DIAGRAMMATIC MONTE CARLO APPLICATIONS

Polarons

Path-integrals

Resonant fermions & Neutron stars

Fermi Hubbard model

Frustrated Quantum magnetism

National Science Foundation
WHERE DISCOVERIES BEGIN
DARPA DSO DEFENSE SCIENCES OFFICE
OPTICAL LATTICE EMULATOR OLE

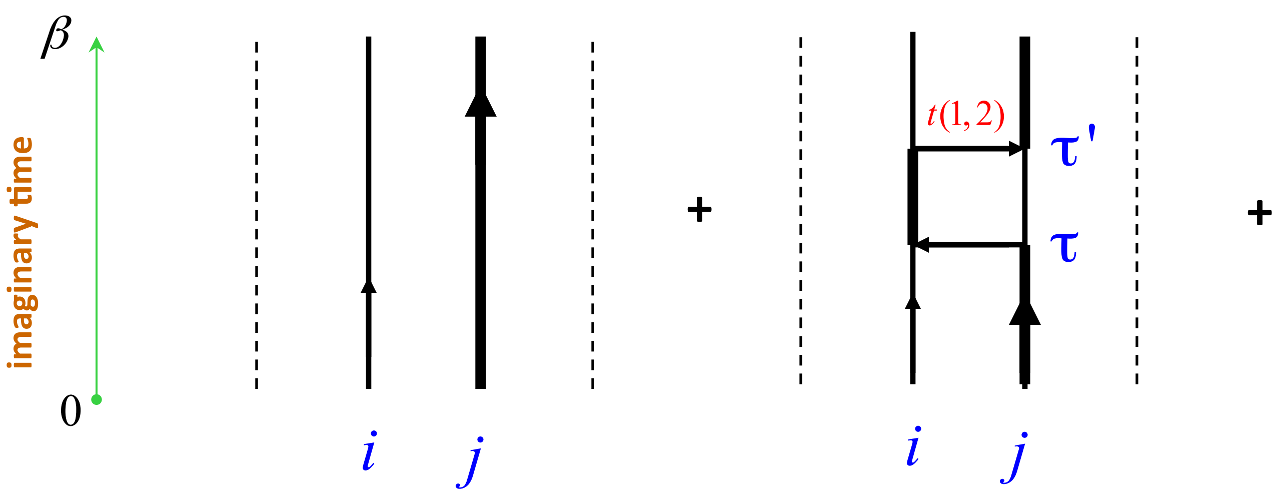
Tallahassee, NHMFL (January 2012)

$$H = H_0 + H_1 = \sum_{ij} U_{ij} n_i n_j - \sum_i \mu_i n_i \;\; - \sum_{<ij>} t(n_i, n_j) b_j^+ b_i$$

Lattice path-integrals for bosons and spins are "diagrams" of closed loops!

$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \mathrm{Tr}\, e^{-\beta H_0}\, e^{-\int_0^\beta H_1(\tau)\, d\tau}$$

$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_0^\beta \int_\tau^\beta H_1(\tau)\, H_1(\tau)\;\; d\tau\, d\tau' + \ldots \right\}$$



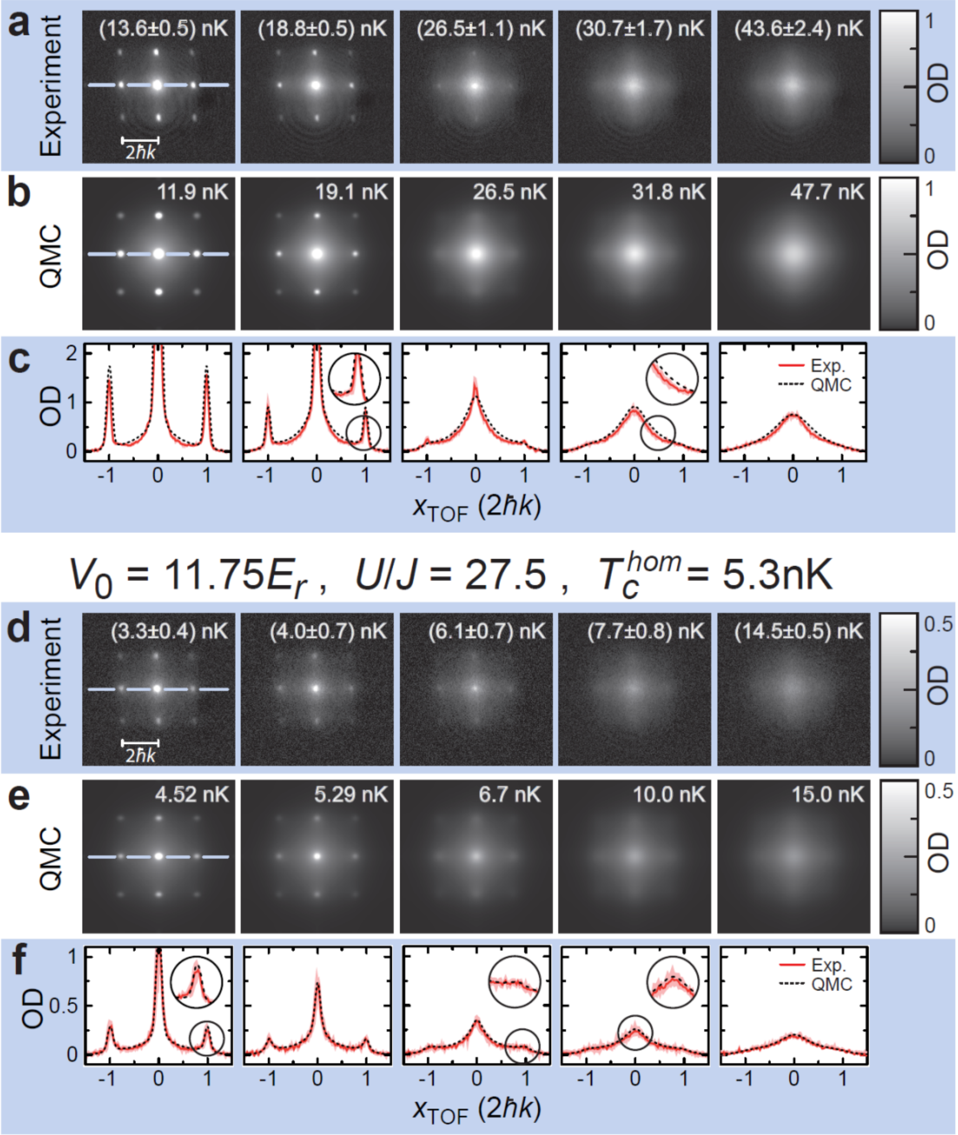
$$|n_i = 0, 1, 2, 0\rangle$$

Simulating Bose-Hubbard model "as is" and comparing to experiments:

(in this example, $N \approx 300000$)

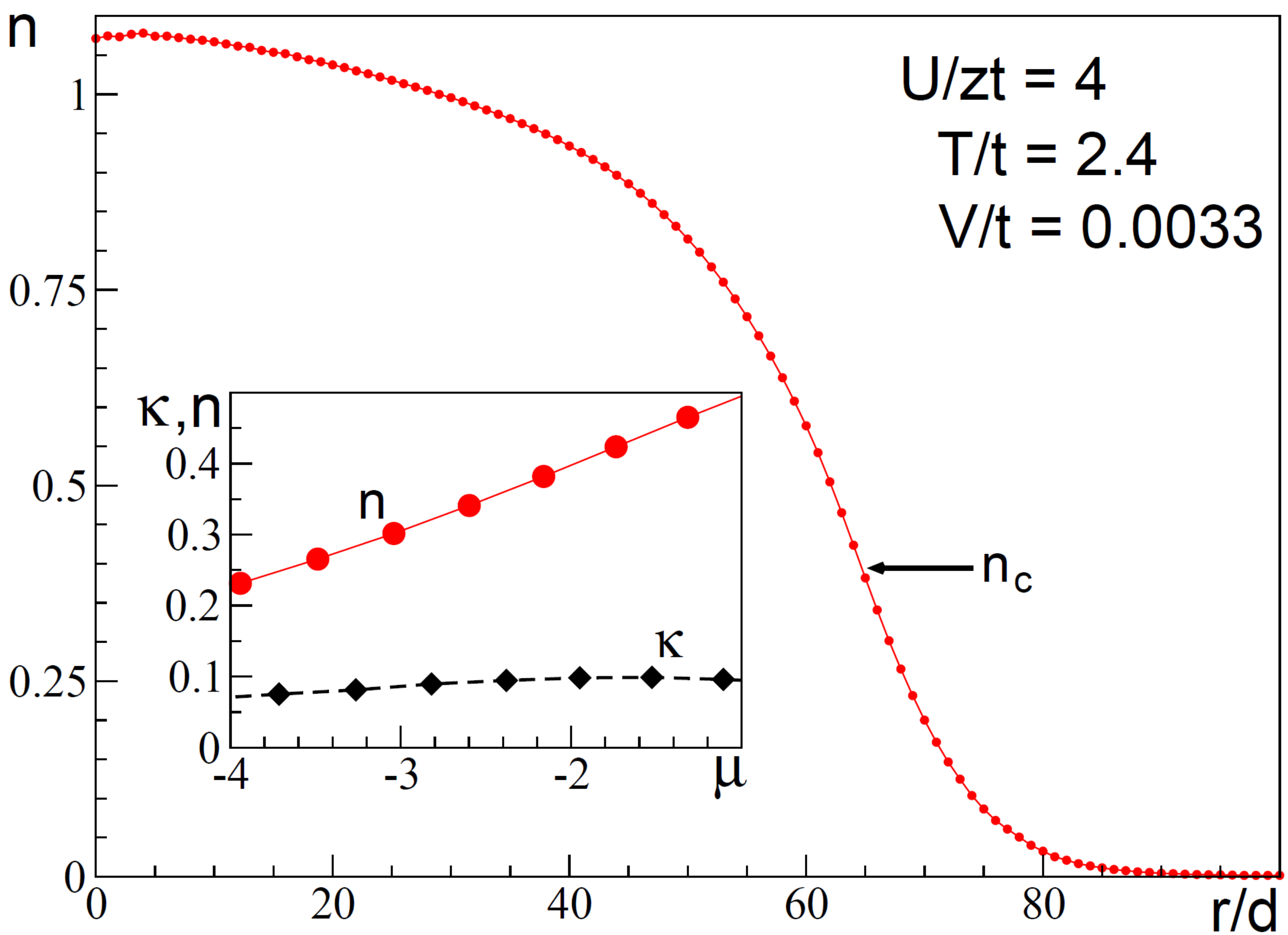
$V_0 = 8E_r$, $U/J = 8.11$, $T_c^{hom} = 26.5$nK

$V_0 = 11.75E_r$, $U/J = 27.5$, $T_c^{hom} = 5.3$nK



Nature Physics, 6, 998–1004, (2010)

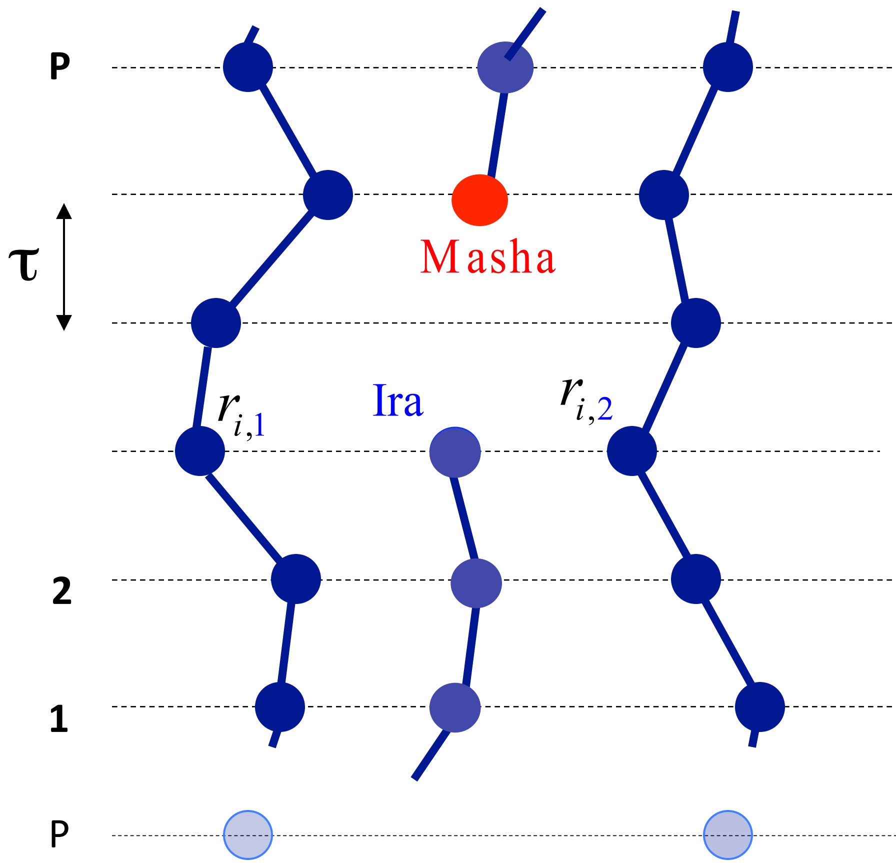
It is realistic to do about 2,000,000 or more particles at temperatures relevant for the experiment.



Phys. Rev. Lett. **103**, 085701 (2009)

Path-integrals in continuous space; He-4 case

$$Z_{WA} = \iiint dR_1 \ldots dR_P \exp\left\{ -\sum_{i=1}^{P=\beta/\tau} \left(\frac{m(R_{i+1}-R_i)^2}{2\tau} + U(R)\tau \right) \right\} + G$$



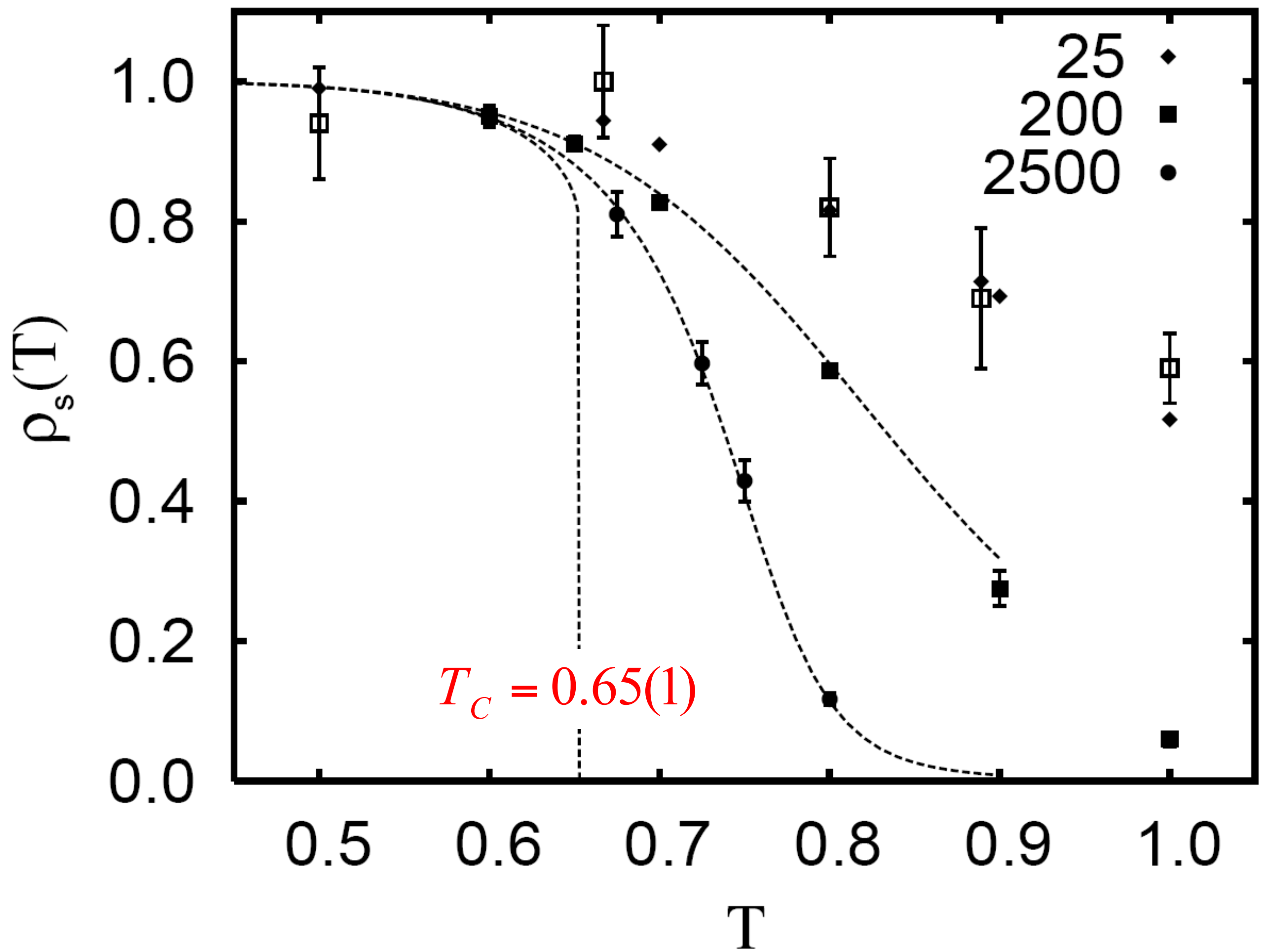
$$R_i = (r_{i,1}, r_{i,2}, \ldots, r_{i,N})$$

Superfluid density: 2D & 3D He-4

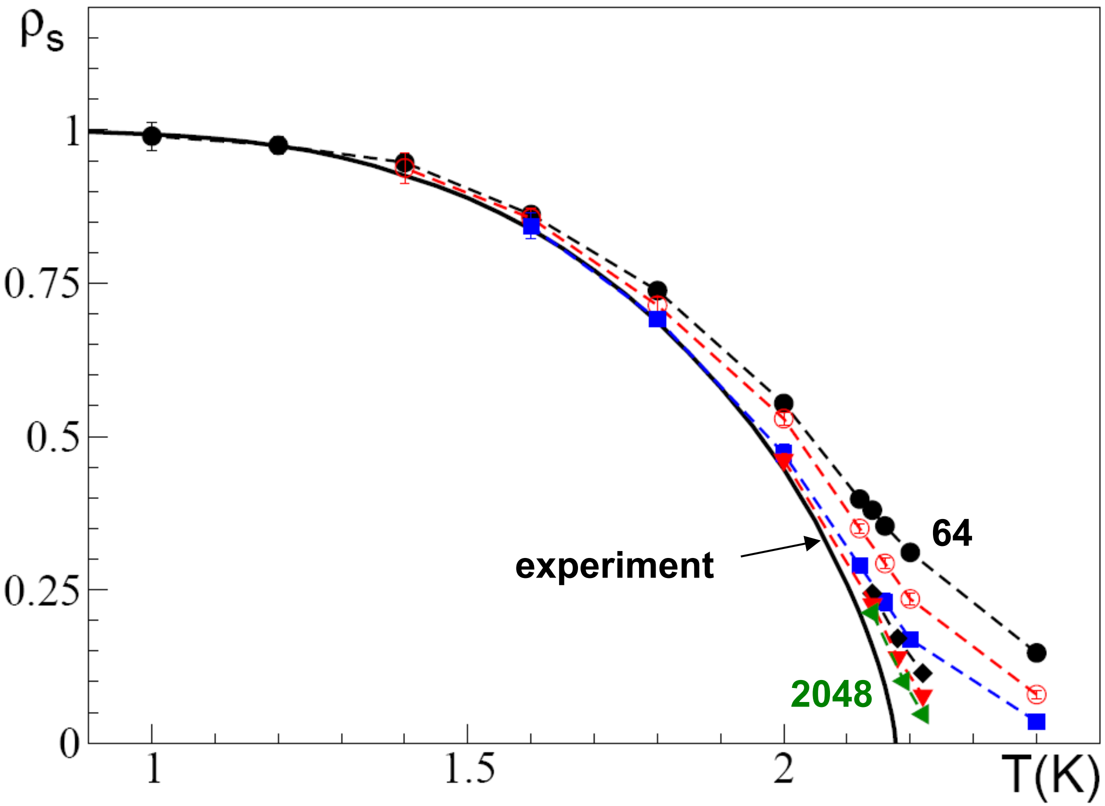
$$\rho_S = \frac{T\langle W^2 \rangle}{Ld}$$

Ceperley, Pollock '87

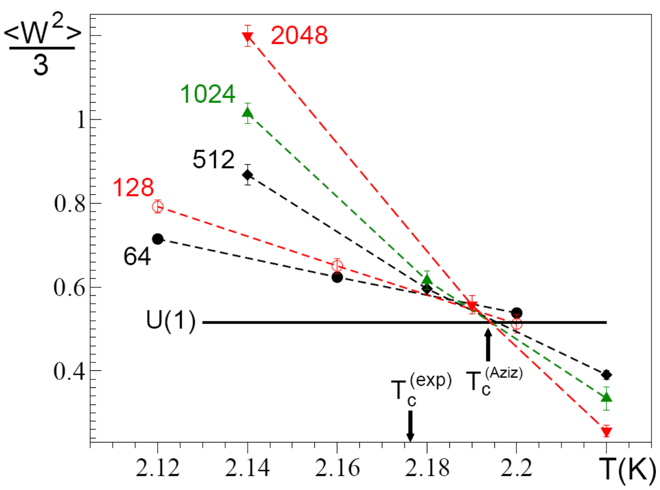
2D @ $(n = 0.0432\ A^{-2})$



3D @ s.v.p.



$$L\rho_S / T = \langle W^2 \rangle / 3$$



$$T_C^{Aziz} = 2.193 \quad \textbf{vs} \quad T_C^{\exp} = 2.177$$

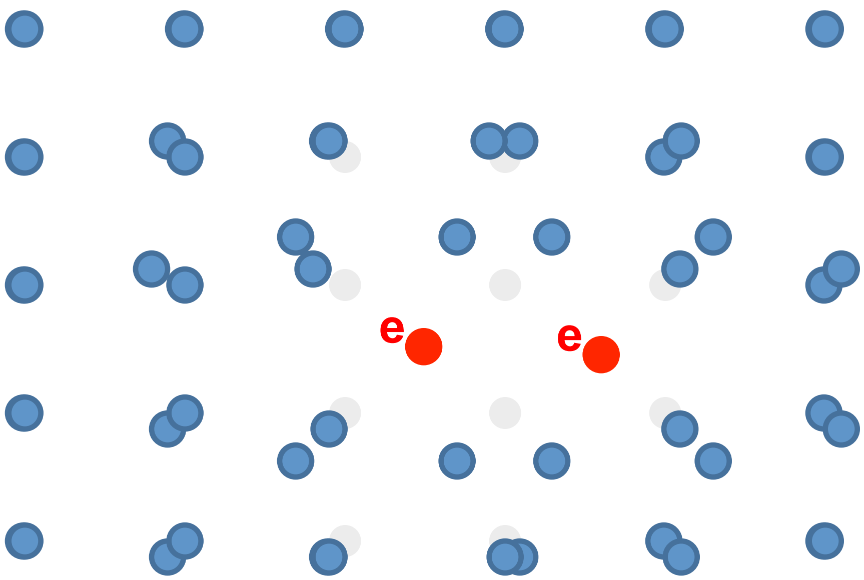
Polaron problem:

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

quasiparticle

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

Electrons in semiconducting crystals (electron-phonon polarons)



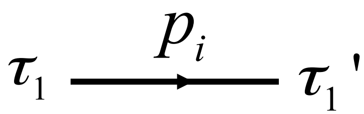
$$H = \sum_p \varepsilon(p) a_p^+ a_p + \quad \textbf{electron}$$

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

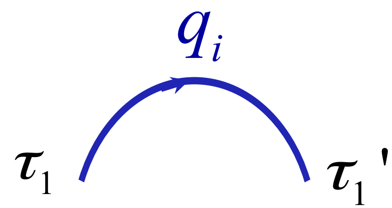
$$\sum_{pq} \left(V_q a_{p-q}^+ a_p b_q^+ + h.c. \right) \quad \textbf{el.-ph. interaction}$$

$$H = \sum_p \varepsilon(p) a_p^+ a_p + \sum_q \omega(p)(b_q^+ b_q + 1/2) + \sum_{pq} \left(V_q a_{p-q}^+ a_p b_q^+ + h.c. \right)$$

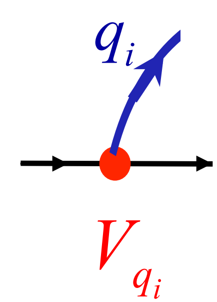
electron | **phonons** | **el.-ph. interaction**



$$e^{-\varepsilon(p_i)(\tau_i' - \tau_i)}$$



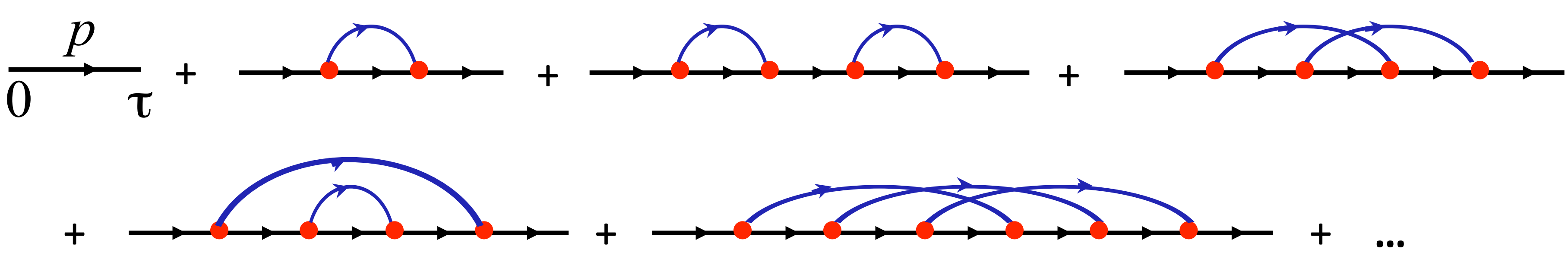
$$e^{-\omega(q)(\tau_i' - \tau_i)}$$



Green function: $G(p,\tau) = \left\langle a_p(0) a^+{}_p(\tau) \right\rangle = \left\langle a_p \, e^{-\tau H} \, a^+{}_p \, e^{\tau H} \right\rangle$

= **Sum of all Feynman diagrams**

Positive definite series in the (p,τ) **representation**



Analysing data: $G(p,\tau \to \infty) \to Z_p e^{-E(p)\tau}$

$Z_p = |C_p|^2$ **probability of getting a bare electron**

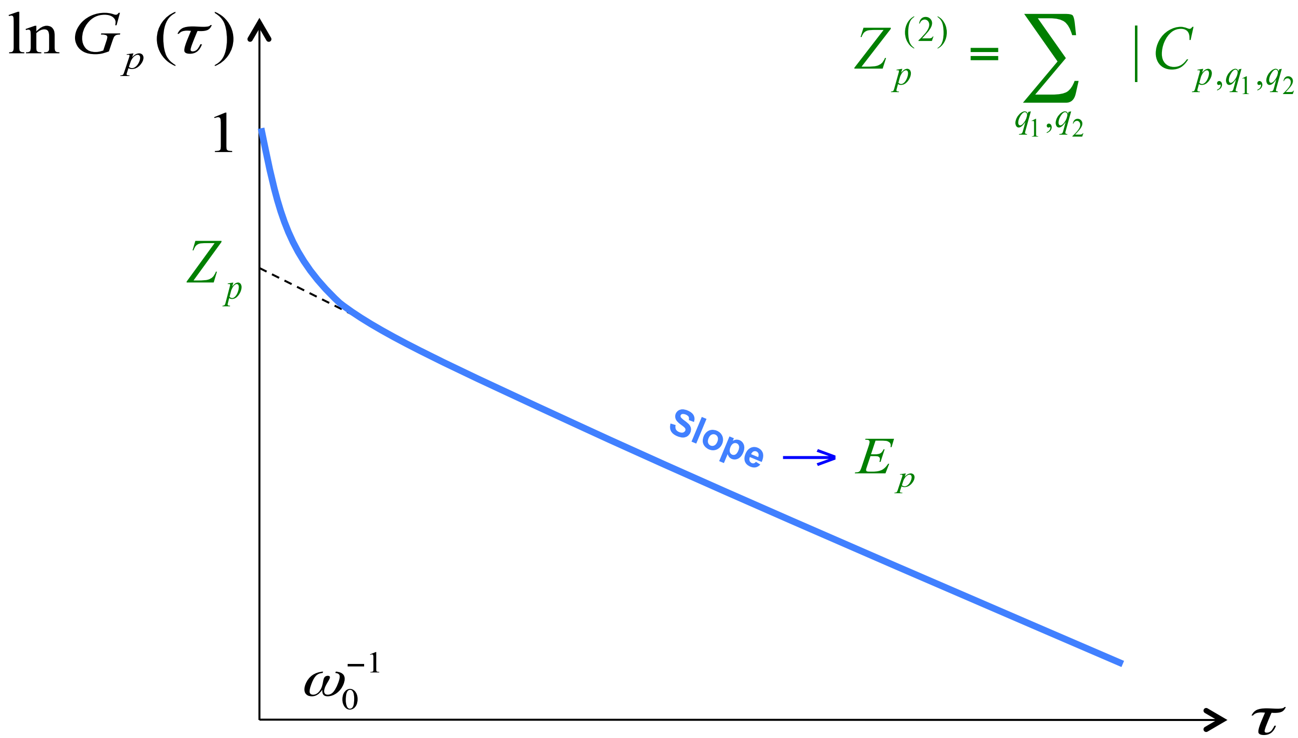
dispersion relation

(Lehman expansion)

$$\left|E_p\right\rangle = C_p\, a_p^\dagger \left|0\right\rangle + \sum_q C_{p,q}\, b_q^\dagger a_{p-q}^\dagger \left|0\right\rangle + \sum_{q_1 q_2} C_{p,q_1,q_2}\, b_{q_1}^\dagger b_{q_2}^\dagger a_{p-q_1-q_2}^\dagger \left|0\right\rangle + \ldots$$

$$Z_p^{(2)} = \sum_{q_1,q_2} |C_{p,q_1,q_2}|^2$$

probability of getting two phonons in the polaron cloud



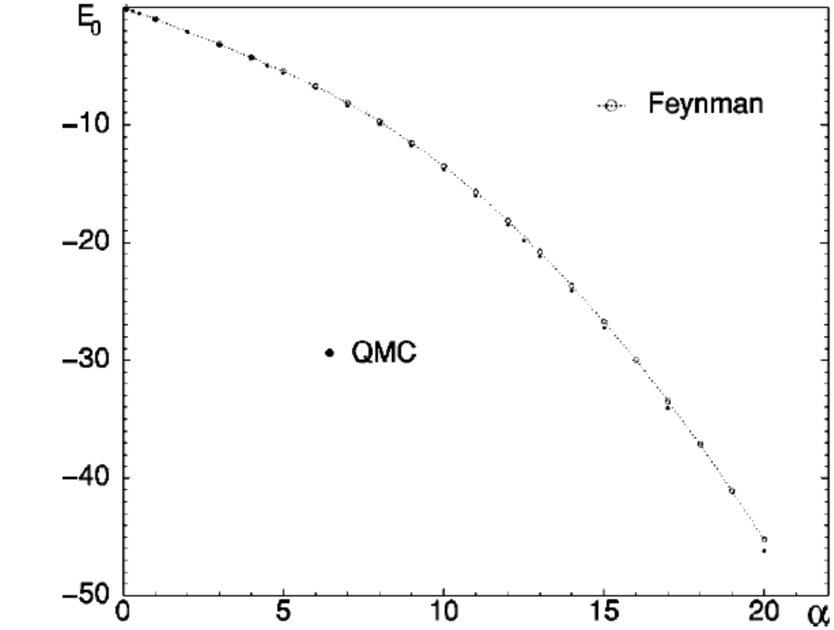


FIG. 4. Bottom of the polaron band E_0 as a function of α. The error bars are much smaller than the point size.

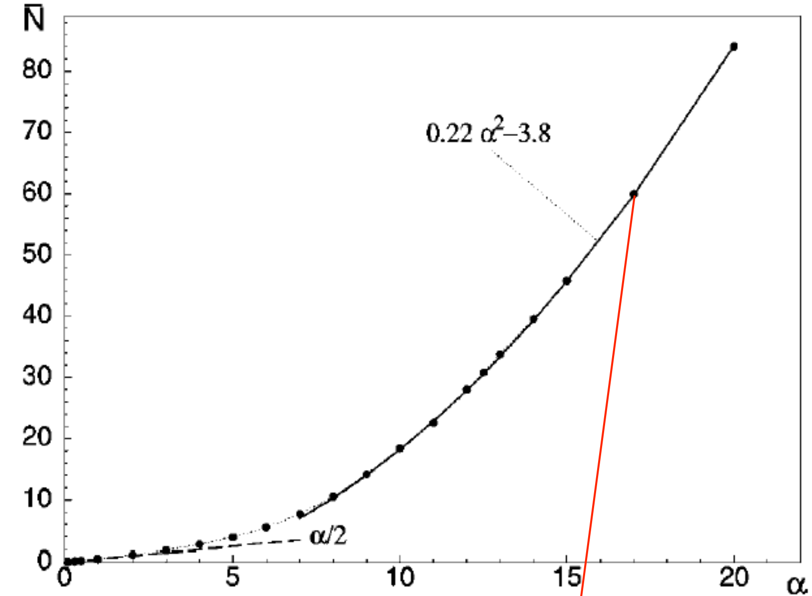
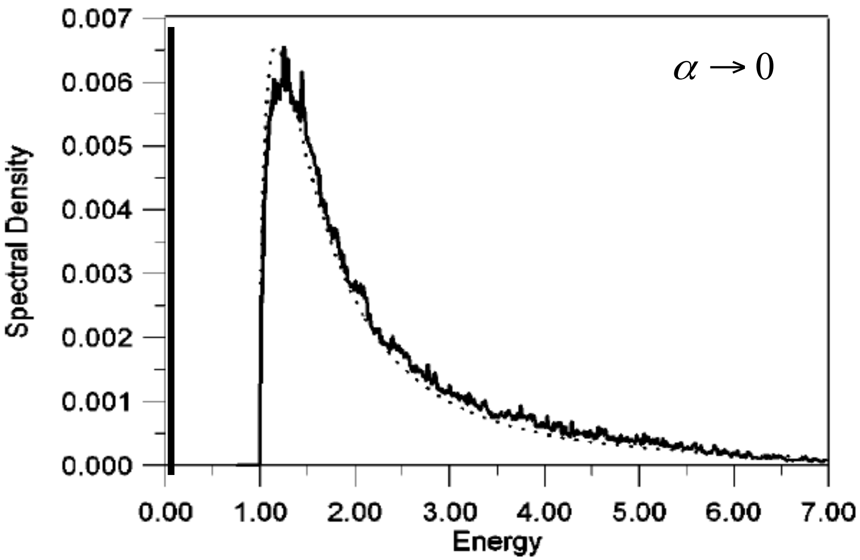
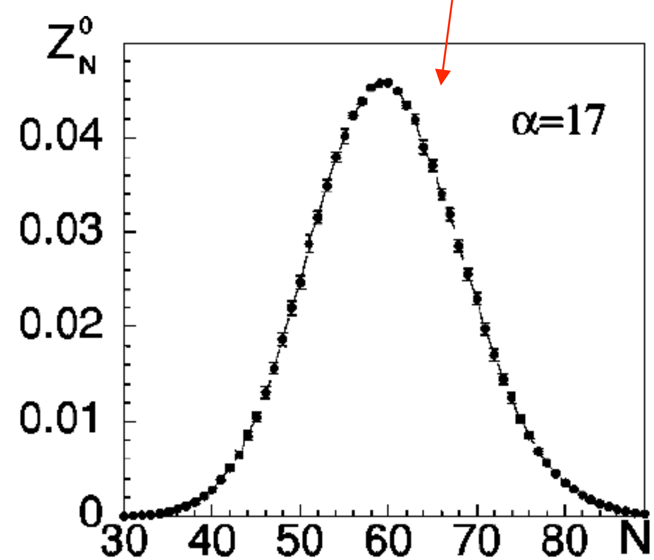
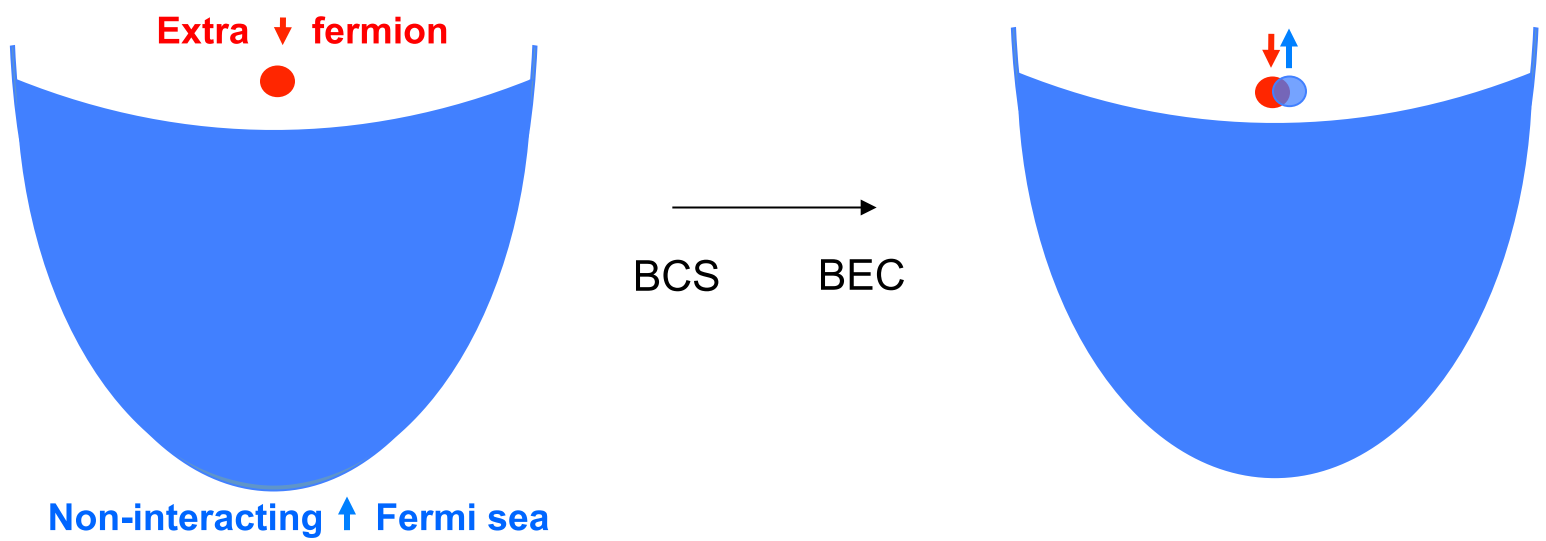


FIG. 8. The average number of phonons in the polaron ground state as a function of α. Filled circles are the MC data (calculated to the relative accuracy better than 10^{-3}), the dashed line is the perturbation theory result (4.1), and the solid line is the parabolic fit for the strong coupling limit.





Fermi-polaron = particle dressed by interactions with the Fermi sea;
orthogonality catastrophe, X-ray singularities, heavy fermions,
quantum diffusion in metals, ions in He-3, etc
Cold resonant Fermi gases: resonant interaction



Fermionic quasiparticle (polaron)

$$E_p(k) = E_p + k^2/2m_p$$

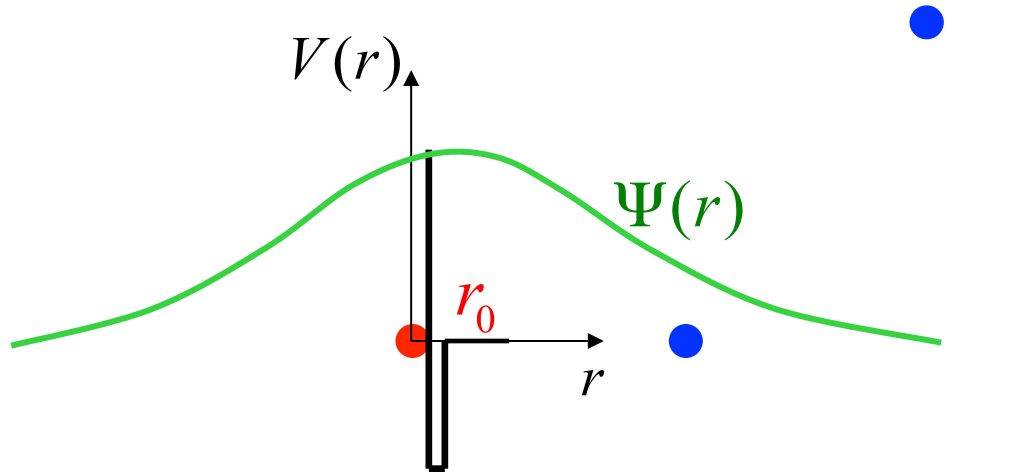
\+ *quasiparticle residue*

Bosonic quasiparticle (molecule)

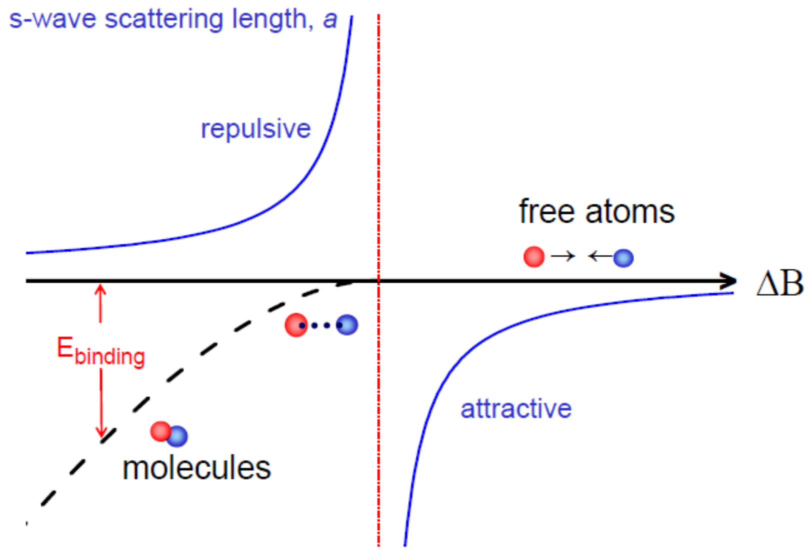
$$E_M(k) = E_M + k^2/2m_M$$

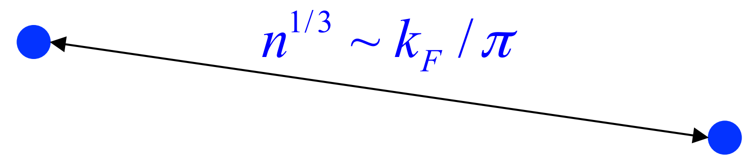
\+ *quasiparticle residue*

Resonant Fermions



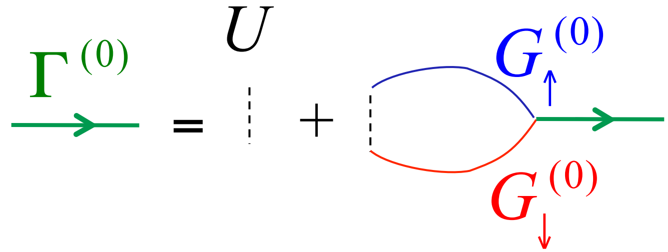
Magnetic-field Feshbach resonance

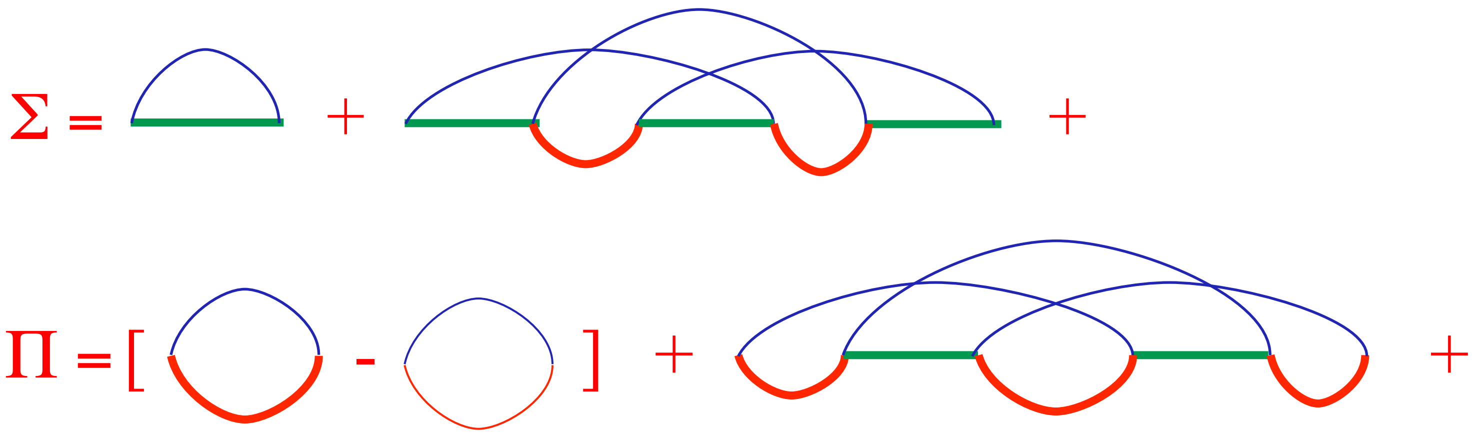




Universal results in the zero-range, $k_F r_0 \to 0$, and thermodynamic limit

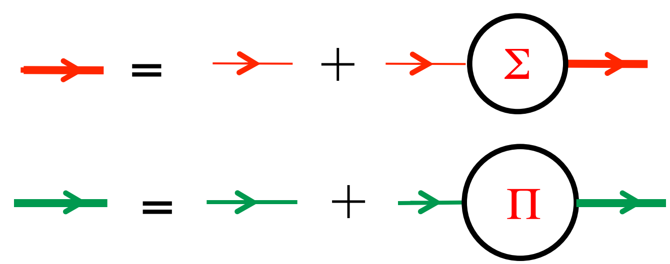
Build diagrams using ladders:
(contact potential)





In terms of "exact" propagators

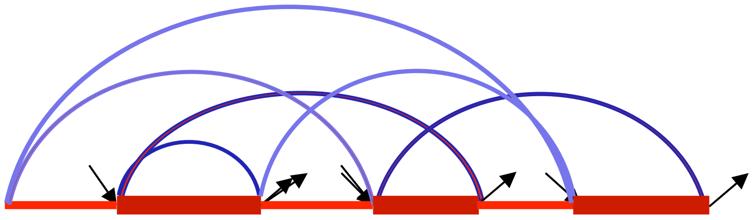
Dyson Equations:



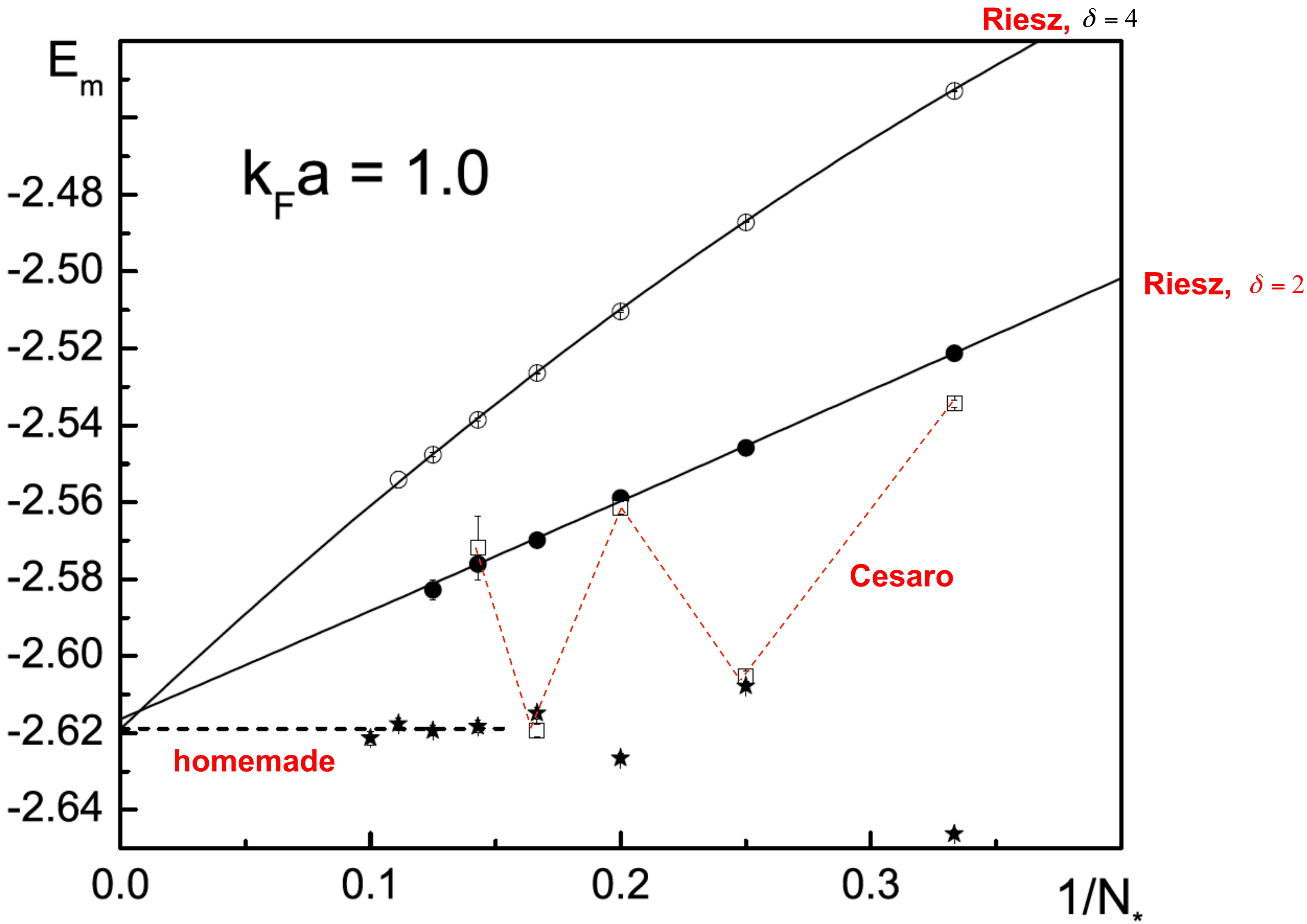
For the rest:

- **develop an ergodic algoritm sampling diagrams for $\Sigma_{\downarrow}$ and $\Sigma_{mol} = \Pi$ which are proper self-energies for polarons and molecules (an appropriate Worm Algorithm does the job)**

Updates:



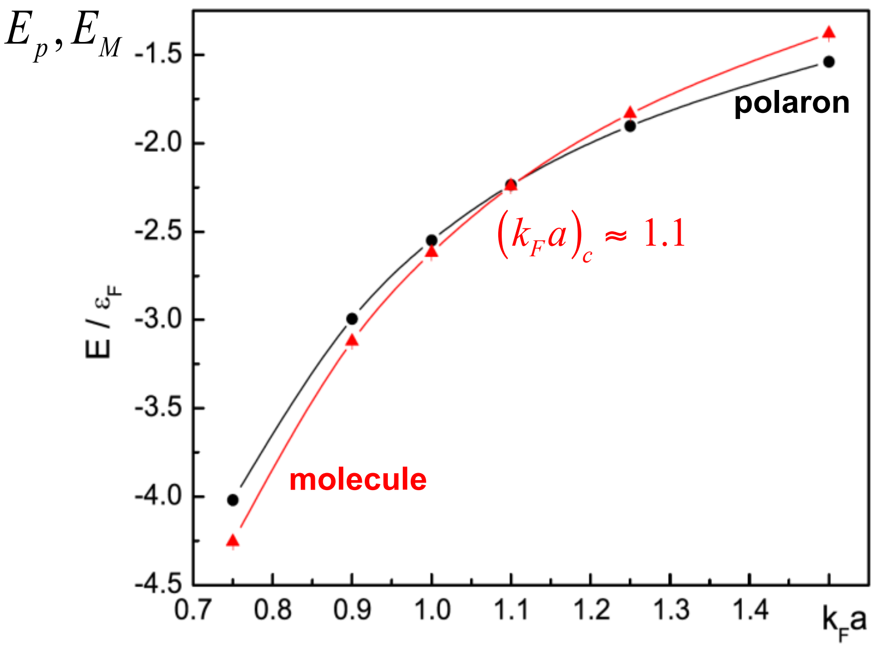
- **calculate self-energies to higher and higher order (up to 11-th)**

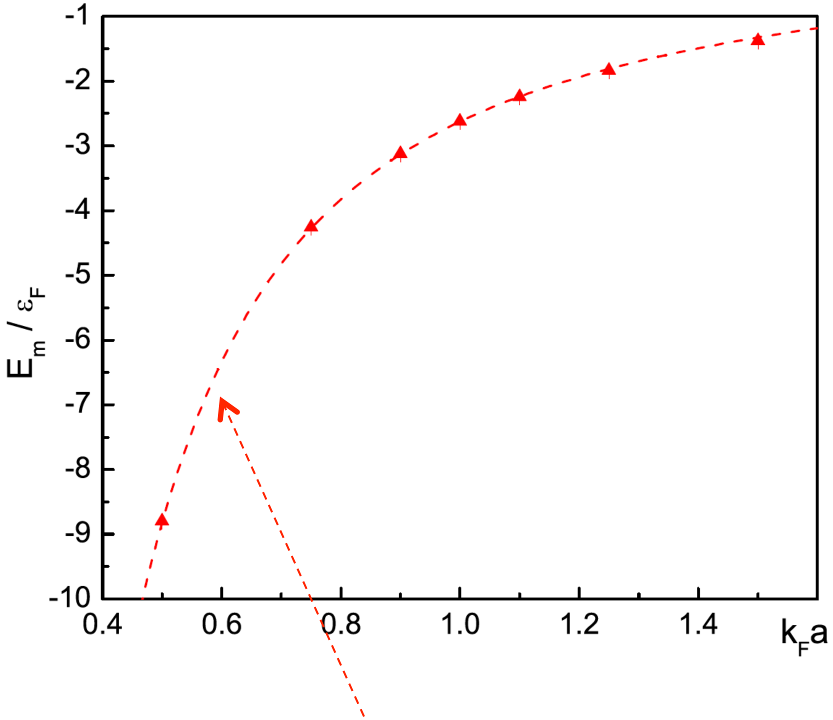


Riesz, δ = 4
Riesz, δ = 2
E_m
$k_F a = 1.0$
-2.48
-2.50
-2.52
-2.54
-2.56
-2.58
-2.60
-2.62
-2.64
Cesaro
homemade
0.0
0.1
0.2
0.3
$1/N_*$

Polaron spectrum from the $G_{\downarrow}(\mathbf{p},\omega)$ **pole:** $\omega - p^2/2m - \Sigma(\mathbf{p},\omega) = 0$

In imaginary time representation: $E - p^2/2m - \int_0^{\infty} \Sigma(\mu_{\downarrow},\mathbf{p},\tau)\, e^{(E-\mu_{\downarrow})\tau} d\tau = 0$

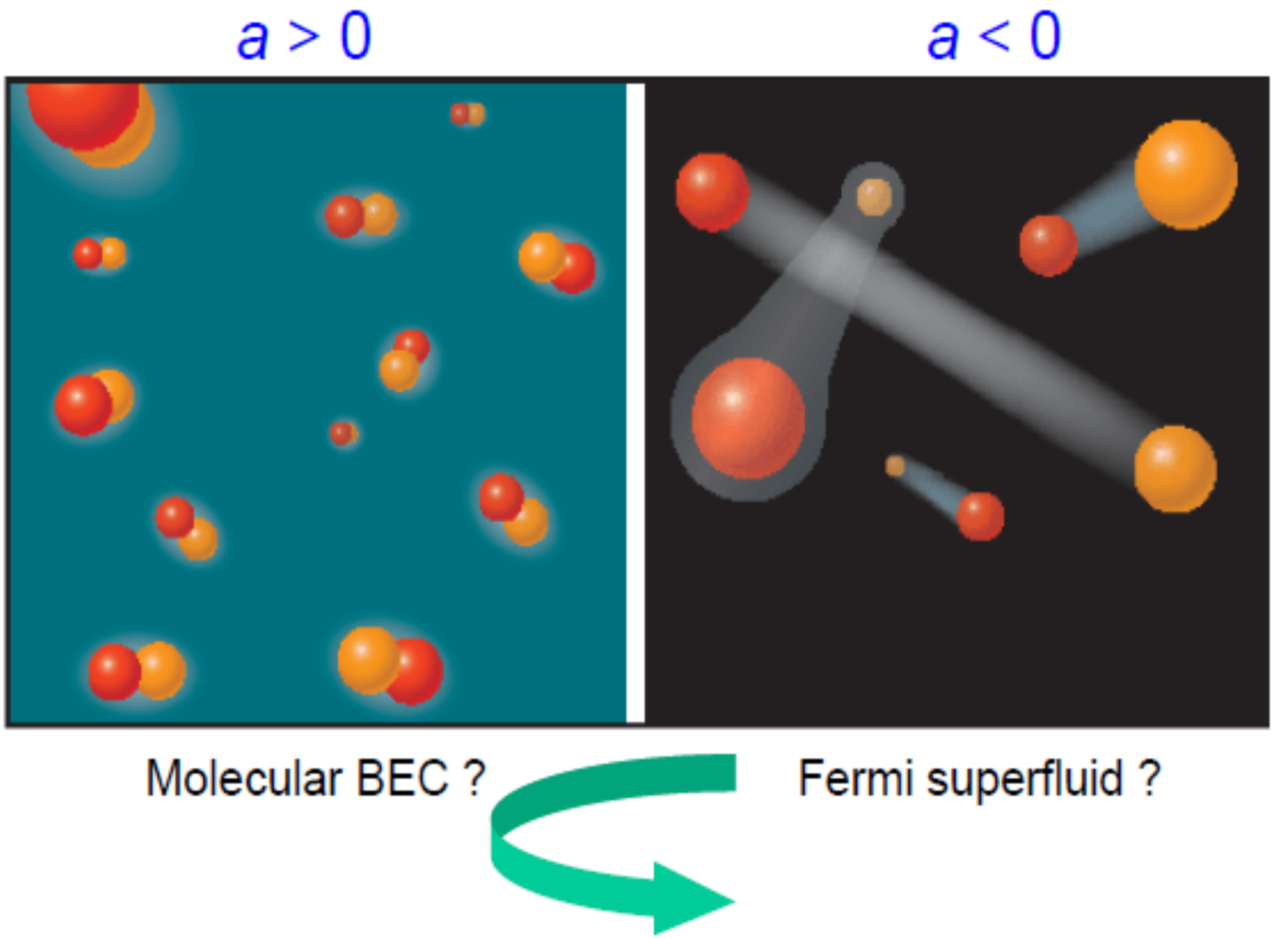




$$E_m = -\frac{1}{ma^2} - \varepsilon_F + \frac{2\pi a_{M\uparrow}}{(2/3)m} n_{\uparrow} \qquad (k_F a \ll 1)$$

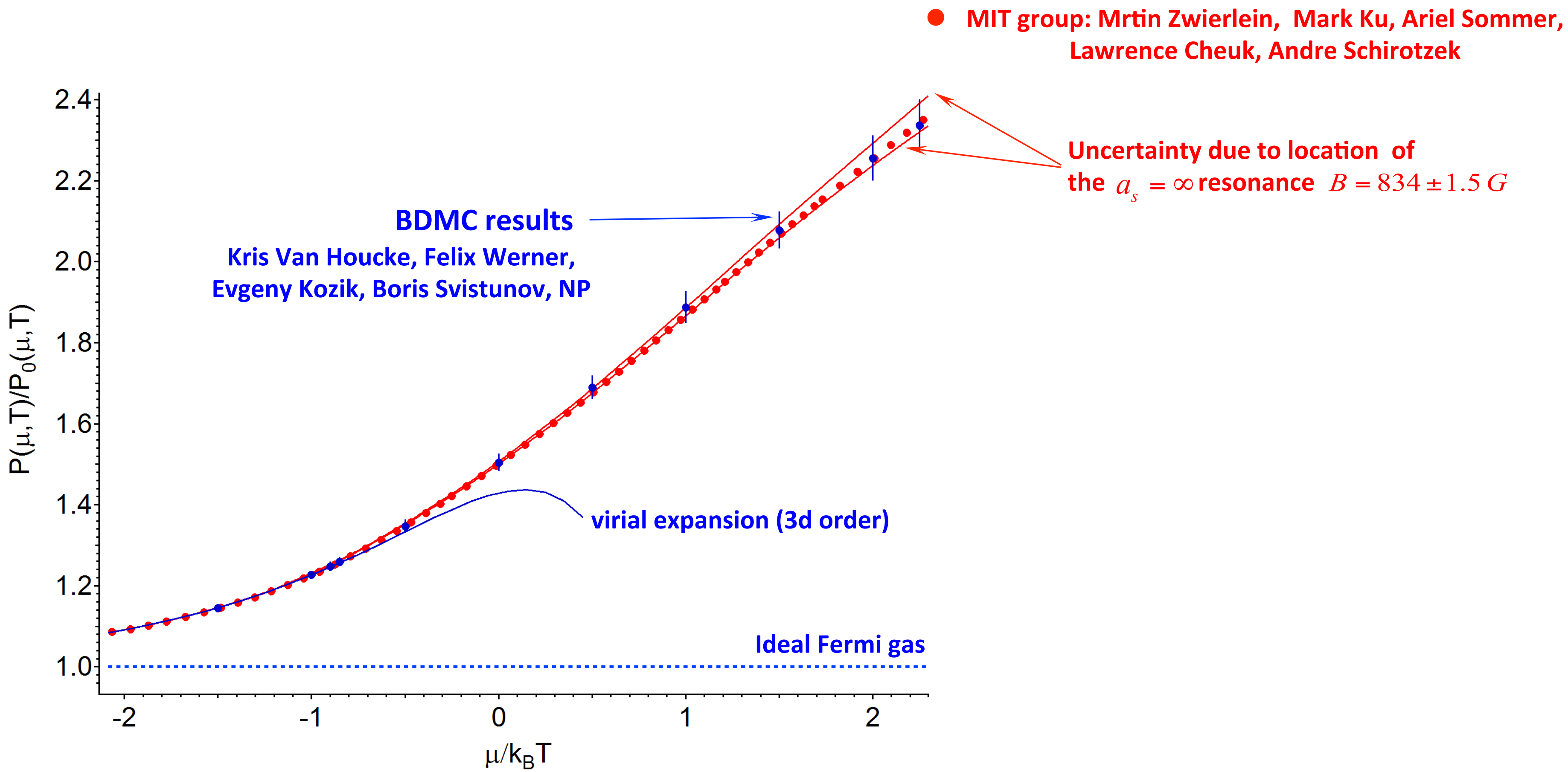
$a_{M\uparrow} = 1.18a$ **Skorniakov, Ter-Martirosian '56**

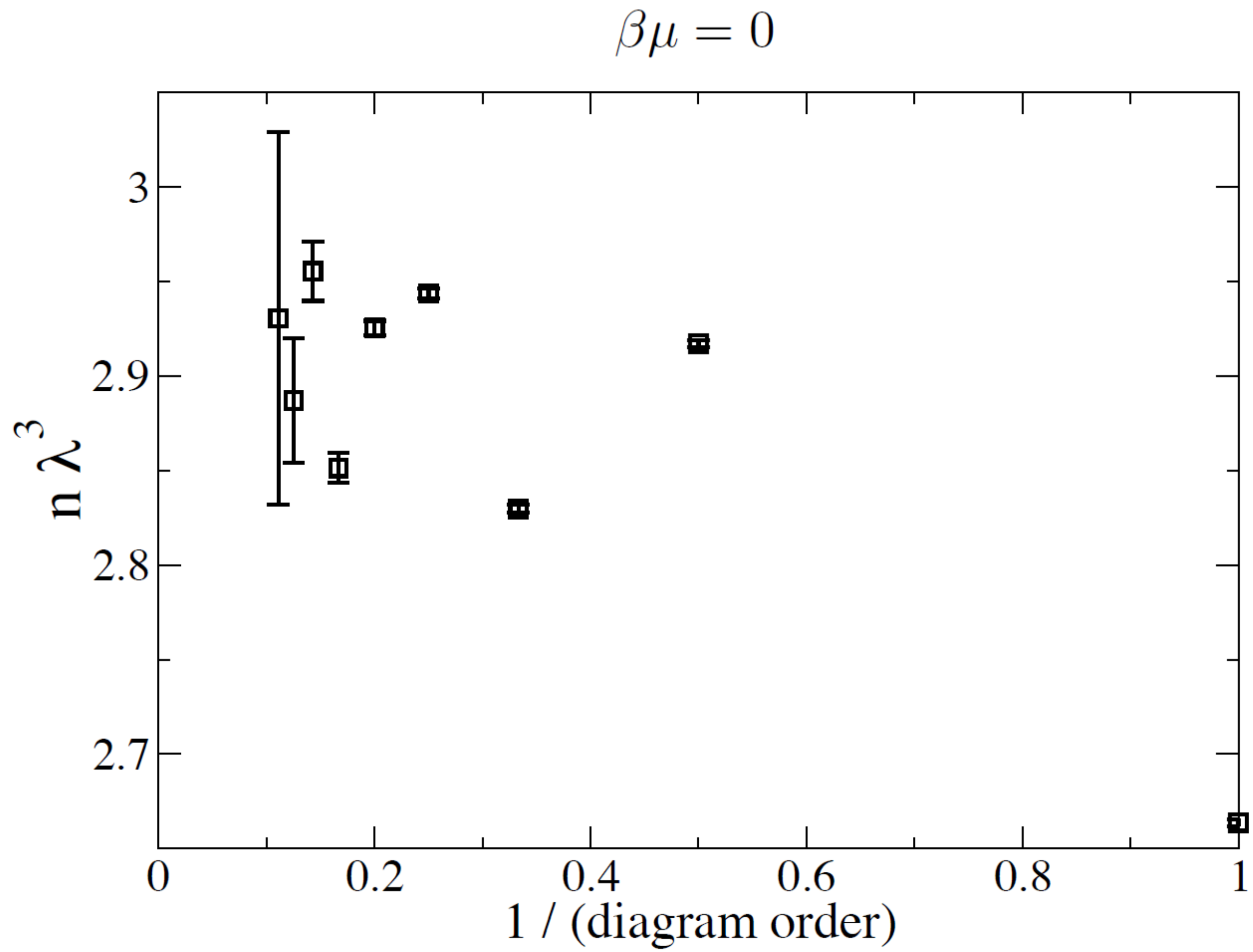
Unpolarized system at unitarity:BCS-BEC crossover



Unitary gas: $k_F a_S \longrightarrow \infty$ **when** k_F **and** ε_F **are the only length/energy scales**

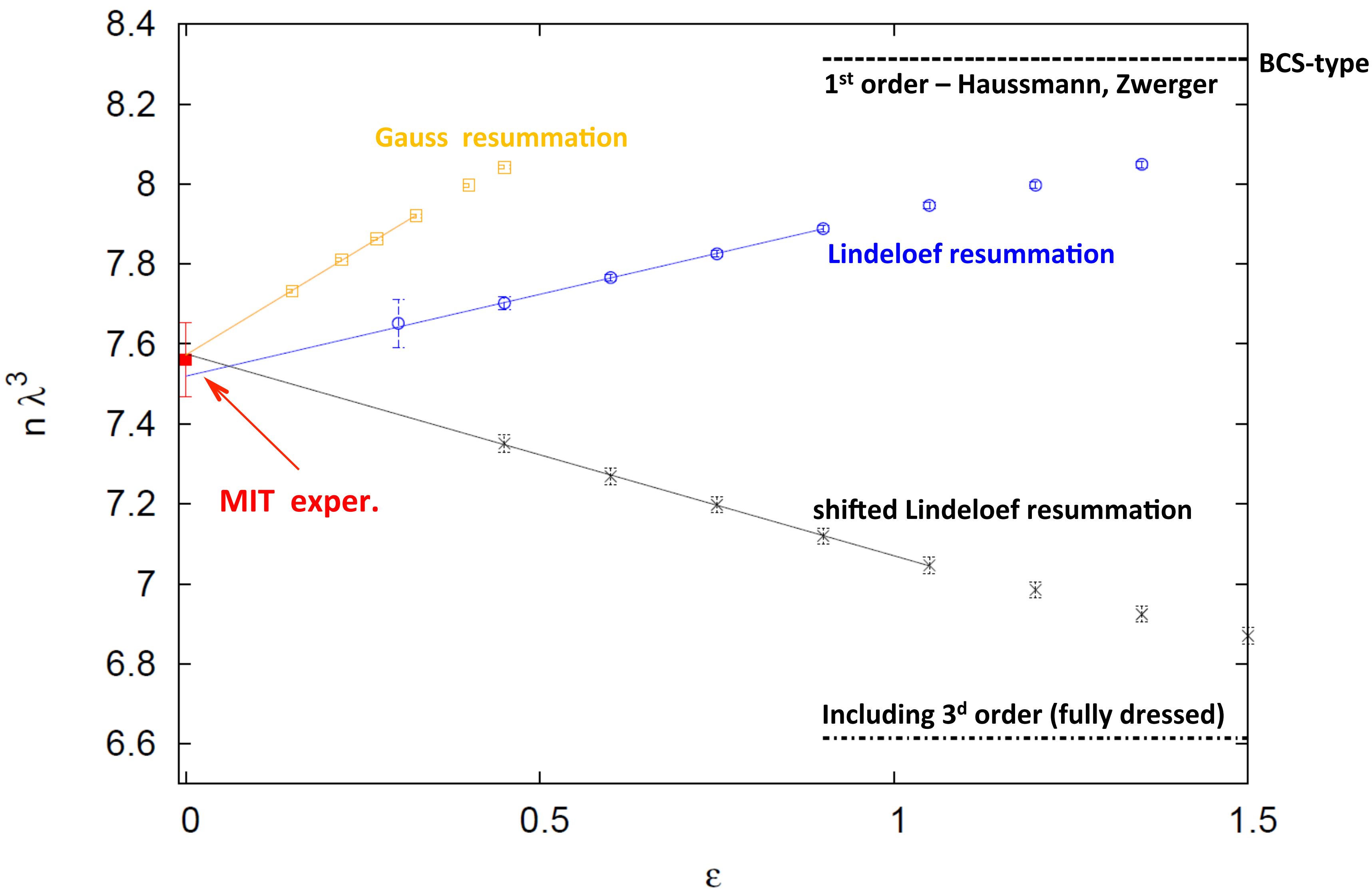
Answering Weinberg's question: cold atoms solve neutron stars





Before resummation the data are not nice looking!

Extraxpolation to the infinite diagram order for density $(\beta\mu = 1)$



controls contributing diagram orders
(the left-most point is effectively order 9 – millions of skeleton diagrams)

Popov-Fedotov trick

Heisenberg model: $$H = \sum_{ij} J_{ij}\, S_i \cdot S_j = \sum_{ij} J_{ij} \left(f^{\dagger}_{i\alpha} \sigma_{\alpha\beta} f_{i\beta} \right) \cdot \left(f^{\dagger}_{j\alpha} \sigma_{\gamma\delta} f_{j\beta} \right)$$

spin-1/2 f-fermions

- **Dynamically, physical config. remains physical at all times**

- **Empty and doubly occupied sites decouple from physical sites and each other**

- **Projecting out unphysical Hilbert space in statistics of** $Z = Tr_f\, e^{-H_f/T}$

$$Z_S = Tr_f\, e^{-\int_0^{\beta} H_f\, d\tau} \prod_i \delta_{n_{i\tau},1}$$

$$\delta_{n_{i\tau},1} \rightarrow \int_0^{2\pi} d\varphi_{i\tau}\, e^{i(n_{i\tau}-1)\varphi_{i\tau}}$$

$$H_f = \sum_{ij} J_{ij} \left(f^{\dagger}_{i\alpha} \sigma_{\alpha\beta} f_{i\beta} \right) \left(f^{\dagger}_{j\alpha} \sigma_{\gamma\delta} f_{j\beta} \right) - \mu \sum_{j\alpha} \left(n_{j\alpha} - 1 \right)$$ **with complex** $\mu = i\pi T/2$

Now: $Z_s = Tr_f\, e^{-H_f/T}$ **, i.e. one number does the job!**

Auxiliary gauge field $\varphi_{i\tau}$

Proof of $Z_S = Tr_f \, e^{-H_f/T}$

Partition function of physical sites in the presence of unphysical ones (K blocked sites)

$$Tr_f \, e^{-H_f/T} = Z_S + \sum_{K=0}^{N} C^K \sum_{\xi_K} Z_S^{(\xi_K)}$$

Number of unphysical sites with n=2 or n=0

Partition function of the unphysical site

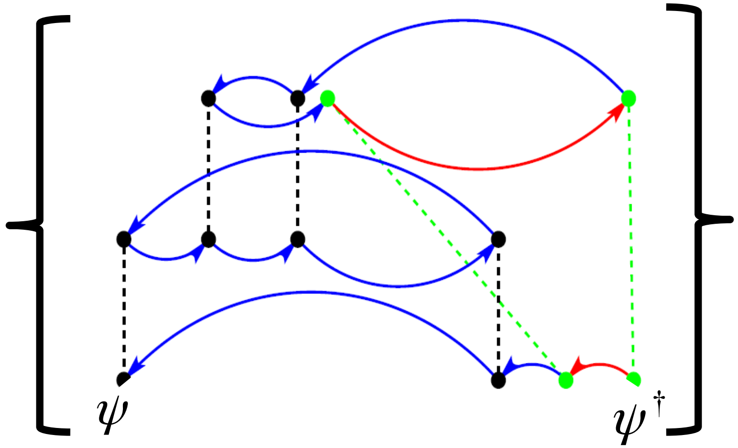
configuration of unphysical sites

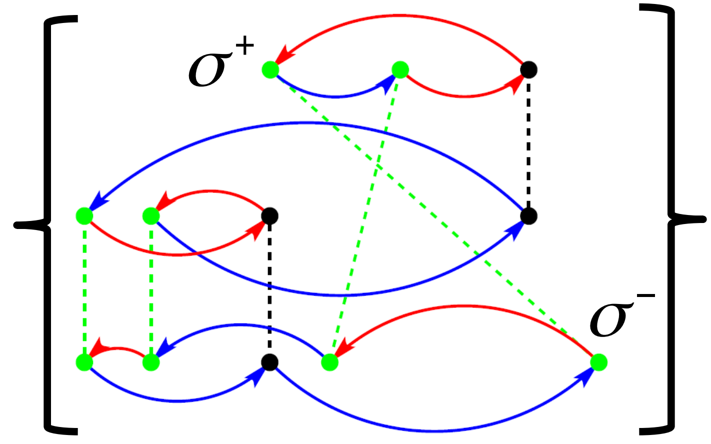
$$\Downarrow$$

$$C = \sum_{n=0,2} e^{\mu(n-1)/T} = e^{-i\pi/2} + e^{i\pi/2} = 0$$

$$H_f = H_0 + H_{\text{int}} = -\frac{i\pi T}{2} \sum_{j\alpha} \left(n_{j\alpha} - 1\right) + \sum_{ij} J_{ij} \left(f_{i\alpha}^{\dagger} \sigma_{\alpha\beta} f_{i\beta}\right) \cdot \left(f_{j\alpha}^{\dagger} \sigma_{\gamma\delta} f_{j\beta}\right)$$

standard diagrammatics for interacting fermions starting from the flat band.

$\Sigma =$ 

$\Pi =$ 

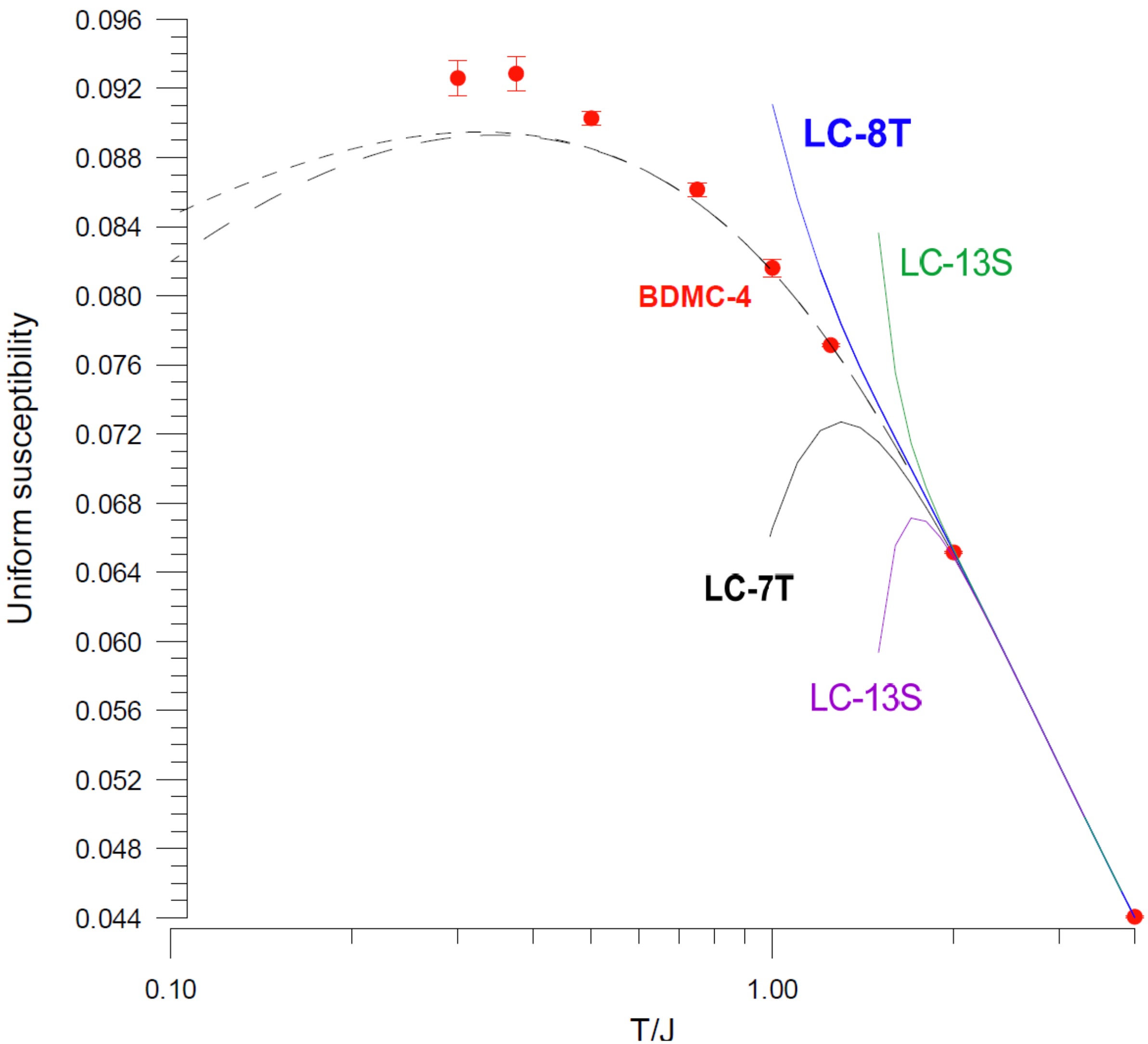
$$G_\sigma = G_\sigma^{(0)} + G_\sigma^{(0)} \Sigma_\sigma G_\sigma$$

$$\hat{U} = \hat{J} - \hat{J} \cdot \hat{\Pi} \cdot \hat{U}$$

Main quantity of interest is magnetic susceptibility

$$\hat{\chi} = \frac{\hat{\Pi}}{(1 + \hat{J} \cdot \hat{\Pi})}$$

Preliminary data; BDMC up to order 4 for triangular lattice Heisenberg anti-ferromagnet.

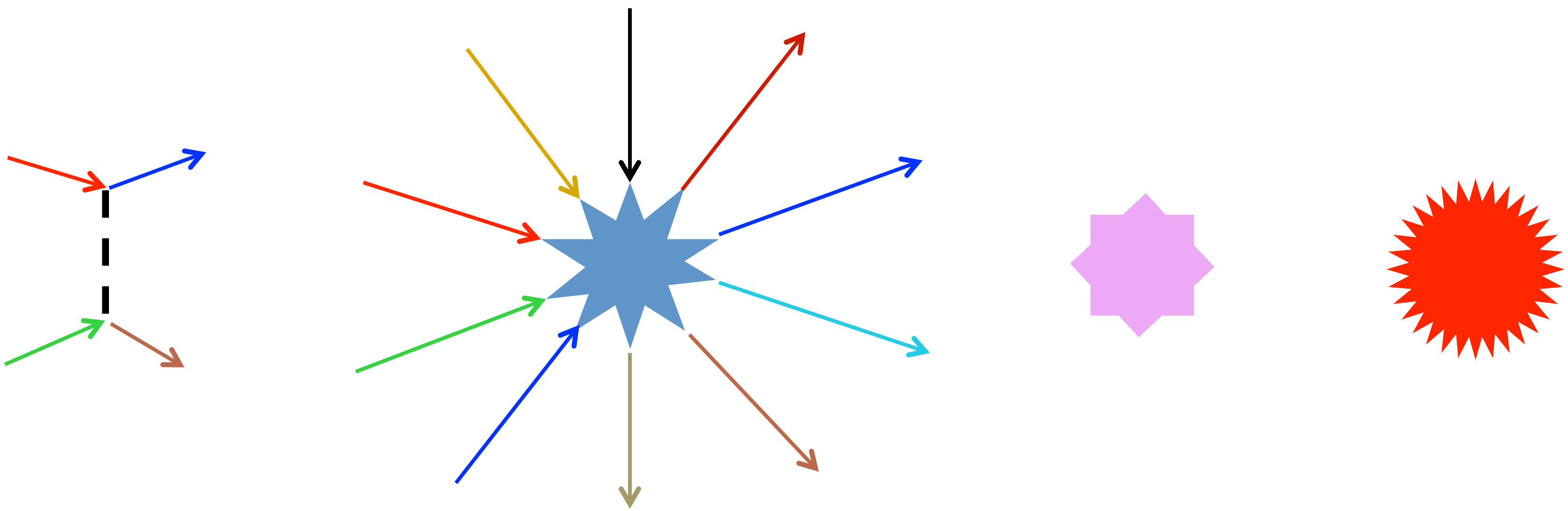


: linked cluster expansion
Rigol, Bryant, Singh '07

1. Sign-blessing works
2. Self-consistency prevents divergence
3. Careful cooling is required for T<< T_{MF}

Generalizations: Arbitrary spin model ✓
Arbitrary lattice boson model with n < MAX ✓
Diagrammatics with expansion on t, not U ! ✓

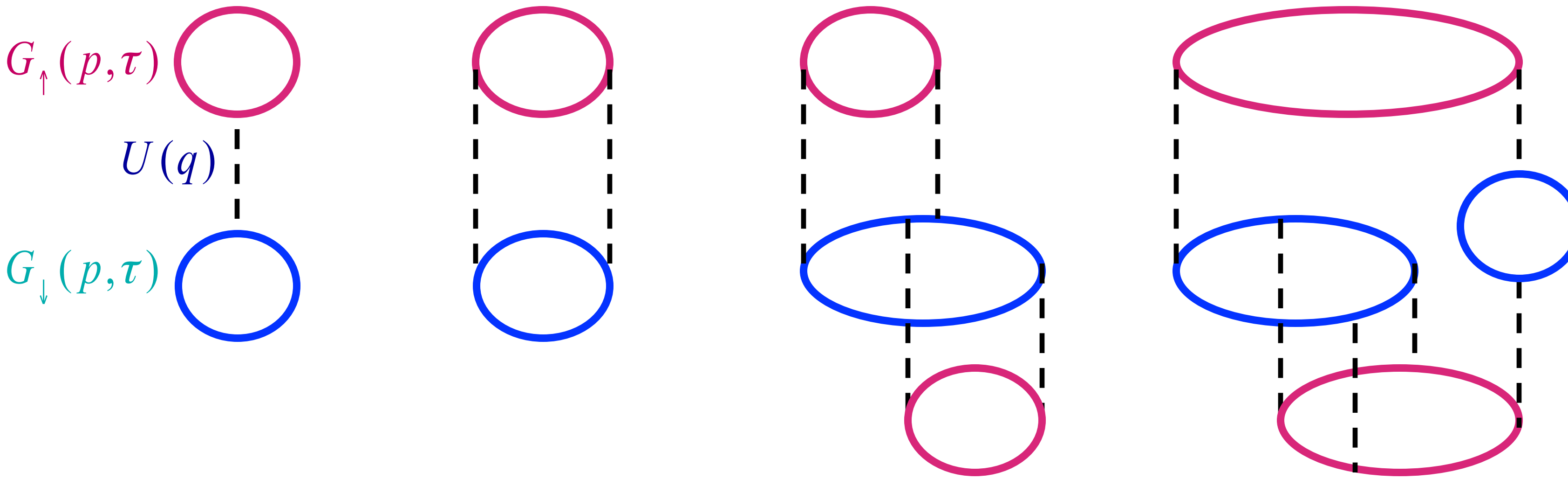
Prise to pay: diagrammatic elements with many "legs"



If nothing else, definitely good for Nature cover !

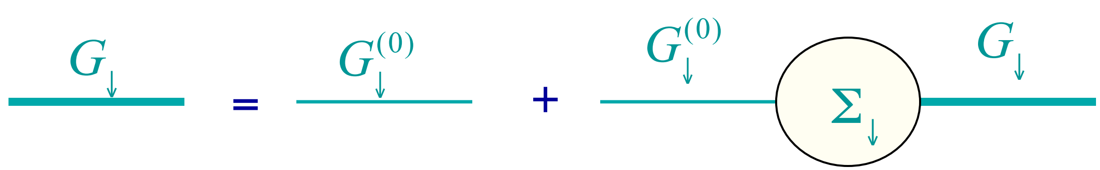
Diagrammatic Monte Carlo in the generic many-body setup

1. Stochastic summation of connected Feynman diagrams for self-energy
   ξ (controls the typical diagram order)



2. Self-consistent feed-back in the form of Dyson, T-matrix, RPA, etc. Eqs.

e.g.



3. Extrapolation to $\xi \to \infty$ (asymptotic and divergent series can be dealt with)

2D Fermi-Hubbard model in the Fermi-liquid regime

$U/t = 4$

$\mu/t = 1.5 \rightarrow n \approx 0.6$

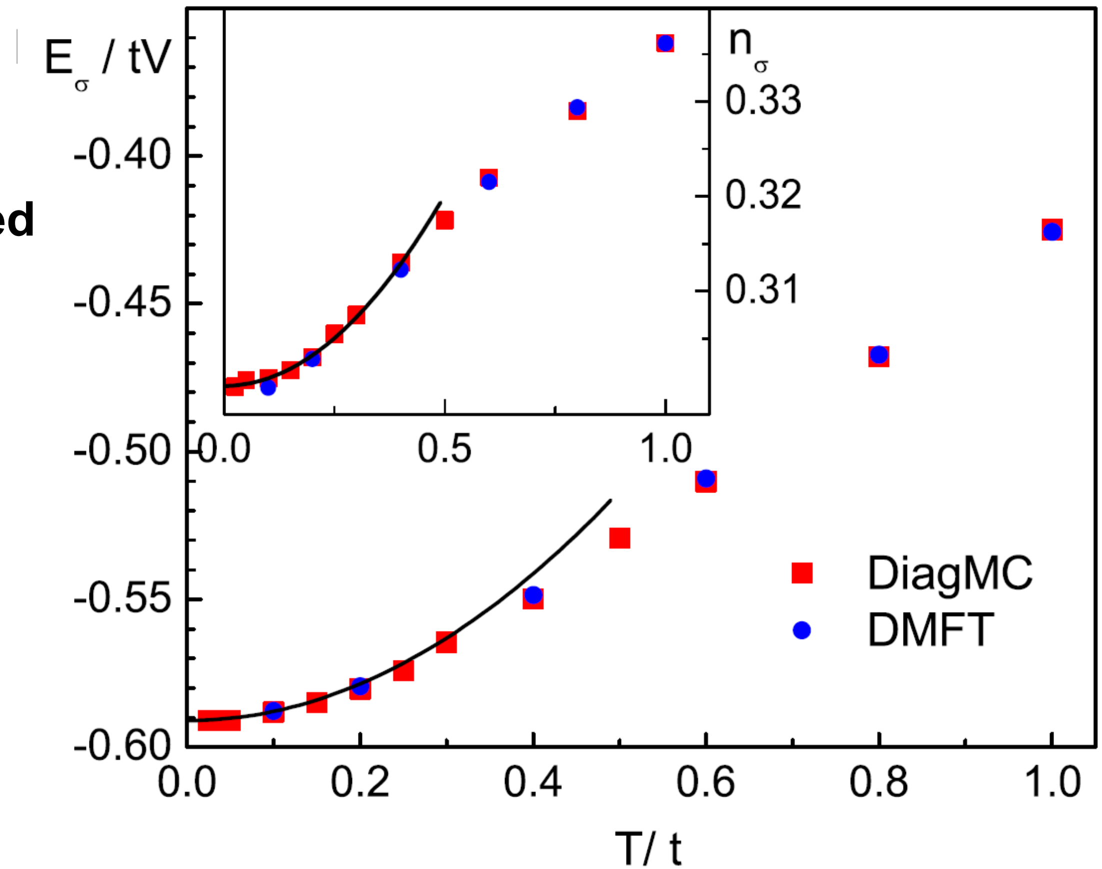
$T/t > 0.025 : \; E_F/100$

Fermi –liquid regime was reached

Bare series convergence: yes, after order 4

$$E(T) - E(0) = (\rho_F + \rho_F' E_F)\frac{\pi^2 T^2}{6}$$

$$n(T) - n(0) = \rho_F' \frac{\pi^2 T^2}{6}$$



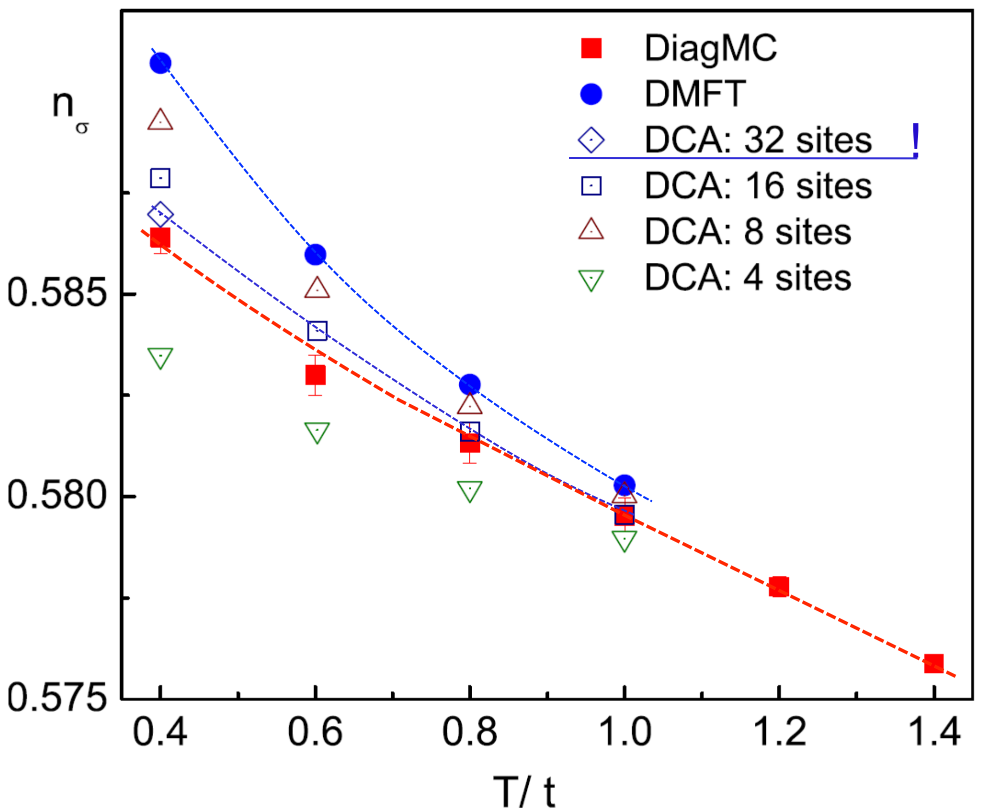
2D Fermi-Hubbard model in the Fermi-liquid regime

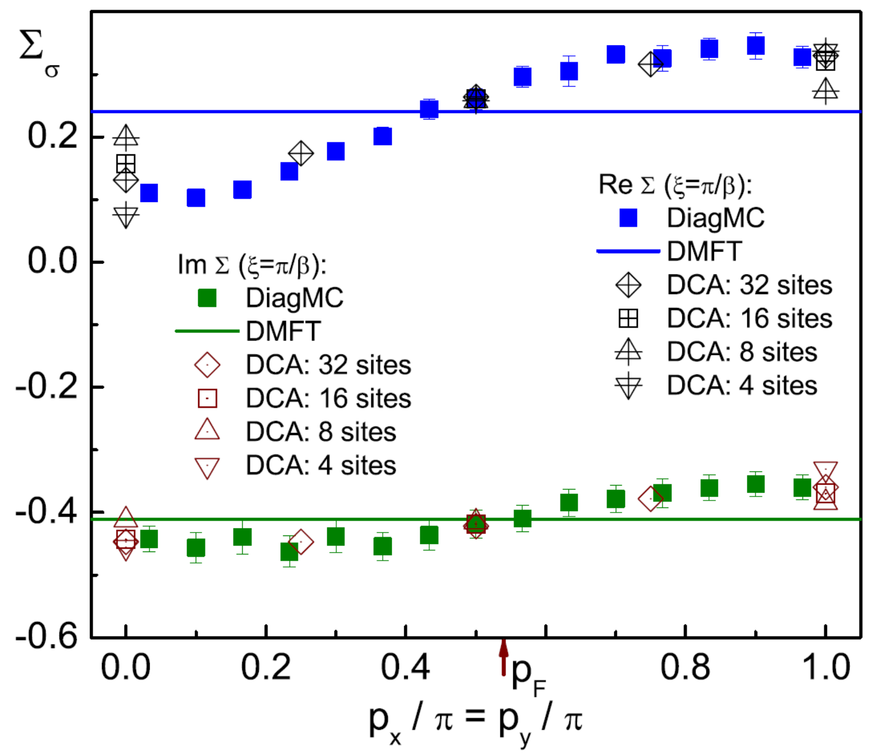
$U/t = 4$

$\mu/t = 3.1 \rightarrow n \approx 1.2$

$T/t \geq 0.4: \; E_F/10$

Comparing DiagMC with cluster DMFT (DCA implementation)





$$\Sigma(\omega_0 = \pi T, p_x = p_y)$$

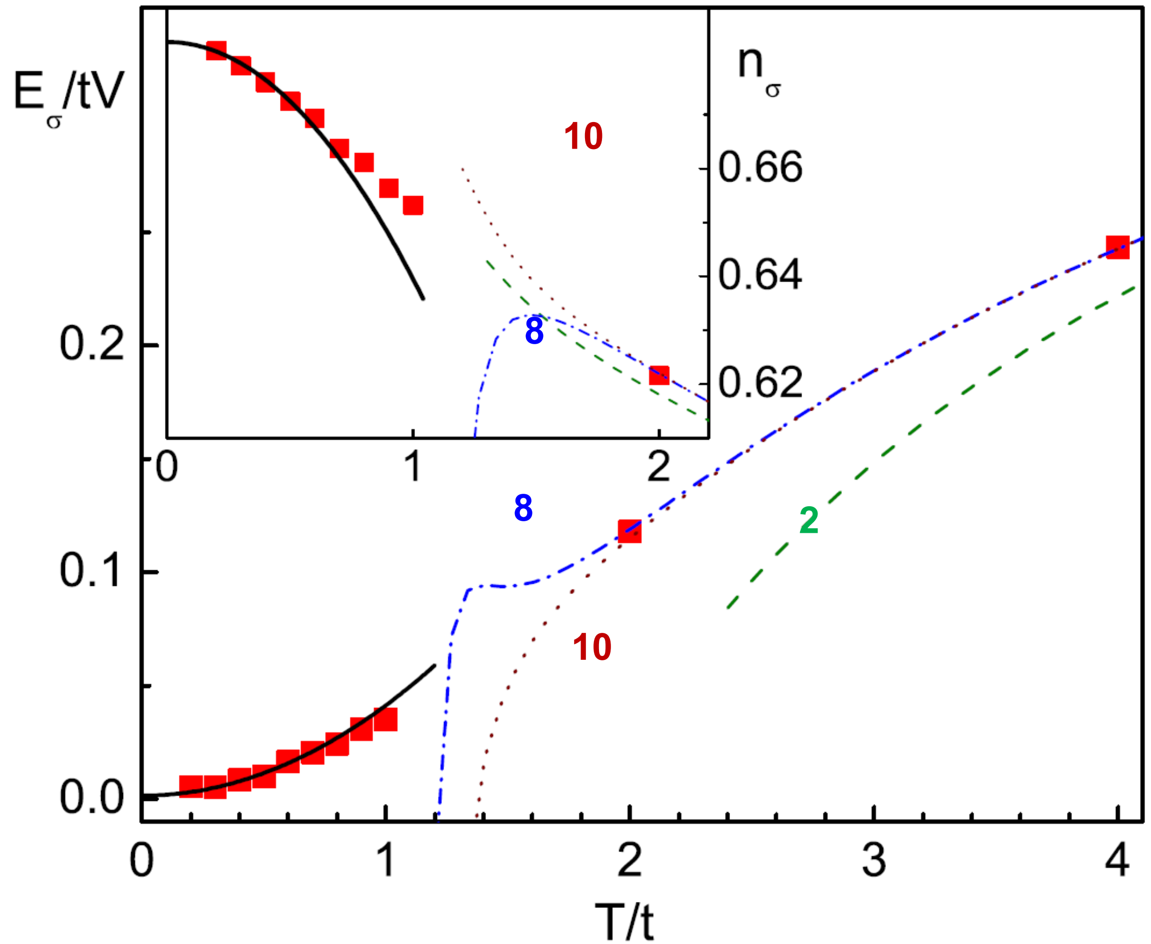
3D Fermi-Hubbard model in the Fermi-liquid regime

$U/t = 4$

$(\mu - nU)/t = 1.5 \rightarrow n \approx 1.35$

$T/t \geq 0.1: \; E_F/50$

DiagMC *vs* high-T expansion in t/T (up to 10-th order)



Conclusions/perspectives

The crucial ingredient, the sign blessing phenomenon, is present in all models (so far)

BDMC for skeleton graphs works all the way to the critical point in strongly correlated Fermi systems

⇩

"Higher-level" self-consistent formulations; 3-point vertex to begin with

New models & broken phases, i.e. nothing is off the table …