hubbard model.

Homotopic action $S(w)$

For our purposes, by the homotopy we mean an analytic transformation of a certain bilinear action $S(w=0)$ into a physical one, $S(w=1)$, controlled by a single parameter w.

Example 1. $S(w) \, = \, (1-w)\, S_{\rm eff}^{(0)} \, + \, w\, S_{\rm phys}$

Example 2. $S(w) \, = \, (1-w)\, S_{\rm eff}^{(0)} \, + \, w(1-w)\, S_{\rm eff}^{(\rm int)} \, + \, w\, S_{\rm phys}$

A **controlled way** of (most broadly understood) regrouping of diagrammatic contributions; ultimately resulting in a convergent Taylor series in powers of homotopic parameter w.

Important example

High-order diagrammatic expansion around BCS theory

G. Spada,[1,2,3,*] R. Rossi,[4,5,†] F. Šimkovic,[6,7] R. Garioud,[6,7] M. Ferrero,[6,7] K. Van Houcke,[2] and F. Werner[1,‡]

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We demonstrate that summation of connected diagrams to high order on top of the BCS hamiltonian is a viable generic unbiased approach for strongly correlated fermions in superconducting or superfluid phases. For the 3D attractive Hubbard model in a strongly correlated regime, we observe convergence of the diagrammatic series, evaluated up to 12 loops thanks to the connected determinant diagrammatic Monte Carlo algorithm. Our study includes the polarized regime, where conventional quantum Monte Carlo methods suffer from the fermion sign problem. Upon increasing the Zeeman field, we observe the first-order superconducting-to-normal phase transition at low temperature, and a significant polarization of the superconducting phase at higher temperature.

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More examples

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **93**, 161102(R) (2016)

Shifted-action expansion and applicability of dressed diagrammatic schemes

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While bare diagrammatic series are merely Taylor expansions in powers of interaction strength, dressed diagrammatic series, built on fully or partially dressed lines and vertices, are usually constructed by reordering the bare diagrams, which is an *a priori* unjustified manipulation, and can even lead to convergence to an unphysical result [E. Kozik, M. Ferrero, and A. Georges, Phys. Rev. Lett. **114**, 156402 (2015)]. Here we show that for a broad class of partially dressed diagrammatic schemes, there exists an action $S^{(\xi)}$ depending analytically on an auxiliary complex parameter ξ, such that the Taylor expansion in ξ of correlation functions reproduces the original diagrammatic series. The resulting applicability conditions are similar to the bare case. For fully dressed skeleton diagrammatics, analyticity of $S^{(\xi)}$ is not granted, and we formulate a sufficient condition for converging to the correct result.

PHYSICAL REVIEW B **98**, 195104 (2018)

Full and unbiased solution of the Dyson-Schwinger equation in the functional integro-differential representation

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We provide a full and unbiased solution to the Dyson-Schwinger equation illustrated for ϕ^4 theory in 2D. It is based on an exact treatment of the functional derivative $\partial\Gamma/\partial G$ of the four-point vertex function Γ with respect to the two-point correlation function G within the framework of the homotopy analysis method (HAM) and the Monte Carlo sampling of rooted tree diagrams. The resulting series solution in deformations can be considered as an asymptotic series around $G = 0$ in a HAM control parameter $c_0 G$, or even a convergent one up to the phase transition point if shifts in G can be performed (such as by summing up all ladder diagrams). These considerations are equally applicable to fermionic quantum field theories and offer a fresh approach to solving functional integro-differential equations beyond any truncation scheme.

Shifted action as a simple example of homotopic action

$S[\Psi] = S_0[\Psi] + gS_{\text{int}}[\Psi]$ original action

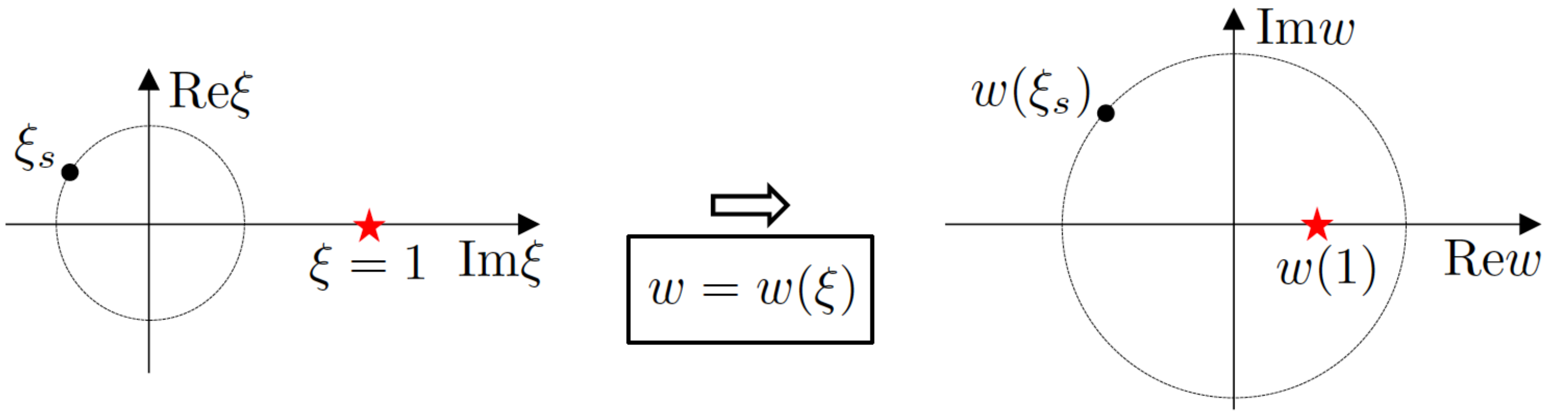
$\tilde{S}[\Psi;\xi] = \tilde{S}_0[\Psi] + \Lambda[\Psi;\xi] + \xi g S_{\text{int}}[\Psi]$ shifted action

The shift: $\Lambda = \sum_{j=1}^{\infty} \xi^j \Lambda_j[\Psi]$, $\tilde{S}_0[\Psi] + \Lambda[\Psi;\xi = 1] = S_0[\Psi]$

Expand in ξ rather than g.

Still problematic if g is large. Would need a conformal map $\xi = \xi(w)$.

Standard routine: shifted action + conformal map



Conformal map as a homotopy

Adding interactions by appropriately small pieces

Quite physical and very illustrative of the general idea of homotopic expansion

Let us take $g = 7$.

$$7 = 3 + 2 + 1 + \tfrac{1}{2} + \tfrac{1}{4} + \tfrac{1}{8} + \ldots$$

$$g(w) = 3w + 2w^2 + w^3 + \tfrac{1}{2}w^4 + \tfrac{1}{4}w^5 + \tfrac{1}{8}w^6 + \ldots$$

no large terms

$$= 3w + \frac{4w^2}{2-w}$$

equivalence with a conformal map

$$g(w=1) = 7$$

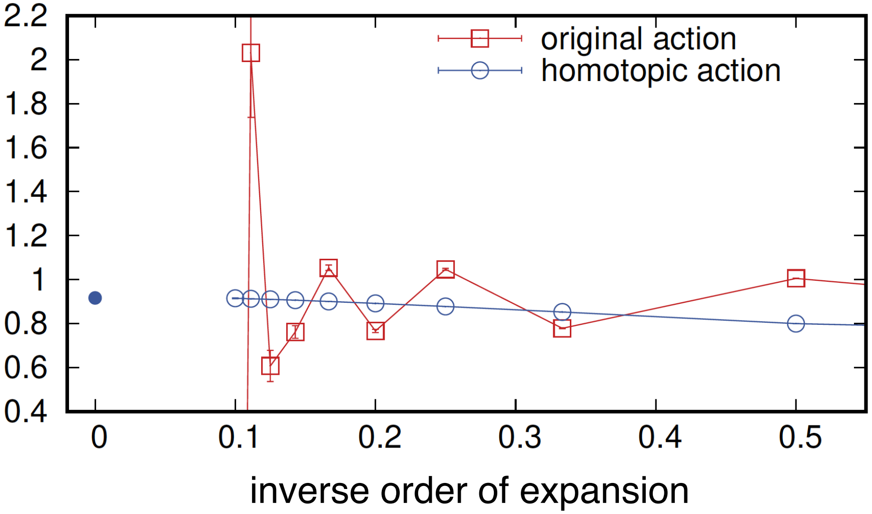
Proof-of-principle simulation for the Hubbard model

$$H = -\sum_{<ij>,\sigma=\uparrow,\downarrow} a^+_{\sigma i} a_{\sigma j} + \xi U \sum_i n_{\uparrow i} n_{\downarrow i} - (\mu + \alpha\xi) \sum_i (n_{\uparrow i} + n_{\downarrow i}), \qquad n_{\sigma i} = a^+_{\sigma i} a_{\sigma i}$$

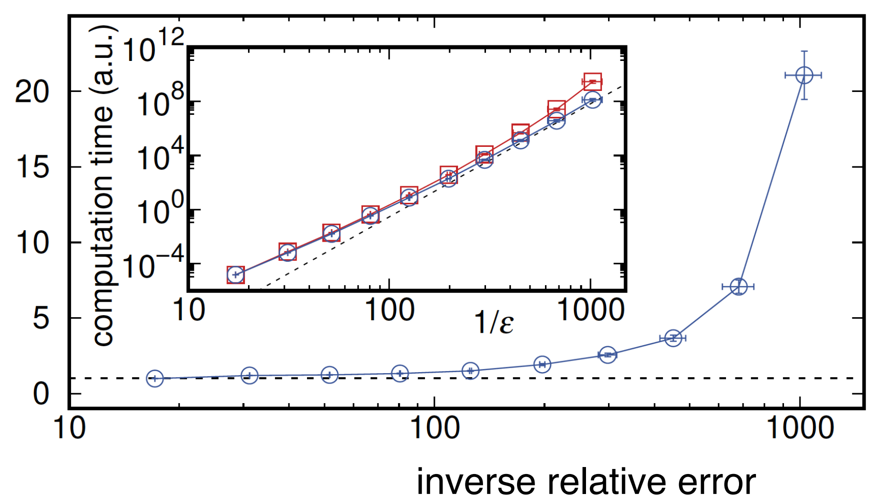
$$T = 0.2, \quad U = 7, \quad \mu = 0.18959, \quad \alpha = 2.5568$$

conformal map: $\xi(w) = \dfrac{12w}{7(1-w)^2}$

density



efficiency gain



“Ultraviolet” regularization. Option 1

Along the shifted-action lines (cf. the symmetry-breaking-restoring trick)

$$\varepsilon(k) \quad \to \quad \varepsilon(k) + \alpha(1-w)k^4$$

modified dispersion

The quartic term prevents a fermionic system from Dyson-collapsing into dense droplets.

"Ultraviolet" regularization. Option 2

Adding interaction by ***momentum dependent*** pieces

Split interaction into momentum shells: $$S_{\mathrm{int}} = \sum_{j=1}^{\infty} S_{\mathrm{int}}^{(j)}$$

Let characteristic momentum of the *j*-th shell increase with *j*.

Introduce homotopic action: $$\bar{S}_{\mathrm{int}}(w) = \sum_{j=1}^{\infty} w^j S_{\mathrm{int}}^{(j)}, \qquad \bar{S}_{\mathrm{int}}(w=1) = S_{\mathrm{int}}$$

In the case of fermions, a finite convergent radius of the homotopic expansion is guaranteed by the Pauli principle, preventing the system from Dyson's collapse.

Convergence at $w = 1$ is then achieved by conformal map.

In conclusion, key questions for future developments

- How to properly group the diagrams?
- How to optimize the choice of homotopic action (both qualitatively and quantitatively)?
- In particular, how to optimize marginal convergence at $w \longrightarrow 1$?