SIGN25 = SIGN is a positive thing!

Nikolay Prokof’ev, UMass, Amherst

Univ. of Bern, Jan. 2025

National Science Foundation
WHERE DISCOVERIES BEGIN

Collaborators (when they were younger …)

Kris van Houcke (ENS, Paris)

Knew that projects will likely fail and no papers will be publish for years but did it anyway

Boris Svistunov UMass., Amherst

Was optomistic but he was tenured …

Felix Werner, ENS

Was pessimistic but did everything to make it work right anyway

Evgeny Kozik, King's College

It is fun only if you do things which others find impossible

Riccardo Rossi, Sorbonne U.

He is simply genius

+SIGN25+ = **Sing is a positive thing!**

Characteristic features/issues of the sign problem

Path-integrals (lattice or continuous), stochastic series expansions, …

…

$$\langle Q \rangle = \frac{\sum_{i=1}^{K} Q_i W_i}{\sum_{i=1}^{K} W_i} \equiv \frac{\sum_{i=1}^{K} Q_i s_i |W_i|}{\sum_{i=1}^{K} s_i |W_i|} \xrightarrow[MCsampling]{} \frac{\sum_{i \in MC} Q_i s_i}{\sum_{i \in MC} s_i} \equiv \frac{\langle Qs \rangle}{\langle s \rangle}$$

1. K is too large to evaluate the entire sum, obviously …

2. Both **numerator** $\langle Qs \rangle \to 0$ and **denominator** $\langle s \rangle \to 0$ when $K \to \infty$
   i.e. **both** must be known with vanishingly small error bars:

$$t_{CPU} \; ? \; \langle s \rangle^{-2}$$

3. Exponential scaling with (d+1)-dimensional volume: $\langle s \rangle \sim \exp\{-\# \beta L^d\}$
   (data cannot be extrapolated to the thermodynamic limit)

Interacting fermions: What Sign problem?

$$H_{Fermions} = \sum_{k\alpha} (\varepsilon(k,\alpha) - \mu_\alpha) \psi^\dagger_{k\alpha} \psi_{k\alpha} + \frac{1}{2} \sum_{rr'abcd} V_{abcd}(r - r') \psi^\dagger_{r'd} \psi^\dagger_{rc} \psi_{rb} \psi_{r'a} + \dots$$

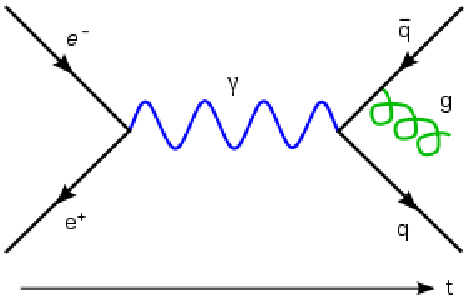
Voltmeter (or any experimentalist):
“I have no clue what you mean …”

Fermions do not have a problem! Theorists do

A similar Hamiltonian with random parameters and unlimited range of support, covers the entire complexity of all known materials and structures in Nature!

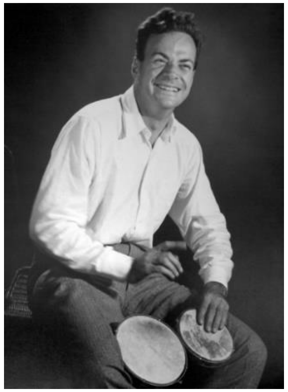
There is no ambition to solve it in one shot, so we consider only regular systems

Feynman Diagrams: the war drum of theoretical physics



$$S = S_0 + \xi S_1 + \xi^2 S_2 + \xi^3 \ldots \qquad (\xi = 1)$$

$$\langle Q \rangle = \frac{\sum_n \langle \Psi_n | Q e^{-S} | \Psi_n \rangle}{\sum_n \langle \Psi_n | e^{-S} | \Psi_n \rangle} = \langle Q \rangle_0 + \xi \langle QB \rangle_0 + \xi^2 \langle QC \rangle_0 + \ \xi^3 \ldots$$



particle A scatters off particle B by virtual exchange of ….

High-order expansion with transparent graphics → math

+ **Thermodynamic limit answers** for physical properties

+ Flexibility: renormalization, mean-fields, summation of infinite sets on the "fly", self-consistent treatments, etc.

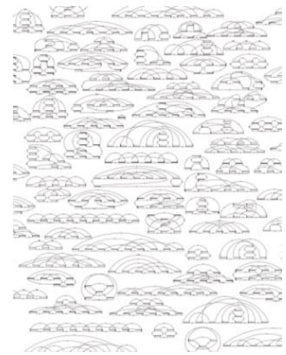
+ "there are Feynman diagrams for almost everything …"

Are Feynman diagrams useful for strongly correlated systems?

Steven Weinberg, Physics Today, Aug. 2011 :

> *"Also, it was easy to imagine any number of quantum field theories of strong interactions but* ***what could anyone do with them****?"*

Factorial number of high-order graphs → need to handle billions of them

$\Sigma = \Bigg\{$  $\Bigg\}$

✓ This talk

Diagrammatic Monte Carlo

Without small parameters, why bother to compute high-order contributions for divergent series?

✓ Boris's talk

Niels Abel, 1828:

> *"Divergent series are the invention of the devil, and it is* ***shameful*** *to base on them any demonstration whatsoever."*

Diagrammatic series:

$$Q(Y)=\sum_{n=0}\xi^{n}\sum_{\Im}\iiint \underbrace{dX_1 dX_2 \mathrm{K}\; dX_n}_{\text{Integration variables}}\;\underbrace{D(n,\Im,X_1,X_2\mathrm{K}\;X_n;Y)}_{\text{Contribution to the answer}}$$

term order

different terms of of the same order (topologies, inte-raction types, …)

$$Q=\sum_{n=0}^{\infty}\xi^{n}a_n \quad \textbf{with Taylor series coefficients} \quad a_n=\sum_{\Im}\iiint dX^{n}\; D(n,\Im,\{X\};Y)$$

or

$$a_n=\iiint dX^{n}\left[\sum_{\Im}D(n,\Im,\{X\};Y)\right]$$

Order n coefficient $a_n = \iiint dX^n \left[\sum_{\mathfrak{I}} D(n, \mathfrak{I}, \{X\}; Y) \right]$

1. K is too large to evaluate the entire sum …

   - Complete sum over $\mathfrak{I}$ can be completed in $n^3 3^n$ operations

2. Both **numerator** $\langle Qs \rangle \to 0$ and **denominator** $\langle s \rangle \to 0$ **…**

   - There is **no denominator**!

   - Numerator approaching zero is a **blessing and a sign of convergent series!**
     a_0, a_1, a_2 – easy
     who cares what is **a_{15}** if it is very small

   SIGN25 = **Sing is a positive thing to have!**

3. Exponential scaling with (d+1)-dimensional volume
   (data cannot be extrapolated to the thermodynamic limit)

   - Connected diagrams are formulated directly in the thermodynamic limit – no need to extrapolate

Computational Complexity Problem (CCP)

[Revelent question: ***How easily can one improve the accuracy of computed answers?*****]**

Let Q and ε be the quantity of interest **in the thermodynamic limit (TL)** and its desired accuracy, respectively.

The numerical scheme is said to have CCP if the CPU time, t_Q***, required to compute*** Q ***with accuracy*** ε ***diverges faster than any polynomial function of*** $\varepsilon^{-1} \to \infty$

The CCQ problem is considered solved if $\ln t_Q \propto \ln \varepsilon^{-1}$

CCP solution by Diagrammatic MC

Define an approximation $$Q_N = \sum_{n=0}^{N} \xi^n a_n = \sum_{n=0}^{N} a_n$$ **(truncated sum)**

For convergent series $\left|\left(Q - Q_N\right)/Q\right| \propto (1/\xi_c)^N$ **with** $\xi_c > 1$ **,**

and accuracy ε **is reached at**

$$n_\varepsilon \propto \ln \varepsilon / \ln(1/\xi_c)$$

For fermions, all order-n contributions can be computed in time [R. Rossi PRL'17**]**

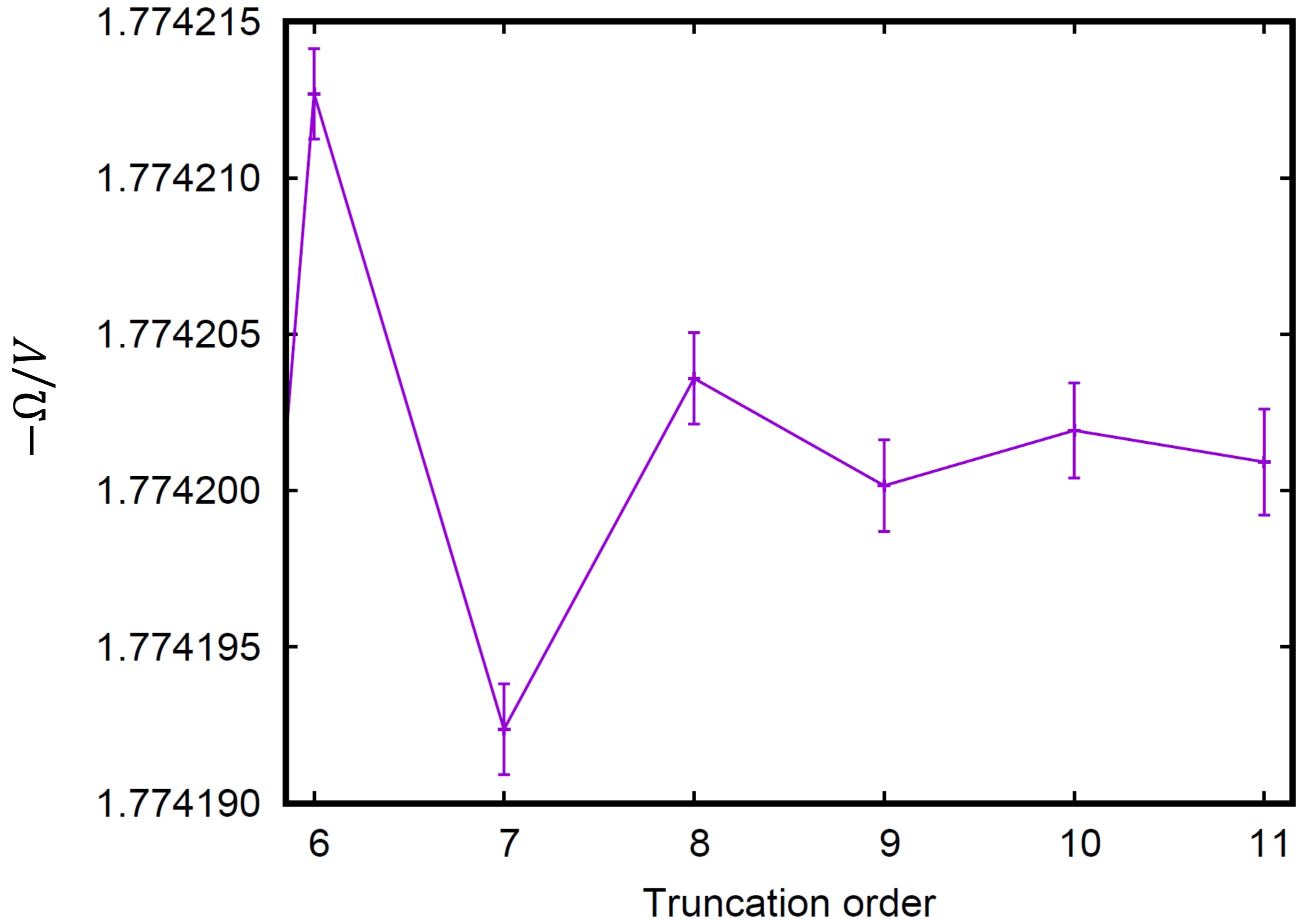
$$\tau_Q(n) \propto e^{\# n}$$

and the CCP is solved! $$\boxed{\ln t_Q(\varepsilon) = \ln \tau_Q(n_\varepsilon) \propto n_\varepsilon \propto \ln \varepsilon^{-1}}$$

When series converge

2D Fermi-Hubbard model $H = -t\sum_{<ij>\sigma} \psi^{\dagger}_{j\sigma}\psi_{i\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$

with $U/t = 2, \quad T/t = 0.125, \quad n = 0.87500(2)$



$E/N = 1.25992(6)$

R. Rossi, PRL '17

Six to five digits (depending on quantity) accuracy for a finite-T answer away from n=1!

Applications so far

Lattice models:

repulsive & attractive Fermi-Hubbard model
frustrated magnetism = flat band fermions
Haldane model (with onsite and Coulomb interactions)
Electron-phonon int. with arbitrary adiabaticity
graphene …
flat band systems (Lieb and Kagome lattices)

Ultracold atoms in continuum:

resonant/unitary fermions

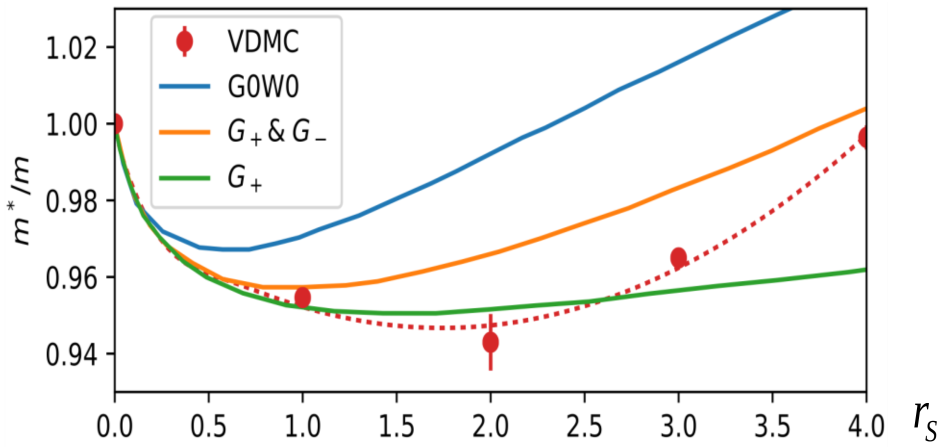
Coulomb gases:

homogeneous electron gas, or jellium liquid
metallic hydrogen chain

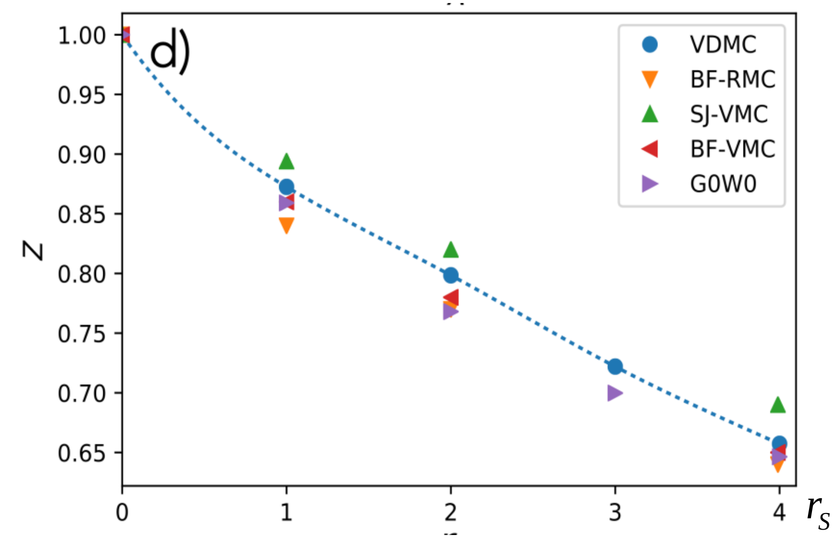
Did not try yet

Real materials,   nuclear matter, magnetic fields, gauge fields …

Uniform Electron Gas



The first unbiased m*/m calculation



Quasiparticle residue
Consistent but more precise

Spin succeptibility χ

r_s	Diagrams	literature
1	1.152(2)	1.15-1.16
2	1.296(6)	1.27-1.31
3	1.438(9)	1.39-1.46
4	1.576(9)	1.51-1.62

Landau parameters from χ **and** m^*

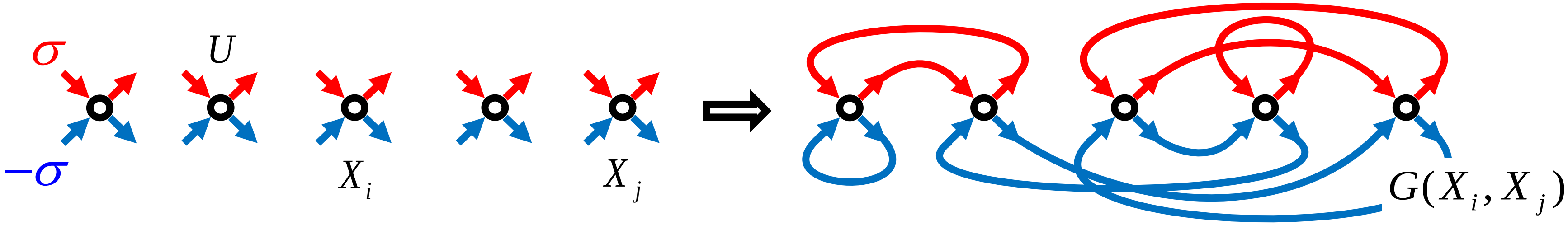
r_s	Z	m^*/m	F_0^a	F_0^s
1	0.8725(2)	0.955(1)	-0.171(1)	-0.209(5)
2	0.7984(2)	0.943(3)	-0.271(2)	-0.39(1)
3	0.7219(2)	0.965(3)	-0.329(3)	-0.56(1)
4	0.6571(2)	0.996(3)	-0.368(4)	-0.83(2)

K. Haule, K. Chen '19-21

For fermions, all order-n contributions can be computed in time $\tau_Q(n) \propto e^{\#n}$

R. Rossi PRL'17

CDet – computing sums of connected diagrams by determinants D **(<u>sign-blessing II</u>)**

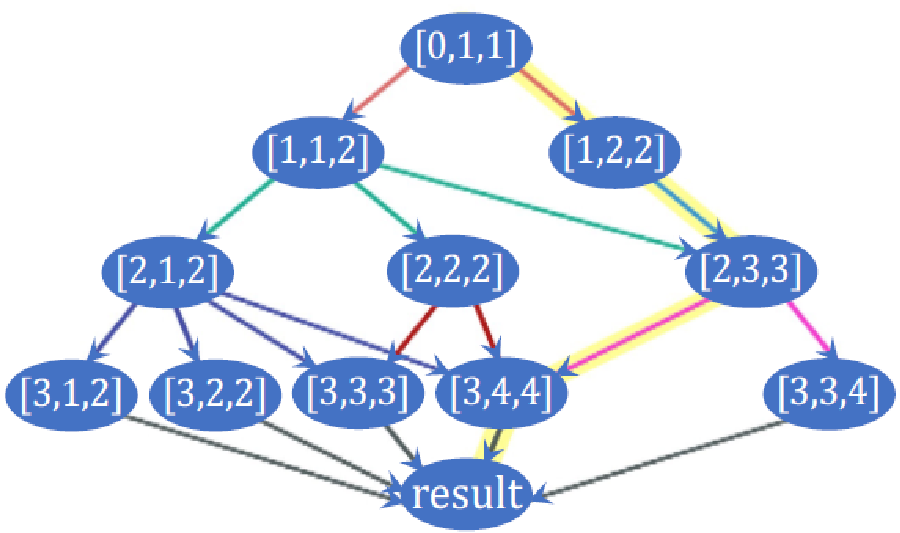


$$C(n) = D(n) - \sum_{\{m\} \not\subseteq n} C(m)\, D(n-m)$$

connected — all — all subsets

Solved for all C(m) in 3^n operations

E. Kozik, Nat. Comm. '24



Explicit (no divisions!) combinatorial summation of graphs.

Not as efficient for n>6, but far more flexible to deal with renormalizations

L. Pitaevskii “ This is the end of theoretical physics …”

Yes, for convergent series.

No, the majority of interesting cases cannot be solved using “black box” approach.
→ **Need to deal with <u>divergent series or reformulate the expansion</u> (∞ # of ways)**
[Boris’s talk]

Feynman diagrams are expansions on top of the Gaussian action for bosons and fermions.
→ **Can one get fractionalized excitations at the end?**

Linear response in the thermal state is possible, but there is no known solution for
→ **Real time dynamics**
(Keldish contour framework is OK only for thermal initial states, but so far only impurity problems were solved)

Generic gauge fields (bosons are a headache)?

Conclusions:

1. **Fermions do not have a sign-problem**

2. **Diag. Monte Carlo for fermions is not subject to FSP and solves the computational complexity problem ($\ln t_Q \propto \ln \varepsilon^{-1}$) if the series "behave".**

3. **Bottleneck is in analytic/math understanding of QFT behavior in the complex plane of the expansion parameter**

Lev Pitaevskii: "This is the end of theoretical physics."

Barak Obama: "Yes we can! But …"