DIAGRAMMATIC MONTE CARLO: WHAT HAPPENS TO THE SIGN-PROBLEM

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Outline

Ising spins vs Feynman Diagrams: Is there any difference from the Monte Carlo perspective?

Acceptable solution to the sign problem?

Yes! (so far …)

Polarons in Fermi systems

Many-body implementation for the Fermi-Hubbard model

Feynman Diagrams: graphical representation for the high-order perturbation theory

$$H = H_0 + H_{\rm int}$$

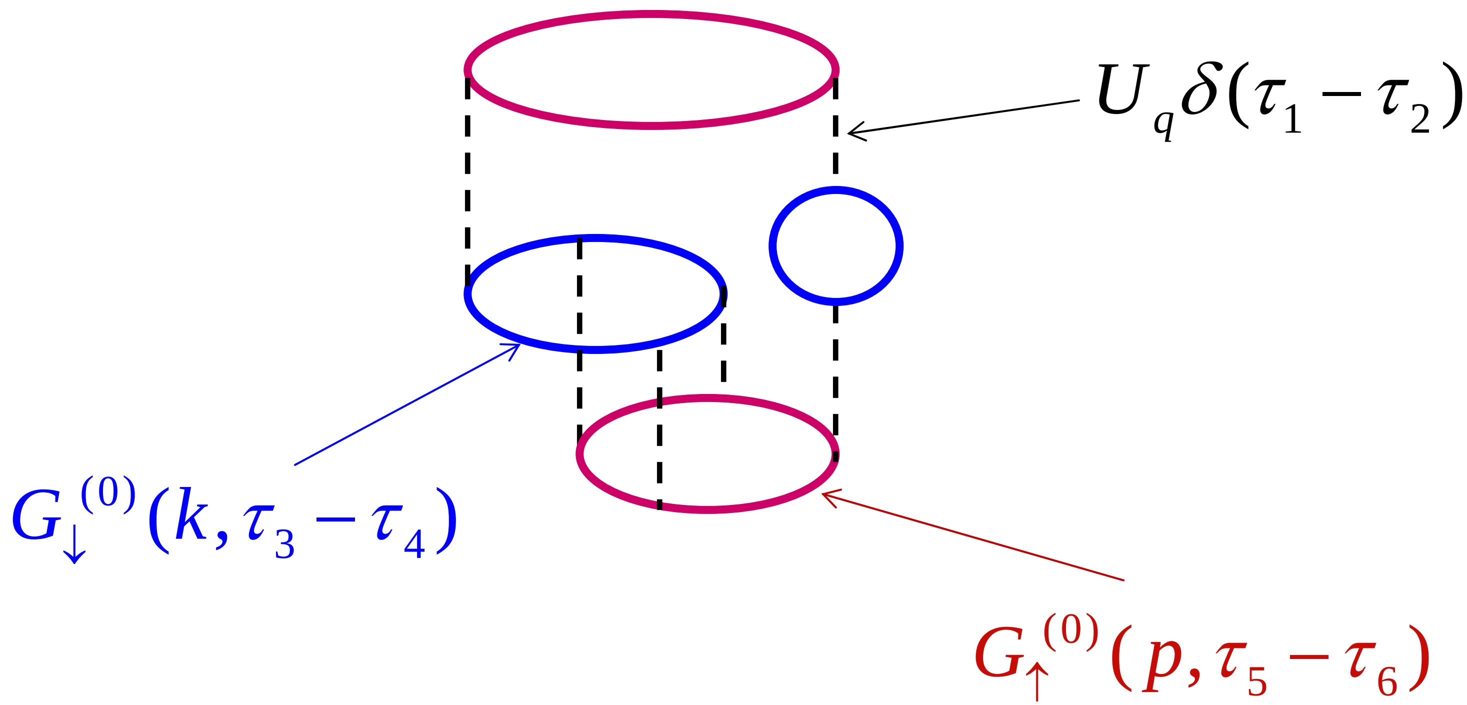
$$\langle A \rangle = \frac{\sum_n \langle \Psi_n | A e^{-H/T} | \Psi_n \rangle}{\sum_n \langle \Psi_n | e^{-H/T} | \Psi_n \rangle} = \langle A \rangle_0 + \langle AB \rangle_0 + \langle AC \rangle_0 + \ldots$$

$\propto H_{\rm int}$ $\qquad \propto H_{\rm int}{}^2$

explicit graphical representation for all terms
and easy rules to convert graphs to math

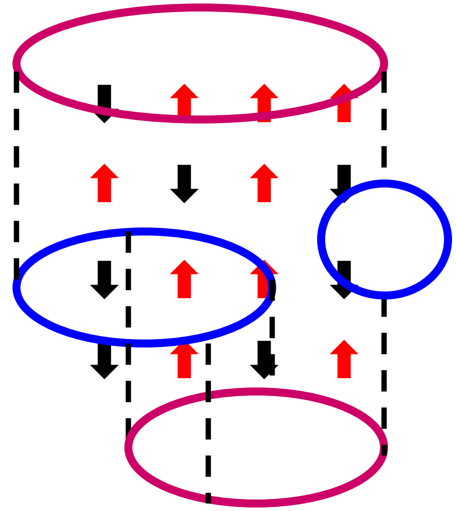
Diagrammatic technique: explicit summation of geometric series "on-the-go" with
self-consistent re-formulation of the diagrams

$$H = \sum_{k,\sigma} (\varepsilon_k - \mu) a^\dagger_{k\sigma} a_{k\sigma} + \sum_{kpq,\sigma\sigma'} U_q a^\dagger_{k-q\sigma} a^\dagger_{p+q\sigma'} a_{p\sigma'} a_{k\sigma'}$$



Configuration space = (diagram order, topology and types of lines, internal variables)

Standard Monte Carlo setup:



- configuration space (depends on the model and it's representation)

- each cnf. has a weight factor W_{cnf} $e^{-E_{cnf}/T}$

- quantity of interest $$\langle A \rangle = \frac{\sum_{cnf} A_{cnf} W_{cnf}}{\sum_{cnf} W_{cnf}}$$

Monte Carlo

$\sum_{cnf}^{MC} A_{cnf}$ configurations generated from the prob. distribution W_{cnf}

$$A(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_n \; W_n(\xi; \vec{x}_1, \vec{x}_2, \ldots \vec{x}_n, \vec{y}) = \sum_{\nu} W_{\nu}$$

term order

different terms of
of the same order

Integration variables

Contribution to the answer

Monte Carlo (Metropolis-Rosenbluth-Teller) cycle:

→ Diagram ν → suggest a change → Accept with probability

$$R_{acc} \sim \frac{|W_{\nu'}|}{|W_{\nu}|} \frac{1}{P_{\nu \to \nu'}(\text{new } \{\vec{x}\})}$$

→

Collect statistics: $A_{counter}(\vec{y}) = A_{counter}(\vec{y}) + sign(\nu)$

sign problem and potential trouble!, but …

Sign-problem

Variational methods
+ universal
- often reliable only at T=0
- systematic errors
- finite-size extrapolation

Determinant MC
+ "solves" $n_{i\sigma} + n_{i-\sigma} = 1$ case
- CPU expensive
- not universal
- finite-size extrapolation

Cluster DMFT/DCA methods
Diagrammatic MC
+ universal
- cluster-size extrapolation
- diagram-order extrapolation

Computational complexity
Is exponential : $\exp\{\#\xi\}$

Cluster DMFT

$$\xi = \left(\frac{\varepsilon_F}{T}\right) L^D$$

linear size

Diagrammatic MC

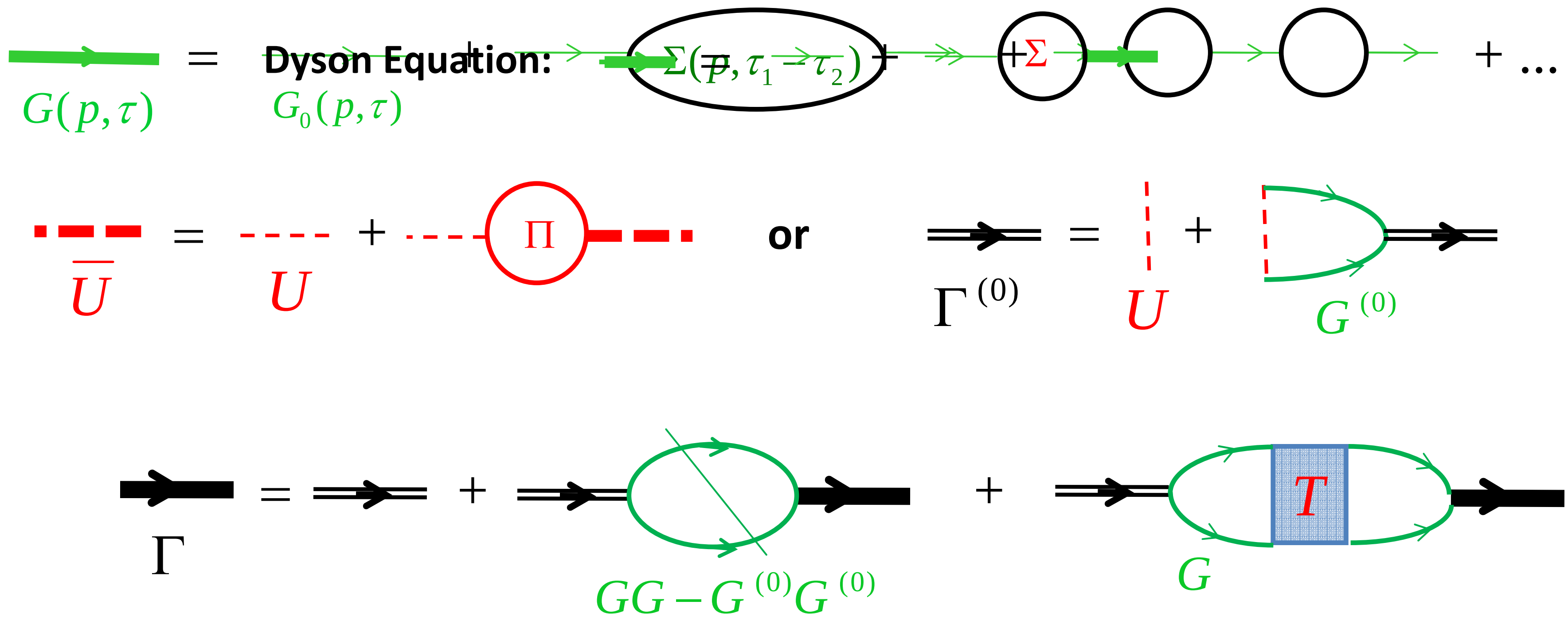
$$\xi = N$$

diagram order

for irreducible diagrams

Further advantages of the diagrammatic technique

Calculate irreducible diagrams for Σ , Π , … to get G , $\bar{U}$, …. from Dyson equations



Make the entire scheme self-consistent, i.e. all internal lines in Σ , Π , … are "bold"

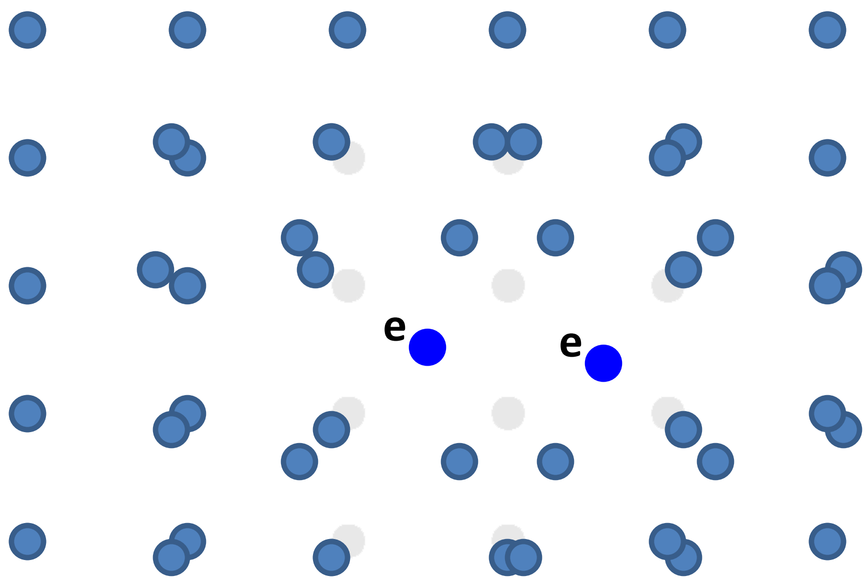
Polaron problem:

$$H = H_{\text{particle}} + H_{\text{environment}} + H_{\text{coupling}} \quad \rightarrow$$

quasiparticle

$$E(p=0),\ m_*,\ G(p,t),\ \ldots$$

Electrons in semiconducting crystals (electron-phonon polarons)



$$H = \sum_p \varepsilon(p) a_p^+ a_p + \quad \textbf{electron}$$

$$\sum_q \omega(p)(b_q^+ b_q + 1/2) + \quad \textbf{phonons}$$

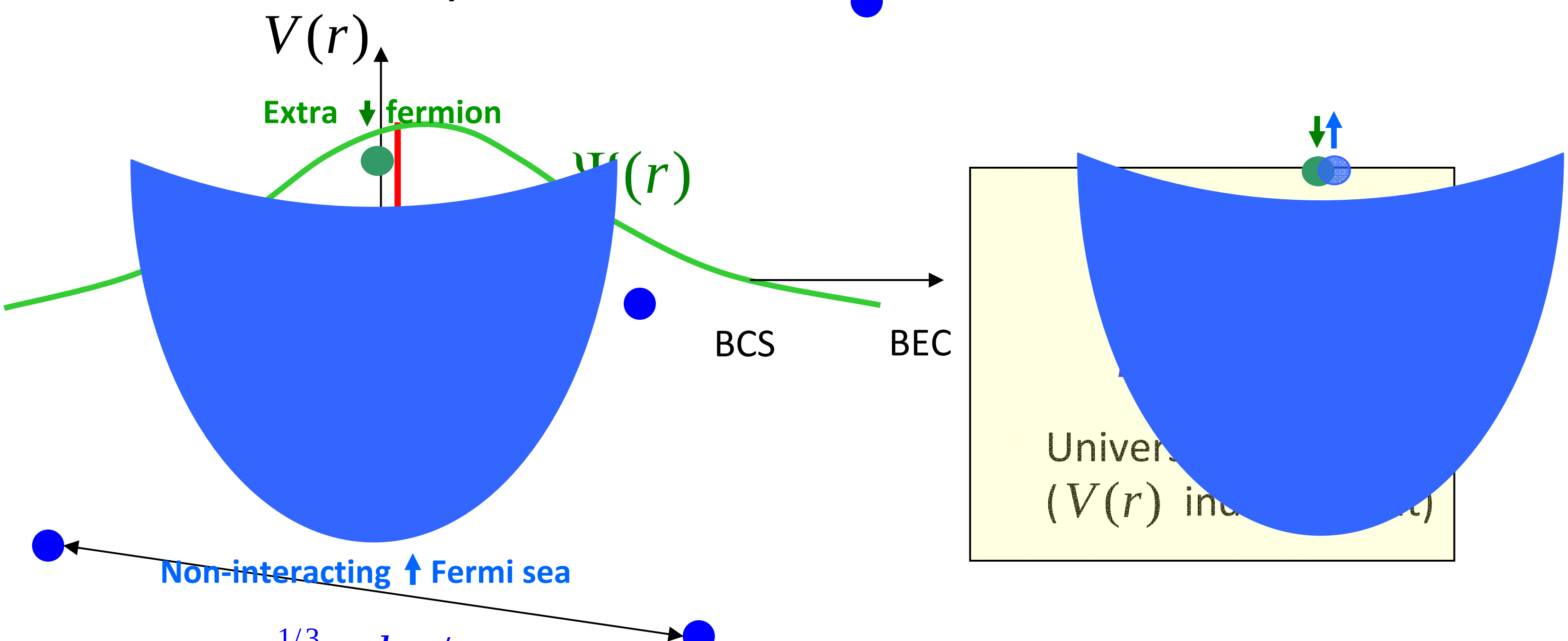
$$\sum_{pq} \left(V_q a_{p-q}^+ a_p b_q^+ + h.c. \right) \quad \textbf{el.-ph. interaction}$$

Fermi-polaron problem: $H = \frac{p^2}{2m} + H_{\text{Fermi sea}} + \int V(r - r')\; n(r')\; dr'$

↓● ●↑

particle dressed by interactions with the Fermi sea:

cold Fermi gases with population strong imbalance
orthogonality catastrophe, X-ray singularities, heavy fermions,
quantum diffusion in metals, ions in He-3, etc.

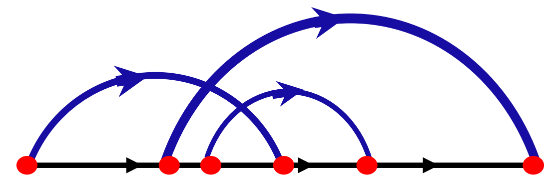


Fermionic quasiparticle (polaron)

Bosonic quasiparticle (molecule)

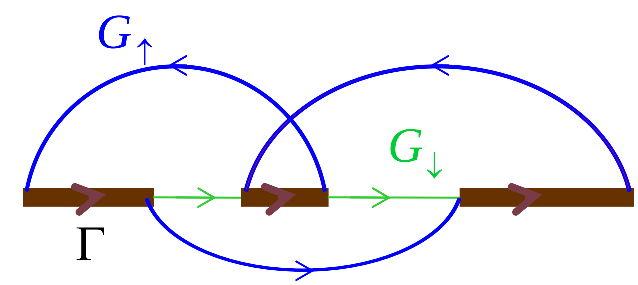
Examples:

Electron-phonon polarons (e.g. Frohlich model) = particle in the bosonic environment.

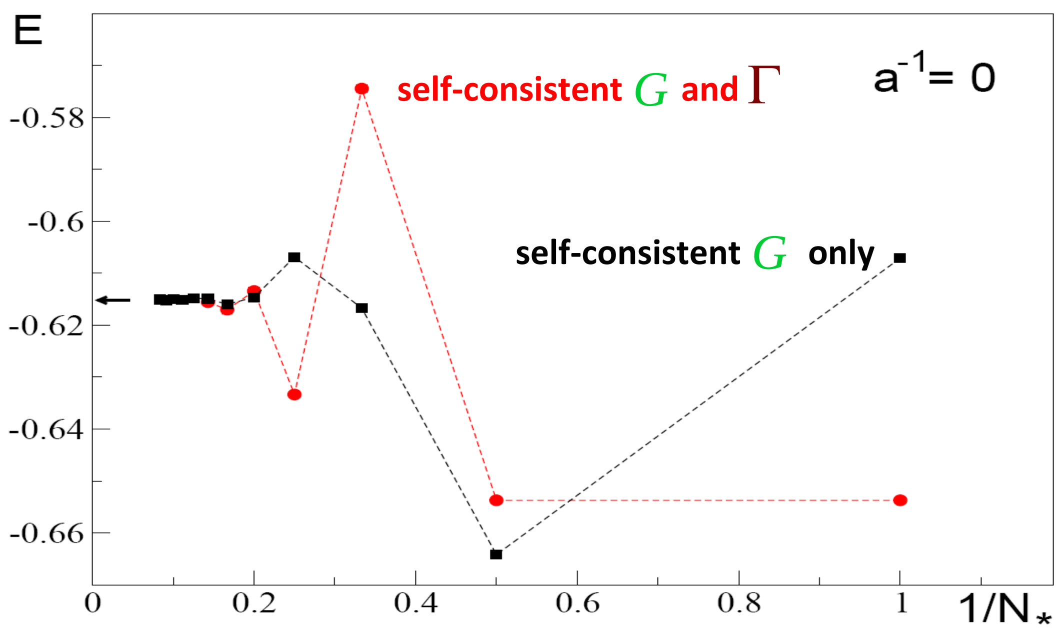


Too "simple", no sign problem, $N \sim 10^2$

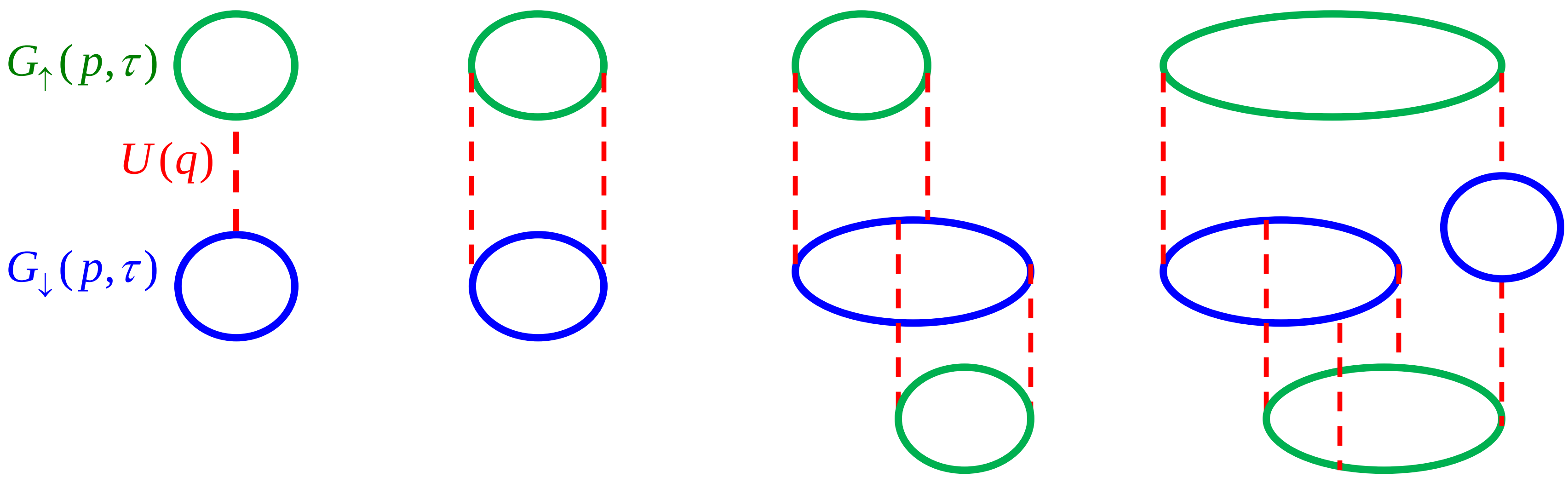
Fermi –polarons (polarized resonant Fermi gas = particle in the fermionic environment.



Sign problem! $N_{max} = 11$



Fermi-Hubbard model: $H = -t \sum_{<ij>,\sigma} a_{i\sigma}\, a^{\dagger}_{j\sigma} + U \sum_{i} n_{i\uparrow}\, n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}$



Self-consistency in the form of Dyson, RPA

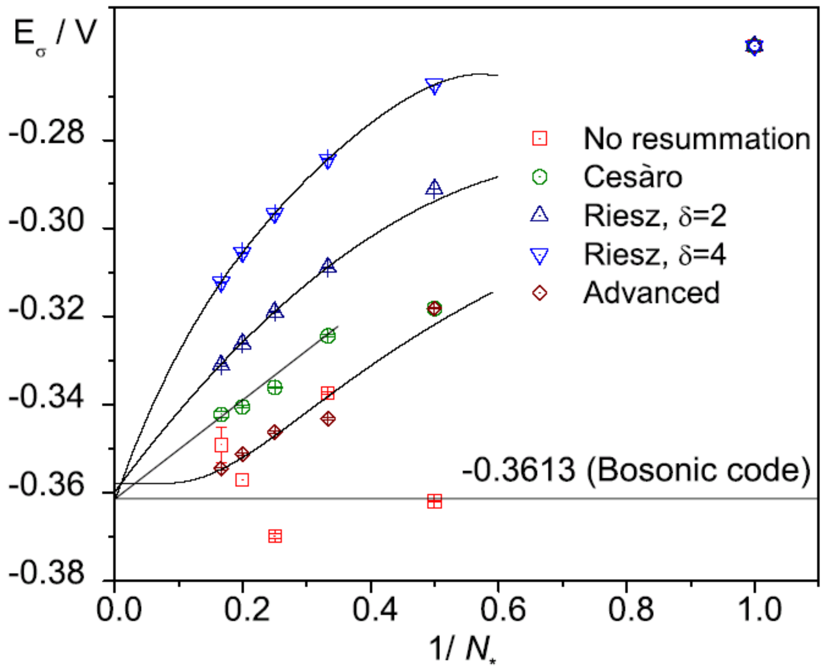
Extrapolate to the $N \to \infty$ **limit.**

1D

$U/t = 4$

$\mu/t = -0.5$

$T/t = 0.3$



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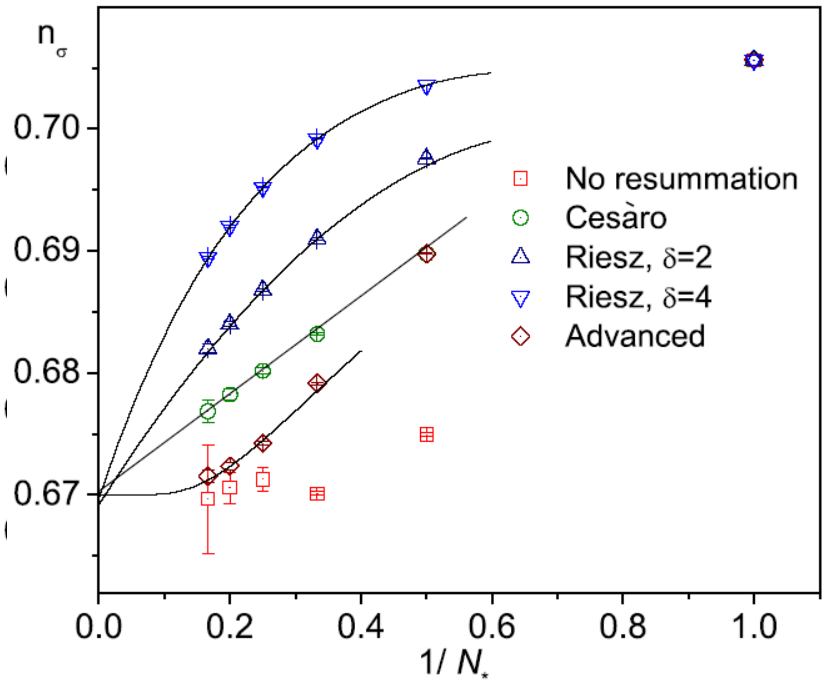
3D

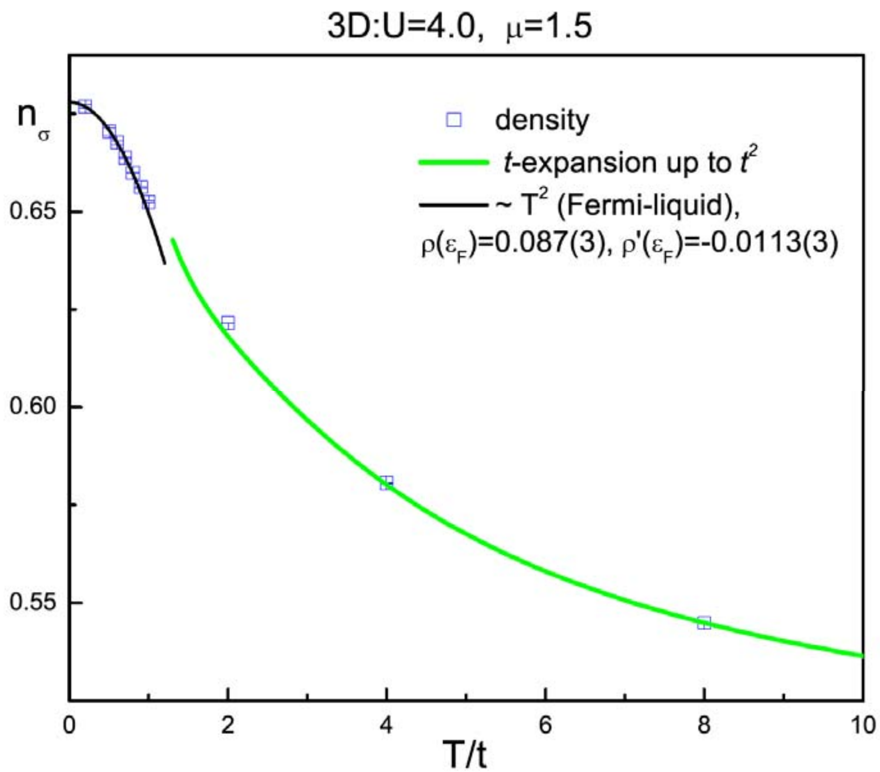
$U/t = 4$

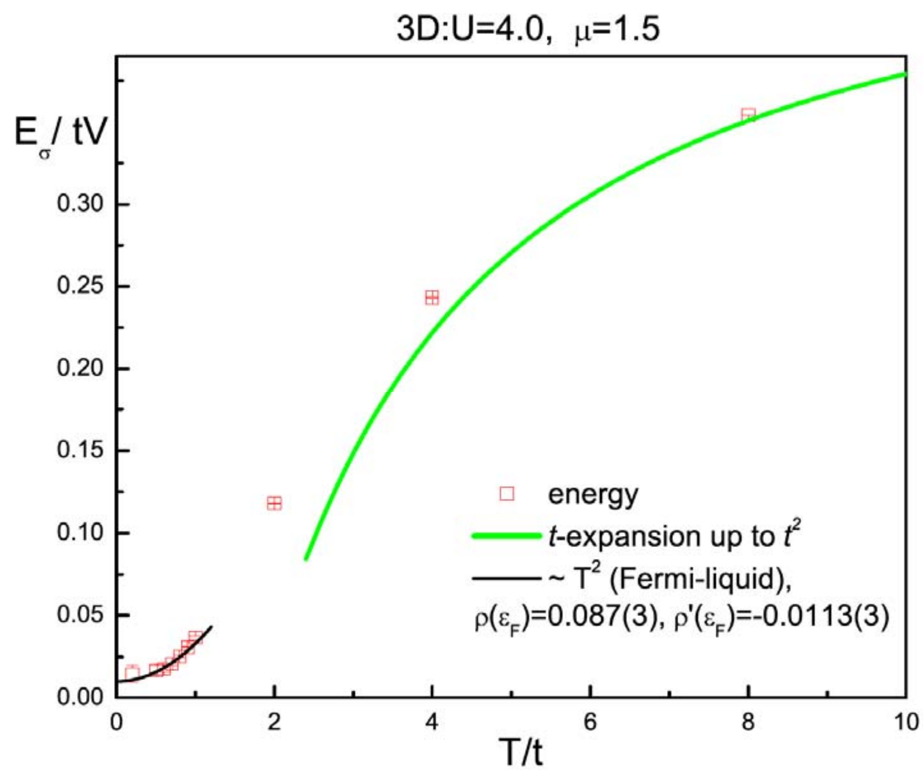
$\mu/t = 1.5$

$T/t = 0.5$



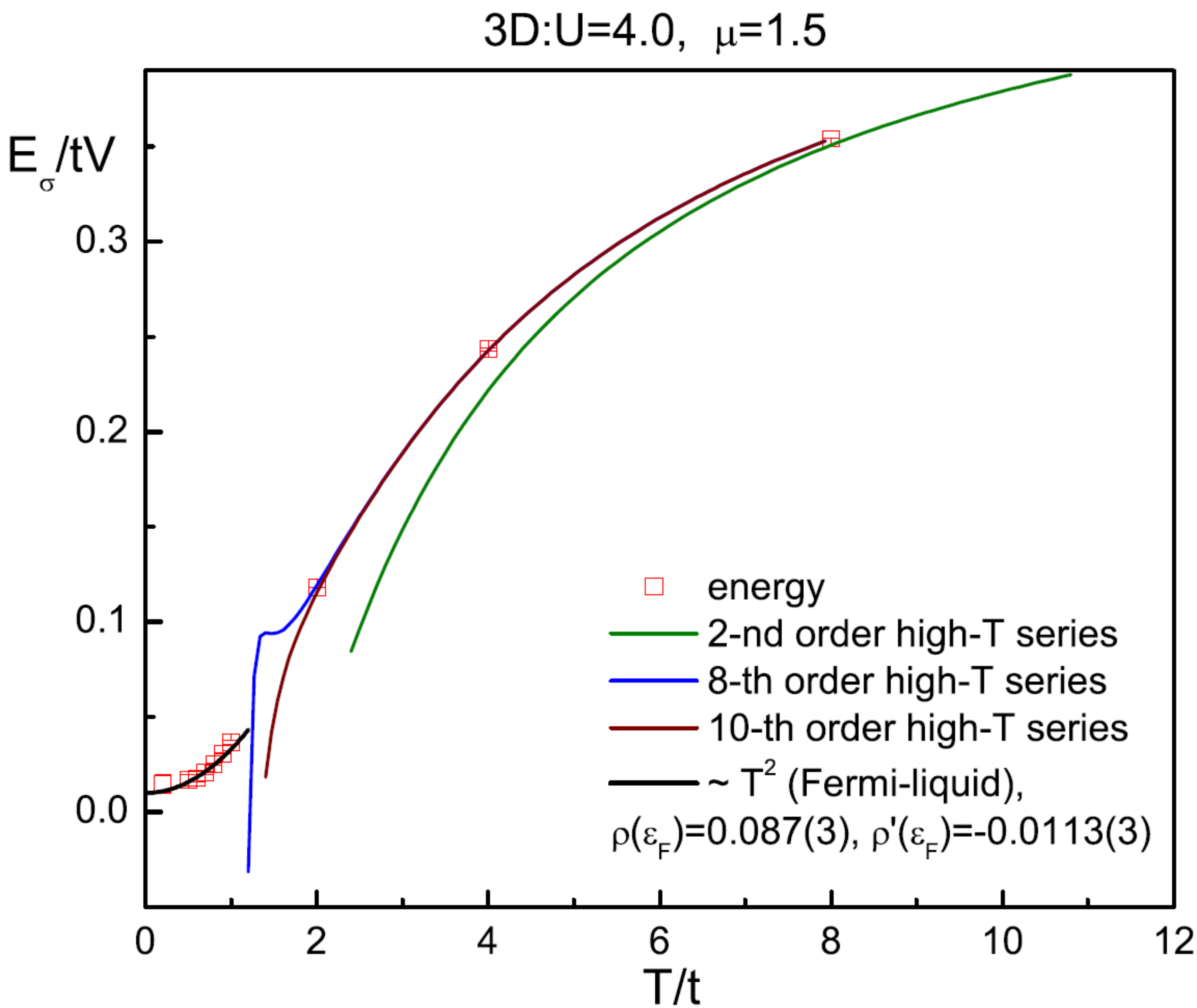
Better quality than in 1D!





In 3D temperatures are low enough $T/zt < 0.03$ to claim Fermi-liquid properties

(using bare propagators so far)


3D:U=4.0, μ=1.5
E_σ/tV
0.0
0.1
0.2
0.3
0
2
4
6
8
10
12
T/t
energy
2-nd order high-T series
8-th order high-T series
10-th order high-T series
~ T^2 (Fermi-liquid),
ρ(ε_F)=0.087(3), ρ'(ε_F)=-0.0113(3)

Conclusions/perspectives

- **Bold-line Diagrammatic series can be efficiently simulated.**

- combine analytic and numeric tools
- thermodynamic-limit results
- sign-problem tolerant (relatively small configuration space)

- **Work in progress**: bold-line implementation for the Hubbard model and the resonant Fermi-gas (G Γ version) and the continuous electron gas, or jellium model (screening version).

- **Next step**: ΓEffects of disorder, broken symmetry phases, additional correlation functions, etc.