Evaluating Matrix Functions by Resummations on Graphs: the method of walk-sums

Simon Thwaite\(^1,\ast \) • Pierre-Louis Giscard\(^2 \)

\(^1\) LS Prof. Schollwöck, Faculty of Physics, LMU Munich  
\(^2\) Clarendon Laboratory, University of Oxford  
\(\ast\)Simon.Thwaite@physik.uni-muenchen.de

Simulating quantum many-body systems

Motivation

Quantum many-body systems with strong correlations are a topic of intense current research interest within both the theoretical and experimental physics communities. A detailed understanding of these systems promises to provide new insights into important condensed-matter and solid-state phenomena such as quantum magnetism, high-T\(_c\) superconductivity, and novel topologically-ordered states of matter.

Path-integral Monte Carlo: strengths and weaknesses

Flexible and scalable computational methods are invaluable for understanding the behaviour of strongly-correlated many-body systems. One key technique is path-integral Monte Carlo, which samples the partition function in the form:

\[ Z(\beta) = \text{Tr} \left[ e^{-\beta H_0 + V} \right] \]

\[ = \text{Tr} \left[ e^{-\beta H_0} \right] \left[ 1 - \int_0^\beta d\tau_1 V(\tau_1) + \int_0^\beta d\tau_2 \int_0^{\tau_2} d\tau_1 V(\tau_2) V(\tau_1) - \cdots \right] \]

PIMC provides extremely accurate results for bosonic systems, but is of limited applicability for fermionic and frustrated systems, due to the infamous sign problem. While a general solution to the sign problem appears to be impossible, progress can be made on a case-by-case basis by searching for more rapidly-convergent expansions to sample.

Walk-sums: new insights into path-integral Monte Carlo

On this poster we introduce a new method for evaluating matrix functions: the method of walk-sums. It is built on two principles:

- A mapping from matrix multiplication to walks on a graph,
- Exploiting structure in the walks to exactly resum certain families of terms.

The method of walk-sums promises to provide new insights into path-integral Monte Carlo and related diagrammatic methods.

Example: deriving the Dyson series

1. Write the Taylor series for \( e^{-\beta H} \), with \( H = H_0 + V \), as a sum over walks:

\[ \exp(-\beta H)_{\alpha \omega} = \sum_{n=0}^{\infty} \sum_{G,\text{loops}} \frac{(-\beta)^n}{n!} H_{\alpha \gamma_1} \cdots H_{\gamma_{n-1} \gamma_n} H_{\gamma_n \omega} \]

2. Take the Laplace transform, \( \mathcal{L}[f(\beta)] = \int_0^\infty f(\beta) e^{-\beta \delta} d\beta \), to get to

\[ \mathcal{L}[\exp(-\beta H)_{\alpha \omega}] = s^{-1} \sum_{m=0}^{\infty} \sum_{G,\text{loops}} (H_{\alpha \gamma_1} s^{-1}) \cdots (H_{\gamma_{m-1} \gamma_m} s^{-1})(H_{\gamma_m \omega} s^{-1}) \]

3. Factorise sum over walks into:

- Sum over loopless walks,
- Sum over self-loops: e.g.

\[ s^{-1} \sum_{m=0}^{\infty} \sum_{G,\text{loops}} (H_{\alpha \gamma_1} s^{-1}) \cdots (H_{\gamma_{m-1} \gamma_m} s^{-1})(H_{\gamma_m \omega} s^{-1}) \]

4. Evaluate the sums over self-loops exactly:

\[ \mathcal{L}[\exp(-\beta H)_{\alpha \omega}] = \sum_{m=0}^{\infty} \sum_{G,\text{loops}} (s - H_{\alpha \gamma_1}) \cdots (s - H_{\gamma_{m-1} \gamma_m})(s - H_{\gamma_m \omega}) \]

5. Invert the Laplace transform to recover the Dyson series.

Factorising walks on graphs into primes

Walk from \( \alpha \) to \( \omega \)

- simple cycle
- compound cycle
- Cycles off \( \alpha, \omega \)
- Path from \( \alpha \) to \( \omega \)

The prime factorisation of a walk

Any walk is a path plus a collection of cycles…

…so any walk is a path plus a recursively nested set of simple cycles!

Resumming all cycles

The prime factorisation of walks allows contributions in the Taylor series from all cycles to be resummed. The result is a sum over paths on the graph:

\[ F(M)_{\alpha \omega} = \sum_{k=0}^{\infty} c_k \sum_{G,\text{paths}} M_{\alpha \gamma_k} \cdots M_{\gamma_{k-1} \gamma_k} M_{\gamma_k \omega} \]

where the resummed cycle contributions are given by

\[ f(M_{\alpha \omega}) = \left[ 1 - \sum_{G,\text{paths}} f(M_{\alpha \gamma_k}) M_{\gamma_k \gamma_{k-1}} \cdots M_{\gamma_{k-1} \gamma_k} f(M_{\gamma_k \gamma_{k-1}}) M_{\gamma_{k-1} \omega} \right]^{-1} \]

where the vertex function \( f \) depends on the form of \( F \). The cycle resummation expresses a matrix function as a continued fraction.

Summary and prospects

Walk-sums are a technique for evaluating matrix functions built on two principles:

- A mapping from matrix multiplication to walks on a weighted directed graph,
- Exploiting structure in the walks to exactly resum certain families of terms.

Current open questions include:

- Can resummations involving only a subset of cycles be found?
- How can the terms in a walk-sum series be generated, or efficiently sampled?
- Can the exact resummations within the walk-sum formalism be used as the basis for an improved path-integral Monte Carlo scheme?

Supporting bodies

Fertig mit der Unterstützung von Alexander von Humboldt Stiftung/Foundation