Diagrammatic Monte Carlo for Strongly Correlated Fermions: Cooper Instability

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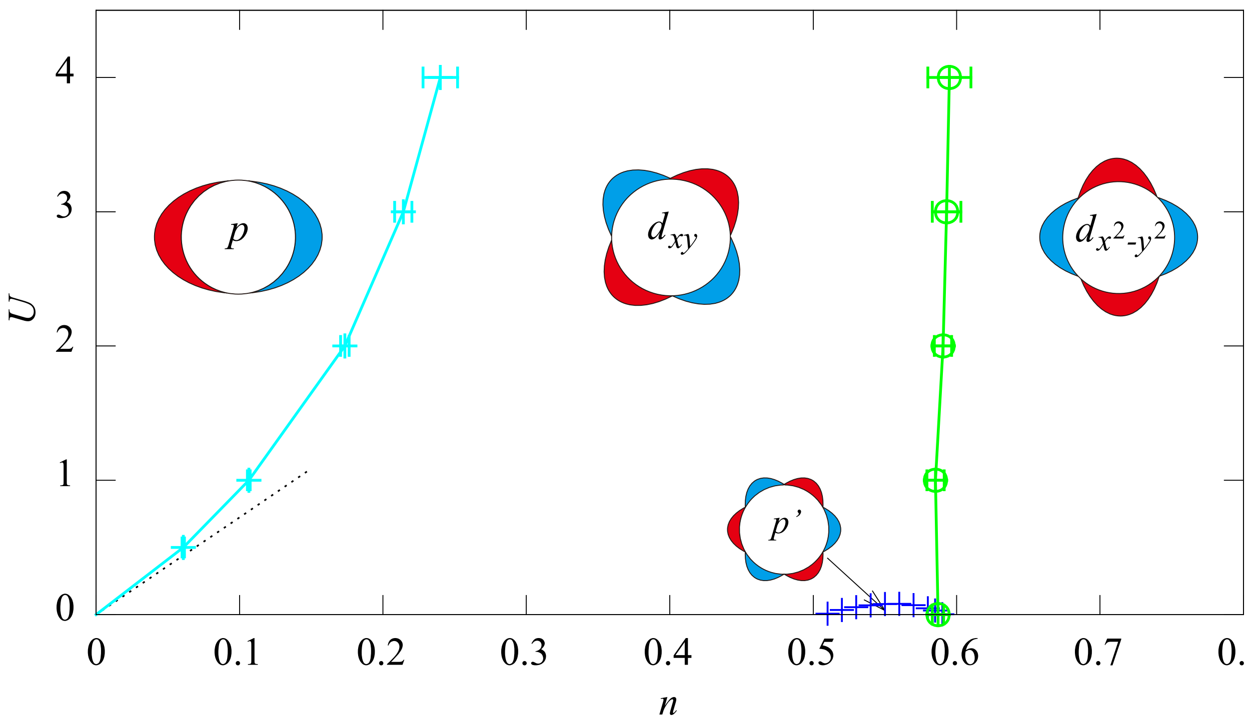
NSF DARPA SIMONS FOUNDATION

Let's start with some results for the Hubbard model…

Ground-State Phase Diagram for Fermi-Hubbard Model in the Emergent BCS Regime

Y. Deng, E. Kozik, N. Prokof'ev and BS, EPL **110**, 57001 (2015)

$$H = -t \sum_{\substack{<ij> \\ \sigma=\uparrow,\downarrow}} a^{+}_{\sigma i} a_{\sigma j} + U \sum_i n_{\uparrow i} n_{\downarrow i} \,, \qquad n_{\sigma i} = a^{+}_{\sigma i} a_{\sigma i}$$



See talk by Nikolay Prokof'ev for more detail.

Fulde-Ferrell-Larkin-Ovchinnikov pairing as leading instability on the square lattice

J. Gukelberger, S. Lienert, E. Kozik, L. Pollet, and M. Troyer (arXiv:1509.05050)

attractive Hubbard model

U/t = -4

quarter filling

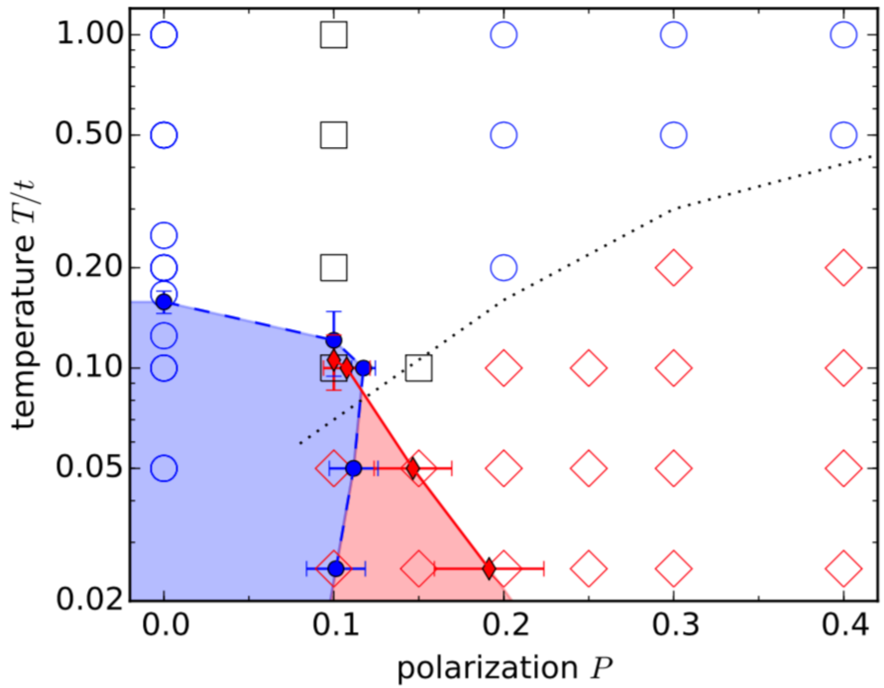


FIG. 1. (all figures: color online). Phase diagram for $U/t = -4$ at quarter filling: The white region is a Fermi liquid. In the blue shaded region, the Fermi liquid is unstable towards conventional ($\boldsymbol{Q} = 0$) pairing. In the red shaded region there is an exclusive FFLO instability with finite pair momentum $\boldsymbol{Q}_*$. Open symbols indicate whether zero- (blue circles) or finite-momentum pairing (red diamonds) is dominant (black squares: no significant difference). The black dotted line separates the two regimes. All lines are guides to the eye.

Cooper instability via linear response

Modify the Hamiltonian: $H \to H + \left(\eta^*_{12}\psi_1\psi_2 + \text{H.c.}\right)$

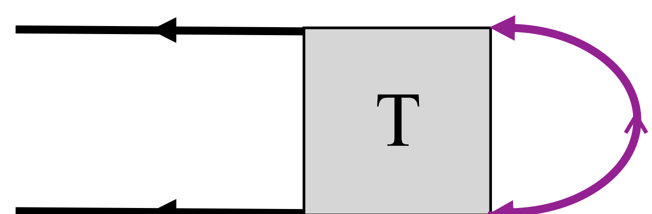
infinitesimally small
symmetry-breaking field

Study linear response $\langle \psi_1\psi_2 \rangle$

Diagrammatically:

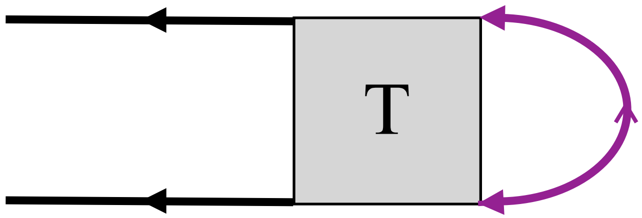
$\langle \psi_1\psi_2 \rangle$

$$= G_{13}G_{24}\eta_{34} +$$



irreducible
(in the Cooper channel)
four-pole vertex

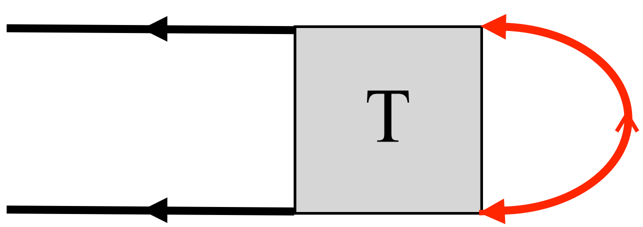
Singular response: eigenvector-eigenvalue problem



$$= G_{13}G_{24}\eta_{34}$$

just some
right-hand side…

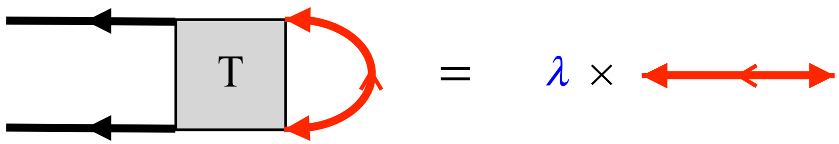
Response diverges when the following eigenvalue becomes equal **1** .



$$= \lambda \times$$

Corresponding eigenvector defines the pairing channel.

(Emergent) BCS regime



In this regime:

The four-pole vertex T is small and essentially independent of temperature.

Green's function has a Fermi-liquid form (close to the Fermi surface):

$$G(\mathbf{k},\xi) \approx \frac{z(\hat{k})}{i\xi - \mathbf{v}_F(\hat{k})\bullet[\mathbf{k}-\mathbf{k}_F(\hat{k})]}$$

Temperature dependence of λ is essentially due to the Green's function factor:

$$\lambda(T) = g\ln\left(\# E_F / T\right) \quad \Rightarrow \quad \boxed{T_c = \# E_F\, e^{-1/g}}$$

$$\boxed{g \ll 1}$$

Diagrams and Diag MC

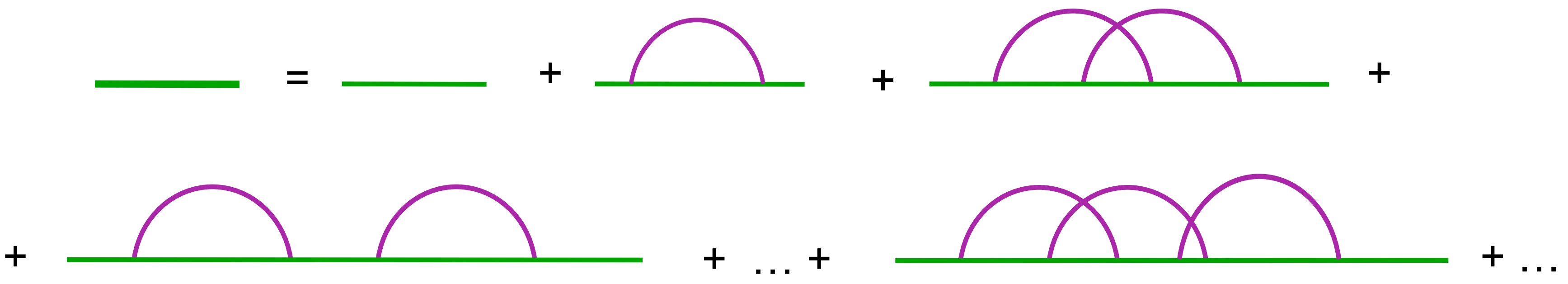
Feynman diagrams

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:

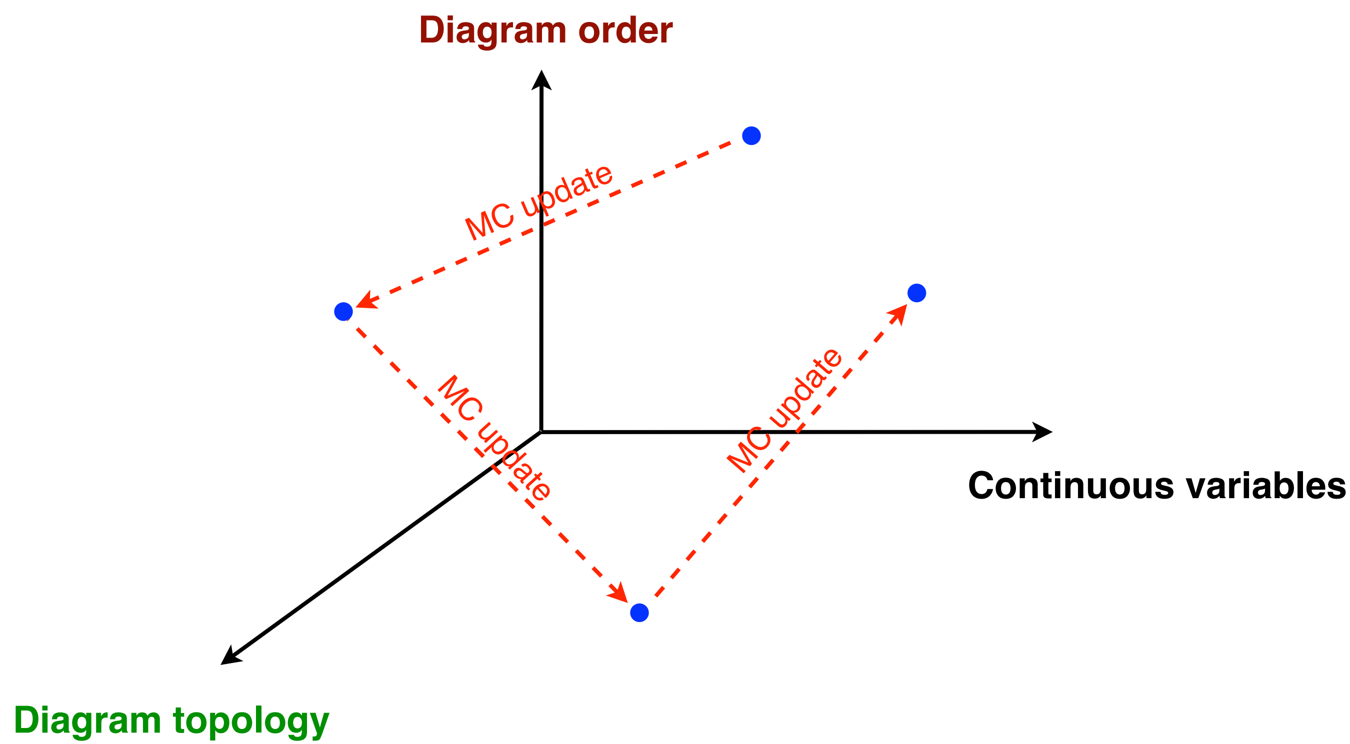


$Q(y)$ **can be sampled by Monte Carlo**

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. 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.

Bold diagrammatics challenged

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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(Received 21 July 2014; published 15 April 2015)

Shifted-action expansion: controlled dressed diagrammatic schemes

R. Rossi, F. Werner, N. Prokof'ev, and BS, 2015

Partial dressing

original action

$$S[\psi] = \langle \psi \,|\, G_0^{-1} \,|\, \psi \rangle + S_{\text{int}}[\psi]$$

auxiliary action

$$S_\xi^{(N)}[\psi] = \langle \psi \,|\, \tilde{G}_N^{-1} + \xi \Lambda_1 + \ldots + \xi^N \Lambda_N \,|\, \psi \rangle + \xi S_{\text{int}}[\psi]$$

expansion parameter

$$\tilde{G}_N^{-1} + \Lambda_1 + \Lambda_2 + \ldots + \Lambda_N = G_0^{-1} \quad \Rightarrow \quad S_{\xi=1}^{(N)} = S$$

equivalence to the original action

self-energies of corresponding orders,
playing the role of counterterms

Full dressing:
sufficient condition for converging to correct answer

(i) The sequence $\tilde{G}_N$ converges and is uniformly bounded.

(ii) The sequence

$$\xi\Lambda_1\left[\tilde{G}_N\right]+\xi^2\Lambda_2\left[\tilde{G}_N\right]+\ldots+\xi^N\Lambda_N\left[\tilde{G}_N\right]$$

converges and is uniformly bounded within a circle $|\xi|<\xi_0$, where $\xi_0>1$.

Resonant Fermions: Dealing with Zero Convergence Radius

Model of Resonant Fermions

(from ultra-cold atoms to neutron stars)

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 .)

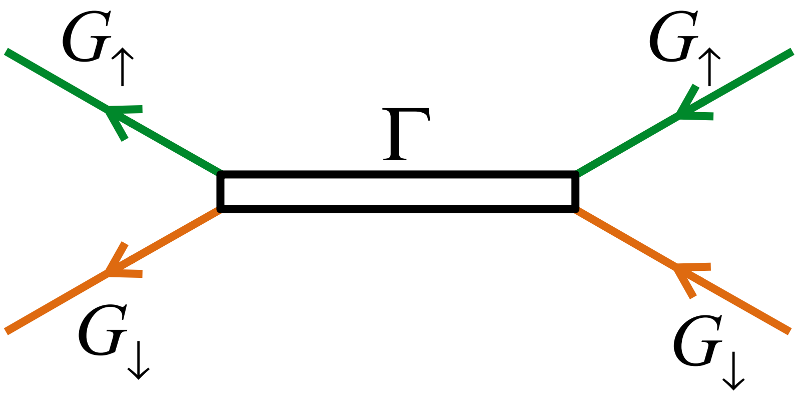
$$c \gg n^{1/3} \sim k_F \quad \Rightarrow$$ BCS regime

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

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

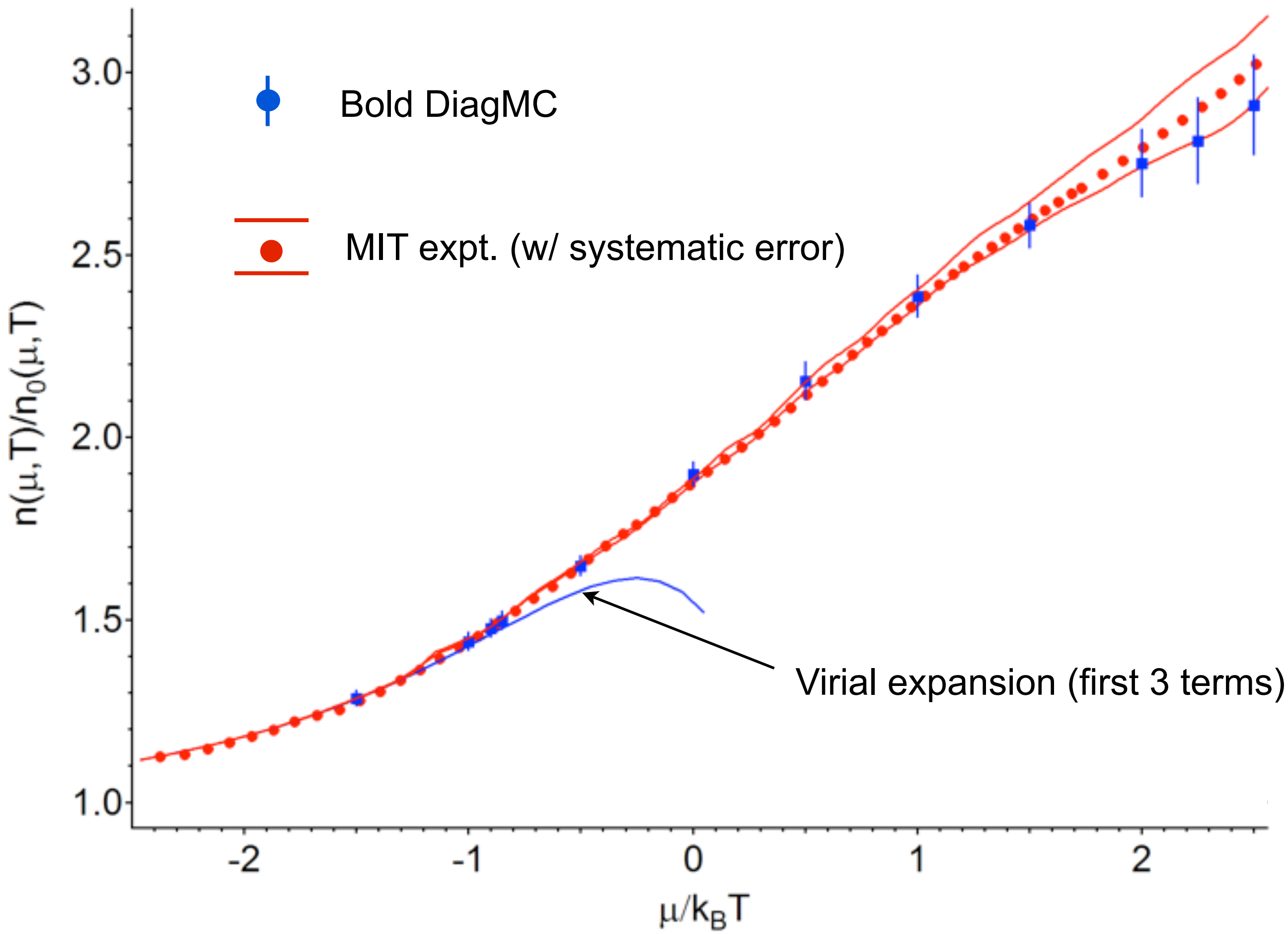
$$c = 0 \quad \Rightarrow$$ unitarity point: scale invariance

Diagrammatics for Resonant Fermions



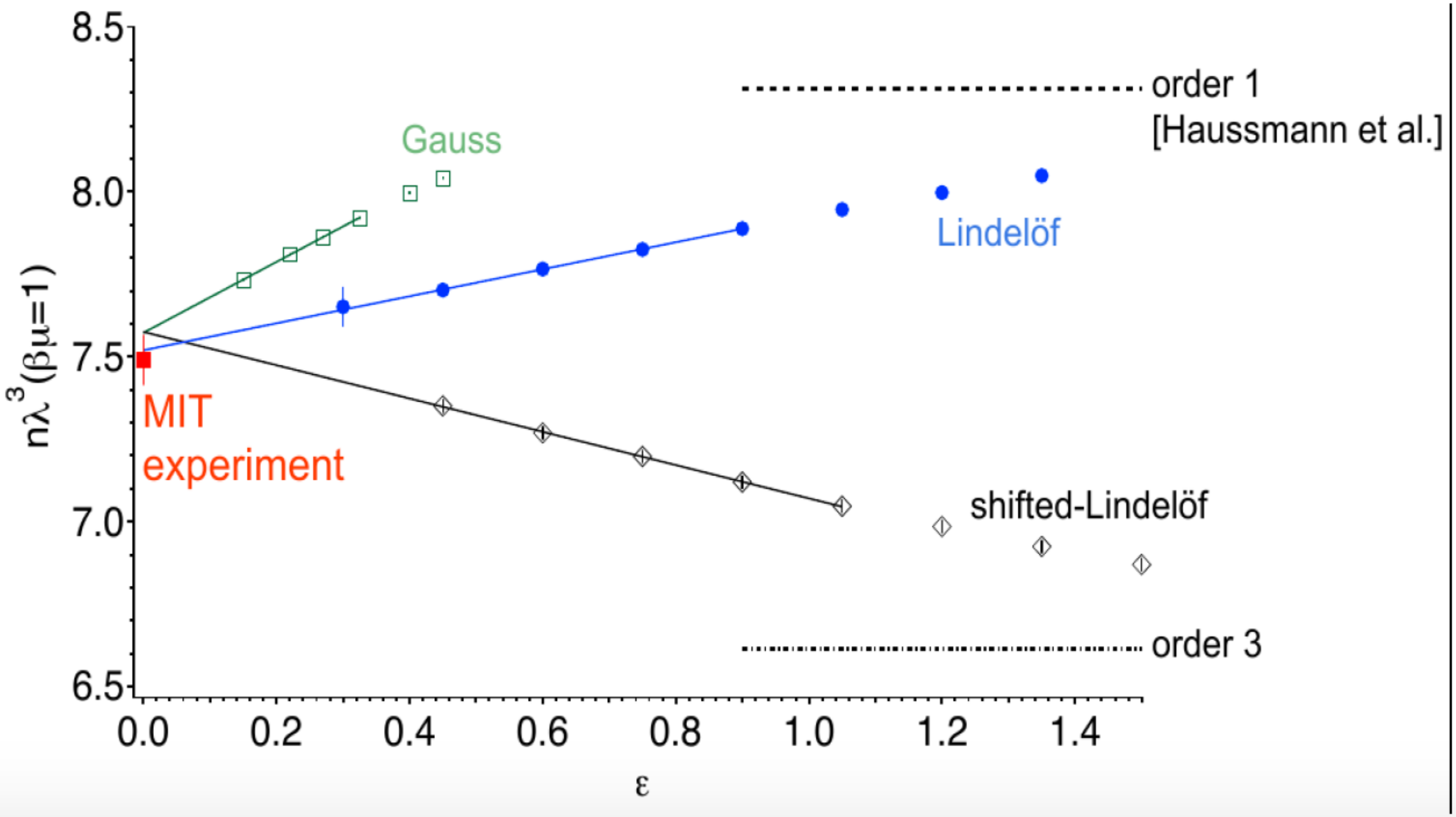
Γ is a pseudo molecule propagator.

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)

Lindelöf resummation: $\lim_{\epsilon \to 0} \sum_{n \geq 0} a_n e^{-\epsilon n \ln n}$ *assuming non-zero radius of convergence*



Resuming divergent series by generalized Borel transformation

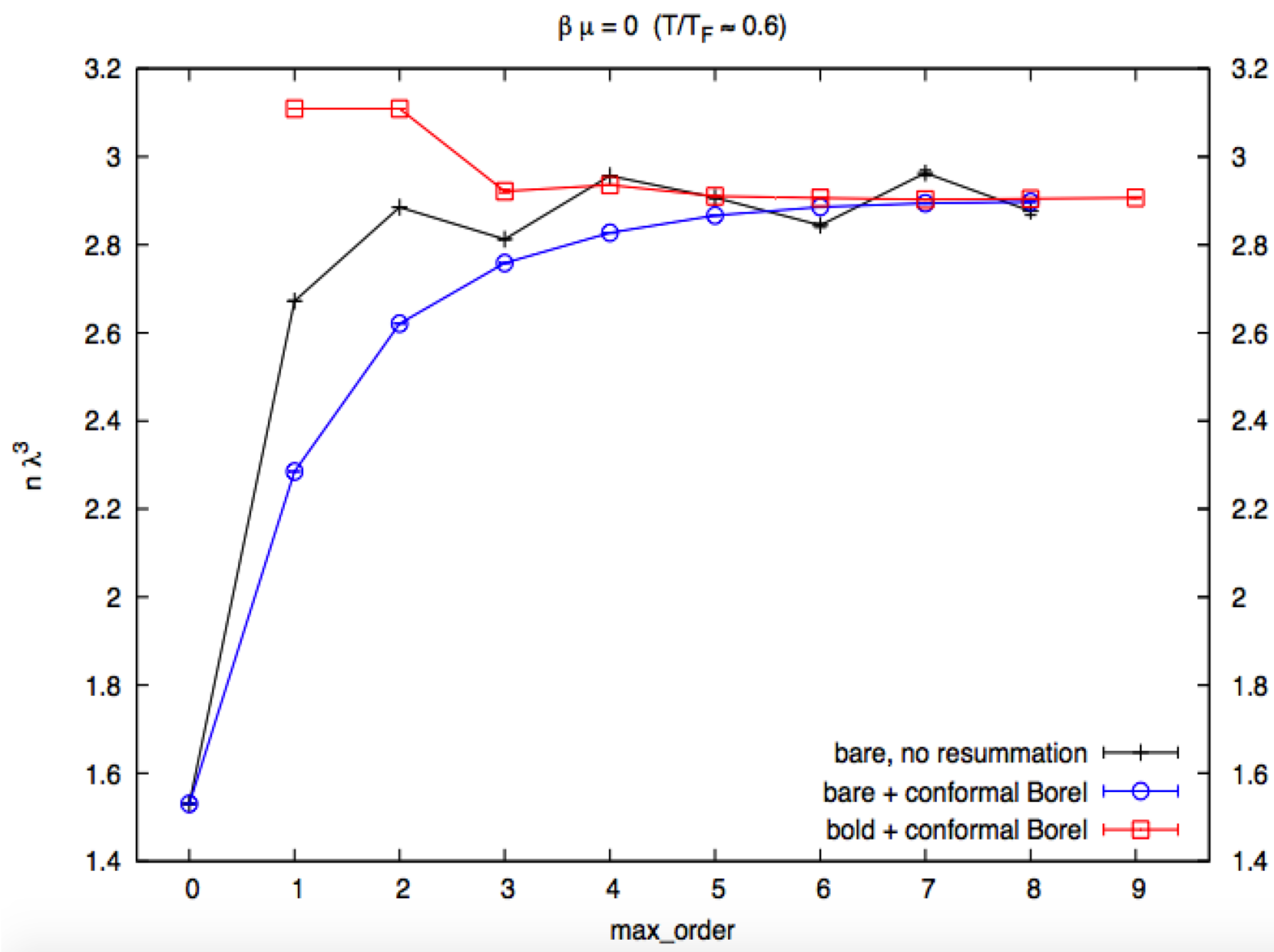
PhD work by Riccardo Rossi (ENS, Paris)

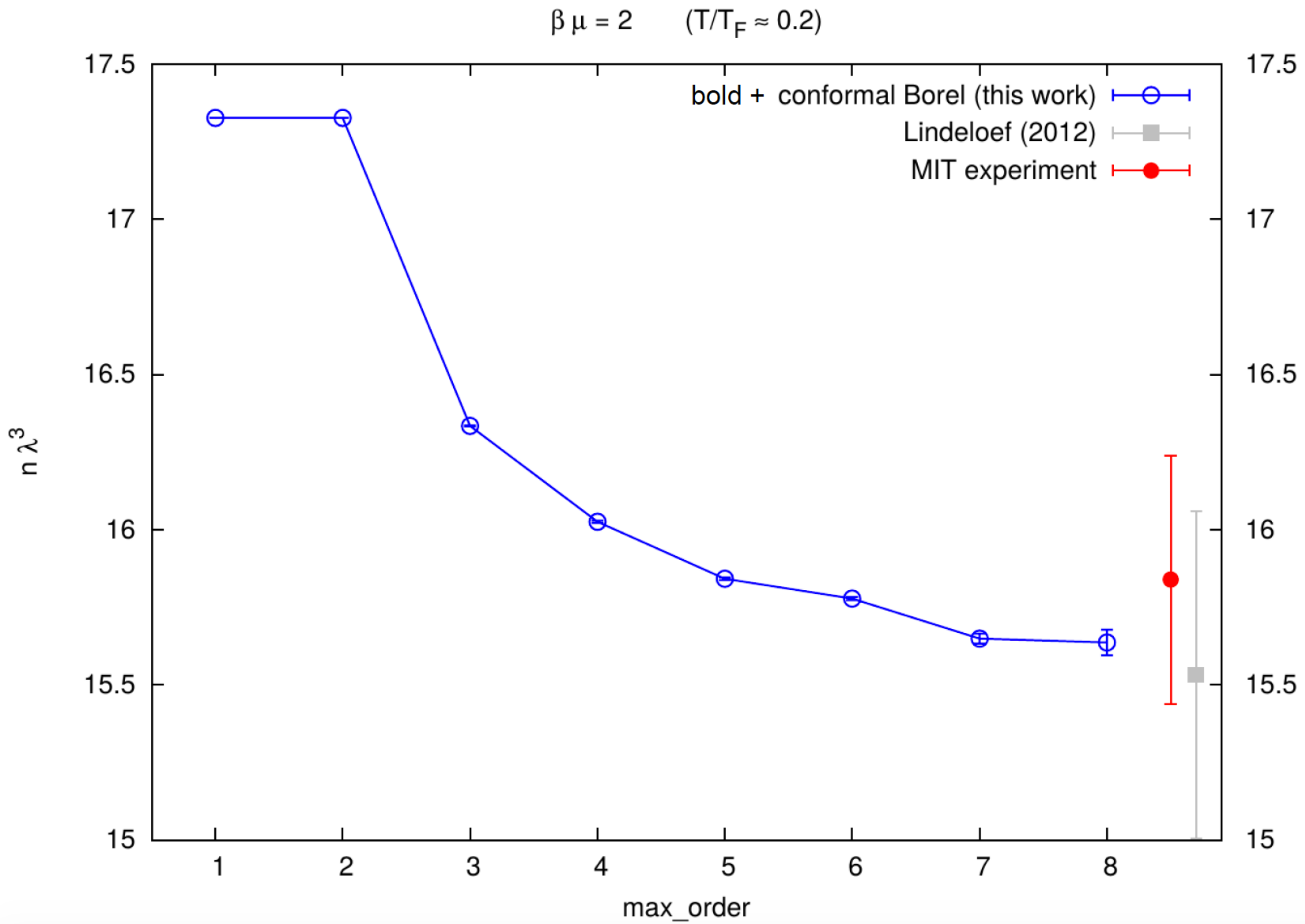
Advisors: Felix Werner and Kris Van Houcke

Idea of optimal resummation:

1. Establish the large-order asymptotic form of the Taylor series (seminal works on the approach are by Lipatov, Brézin, Le Guillou, Zinn-Justin, Parisi, Itzykson, and Zuber).

2. Use this knowledge to adjust the form of the generalized Borel transformation.


β μ = 0 (T/T_F ≈ 0.6)
n λ^3
max_order
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
0
1
2
3
4
5
6
7
8
9
bare, no resummation
bare + conformal Borel
bold + conformal Borel



β μ = 2 (T/T_F ≈ 0.2)
bold + conformal Borel (this work)
Lindeloef (2012)
MIT experiment
n λ^3
max_order
17.5
17
16.5
16
15.5
15
1
2
3
4
5
6
7
8

Order Parameter Susceptibility $\quad \chi = -\Gamma(\mathbf{p} = \mathbf{0}, \Omega_n = 0)$