Homotopic Action: A Pathway to Convergent Diagrammatic Theories

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A small historic piece: where our inspiration for the worm algorithm was coming from.

Simulations of Discrete Quantum Systems in Continuous Euclidean Time

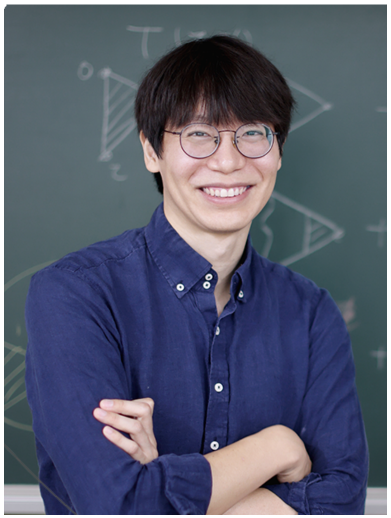
B. B. Beard and U.-J. Wiese

Center for Theoretical Physics, Laboratory for Nuclear Science, and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 27 February 1996)

We propose a new method to study path integrals for discrete quantum systems in which we work directly in the Euclidean time continuum. The method is of general interest. Here it is applied to the Heisenberg quantum antiferromagnet using a continuous-time version of a loop cluster algorithm. This algorithm is exploited to confirm the predictions of chiral perturbation theory in the extreme low temperature regime, down to $T = 0.01J$. A fit of the low-energy parameters of chiral perturbation theory gives excellent agreement with previous results and with experiments. [S0031-9007(96)01873-X]

Homotopic expansions



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“Sign blessing” of diagrammatic Monte Carlo comes at a price…

… of the convergence problem:

Sometimes convergence is slow, some times the series is divergent/ asymptotic, and some times convergence is there but to a wrong result.

Notorious example of the convergence problem

PRL **114,** 156402 (2015) PHYSICAL REVIEW LETTERS week ending 17 APRIL 2015

Nonexistence of the Luttinger-Ward Functional and Misleading Convergence of Skeleton Diagrammatic Series for Hubbard-Like Models

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The Luttinger-Ward functional $\Phi[\mathbf{G}]$, which expresses the thermodynamic grand potential in terms of the interacting single-particle Green's function $\mathbf{G}$, is found to be ill defined for fermionic models with the Hubbard on-site interaction. In particular, we show that the self-energy $\Sigma[\mathbf{G}] \propto \delta\Phi[\mathbf{G}]/\delta\mathbf{G}$ is not a single-valued functional of $\mathbf{G}$: in addition to the physical solution for $\Sigma[\mathbf{G}]$, there exists at least one qualitatively distinct unphysical branch. This result is demonstrated for several models: the Hubbard atom, the Anderson impurity model, and the full two-dimensional Hubbard model. Despite this pathology, the skeleton Feynman diagrammatic series for Σ in terms of $\mathbf{G}$ is found to converge at least for moderately low temperatures. However, at strong interactions, its convergence is to the unphysical branch. This reveals a new scenario of breaking down of diagrammatic expansions. In contrast, the bare series in terms of the noninteracting Green's function $\mathbf{G}_0$ converges to the correct physical branch of Σ in all cases currently accessible by diagrammatic Monte Carlo calculations. In addition to their conceptual importance, these observations have important implications for techniques based on the explicit summation of the diagrammatic series.

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.

Source of our inspiration for homotopic expansions

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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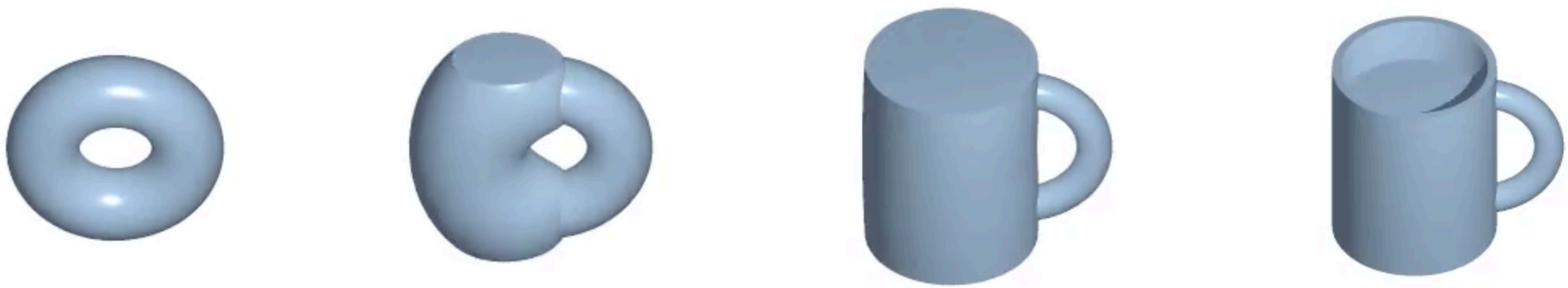
We provide a full and unbiased solution to the Dyson-Schwinger equation illustrated for ϕ^4 theory in 2D. It is based on an exact treatment of the functional derivative $\partial\Gamma/\partial G$ of the four-point vertex function Γ with respect to the two-point correlation function G within the framework 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.

Homotopic transformation

Controlled by a single parameter $w \in [0, 1]$.



$w = 0$ $w = 1/3$ $w = 2/3$ $w = 1$

Conceptual idea: Taylor-expand in powers of homotopic parameter w .

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.

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

Bilinear functionals of Ψ

Expand in ξ rather than g.

Symmetry-broken expansions: important subclass of homotopic (shifted-action-type) expansions

$$S[\Psi;\xi] = S_0[\Psi] + (1-\xi)\,S_*[\Psi] + \xi g S_{\rm int}[\Psi]$$

Bilinear action explicitly breaking certain symmetries of the original action.

Important example of successful symmetry-broken expansion

arXiv:2103.12038

High-order diagrammatic expansion around BCS theory

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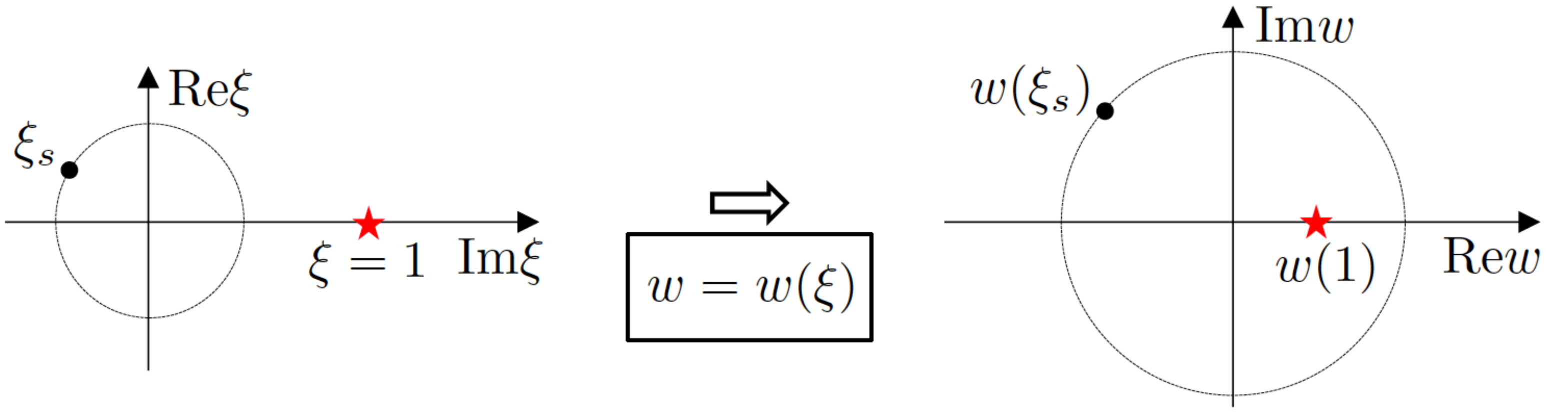
(Dated: June 21, 2023)

We demonstrate that summation of connected diagrams to high order starting from a 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 thermally activated polarization of the superconducting phase well described by quasiparticle theory.

Standard routine: shifted action + conformal map

(When shifted action does not yet yield convergence)



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

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

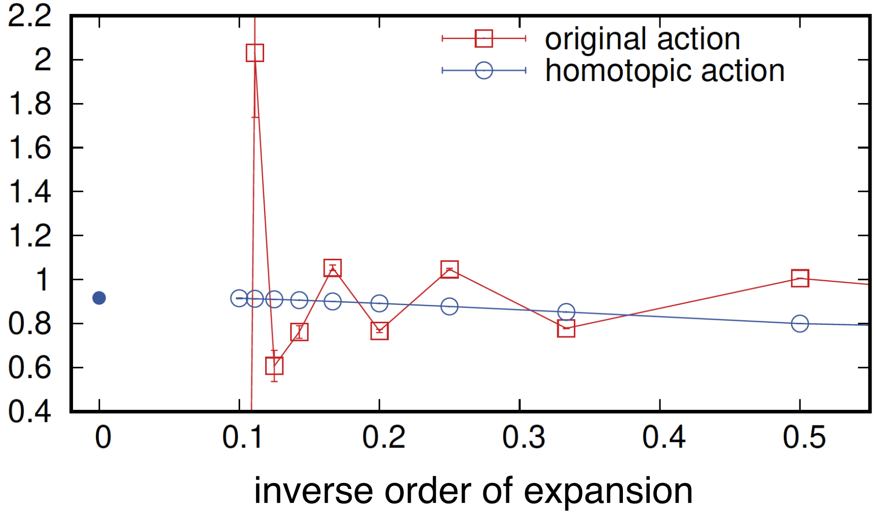
Proof-of-principle simulation for the Hubbard model

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

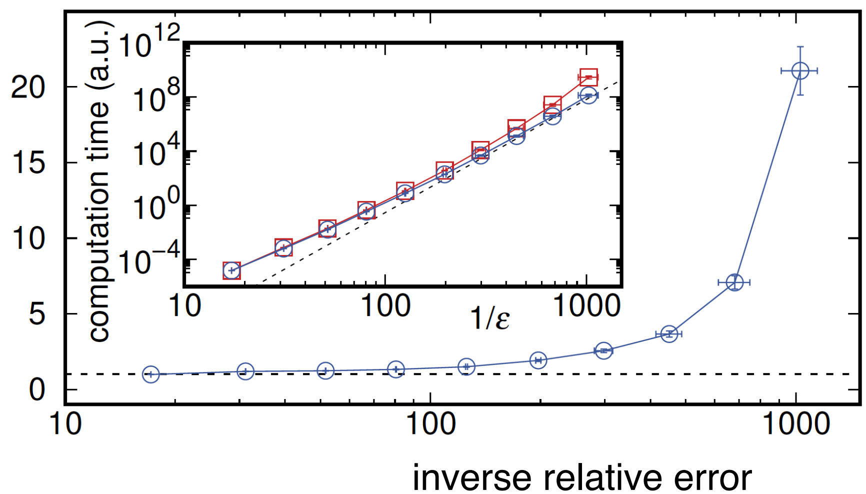
$$T = 0.2, \quad U = 7, \quad \mu = 0.18959, \quad \alpha = 2.5568$$

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

density



efficiency gain



Further ideas

Ultraviolet regularization. Option 1

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

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

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: $$S_{\text{int}} = \sum_{j=1}^{\infty} S_{\text{int}}^{(j)}$$

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

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

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.

Homotopic tools for introducing induced interactions and/or emergent degrees of freedom

$$w(1-w)\,S_{\text{ind}}$$

Effective action describing induced interactions and/or emergent degrees of freedom. The contribution of this term to the total action vanishes at $w \to 0$ and $w \to 1$.

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 $w \to 1$?