Improved lattice operators for non-relativistic fermions

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THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

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Outline

- Improved lattice operators for non-relativistic fermions

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    - Why
    - How
    - Illustrative results

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- Towards asymmetric systems on the lattice via imaginary polarization (if time permits)
  - Why
  - How
  - Mean-field results

"A glance at the imaginary world of ultracold atoms."
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[arXiv:1209.3319]

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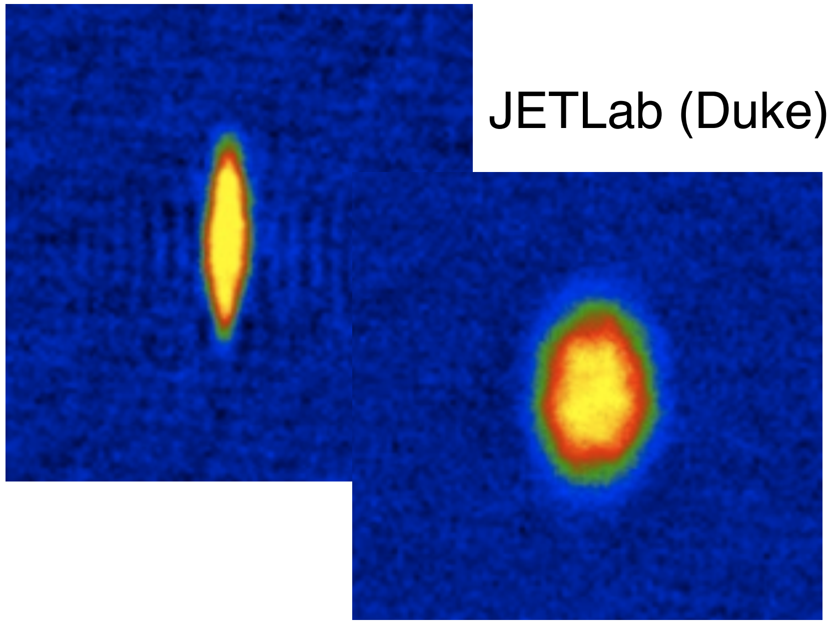
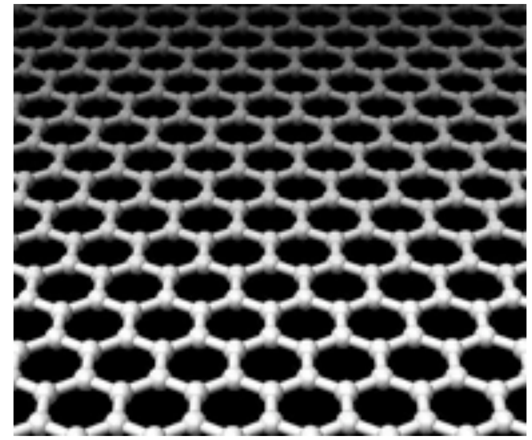
Improved lattice operators

Ultracold Gases



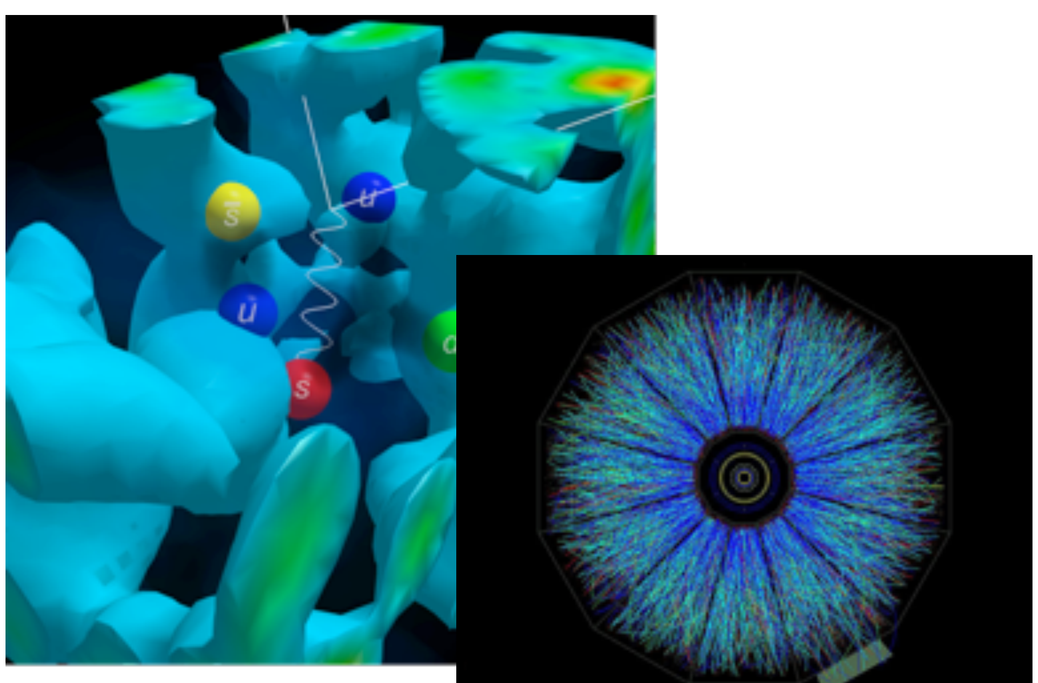
JETLab (Duke)

Condensed Matter Physics

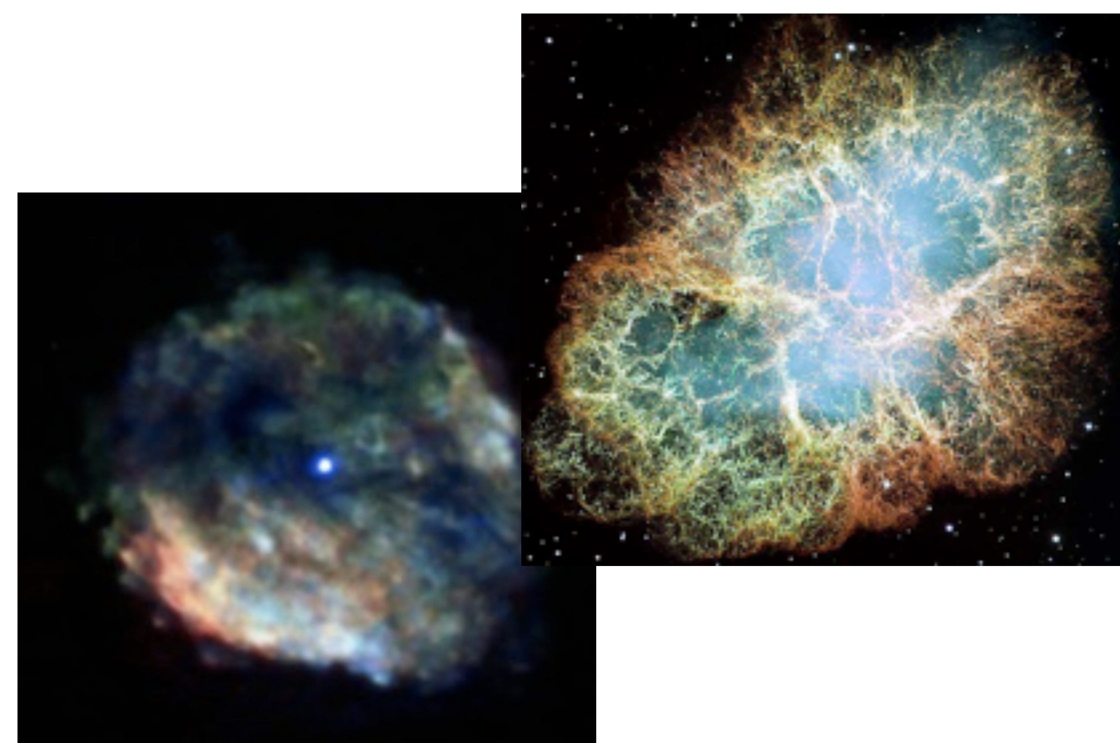


Materials Science

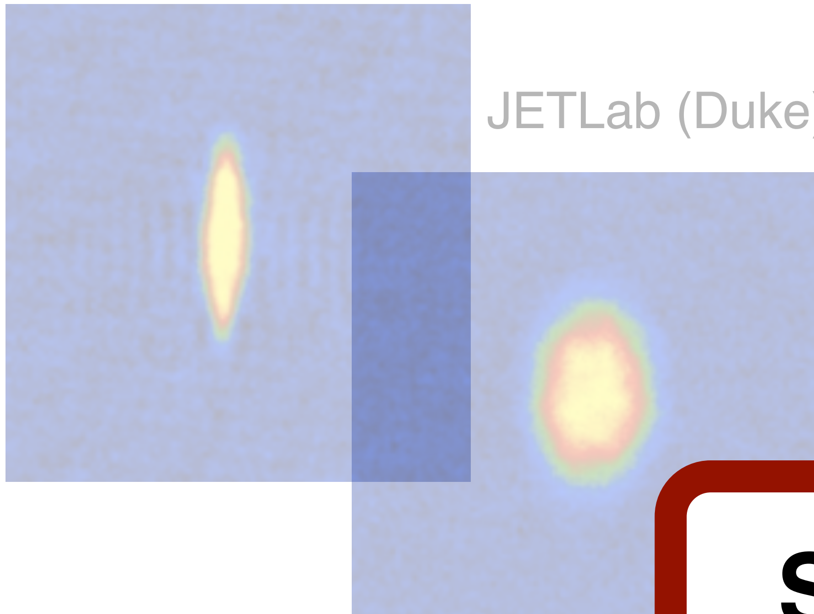
High-Energy Physics, QCD, Low-Energy NP



Astrophysics

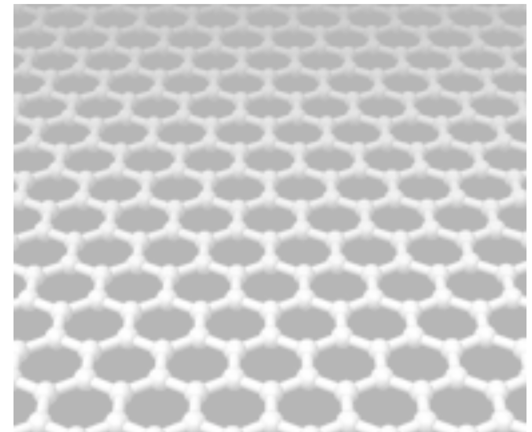


Ultracold Gases



JETLab (Duke)

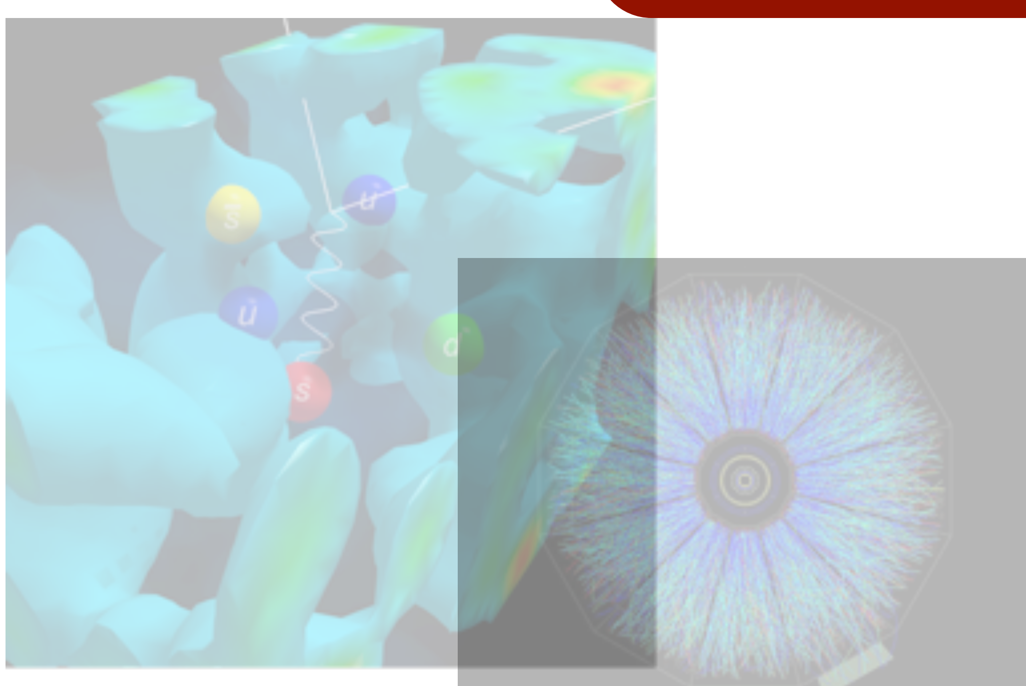
Condensed Matter Physics



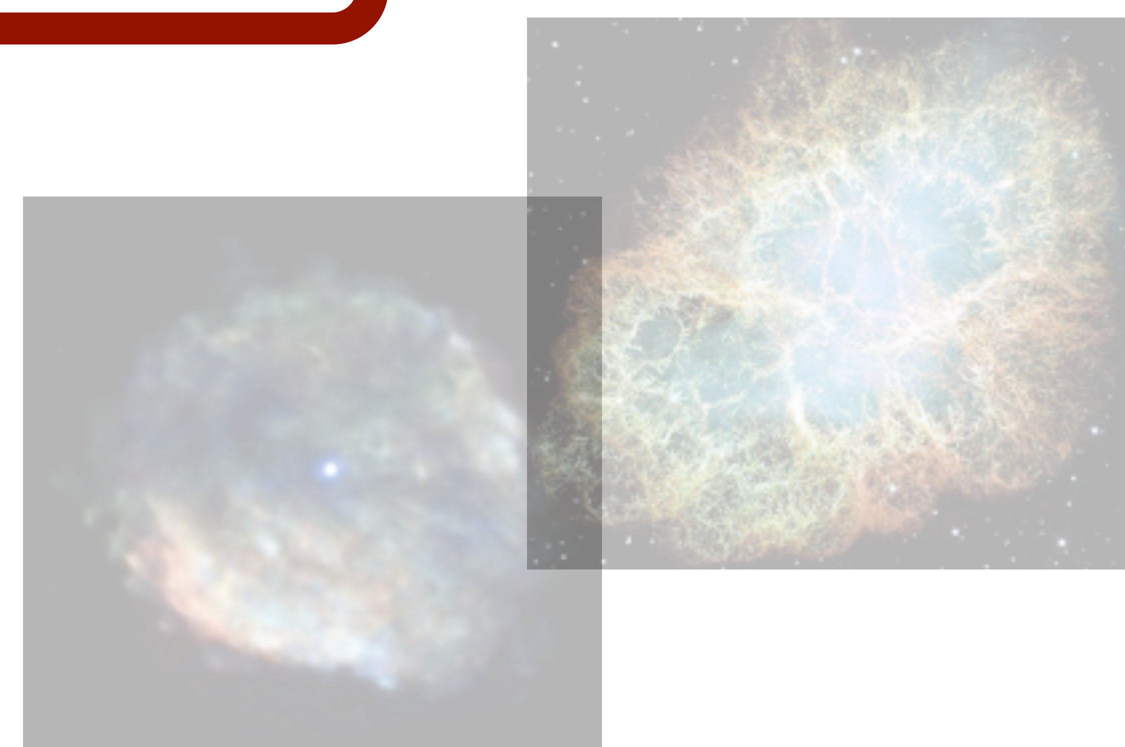
Materials Science

Strongly correlated quantum many-body systems

High-Energy Pl
QCD, Low-Ene



strophysics
ly neutron stars)



In all of these cases...

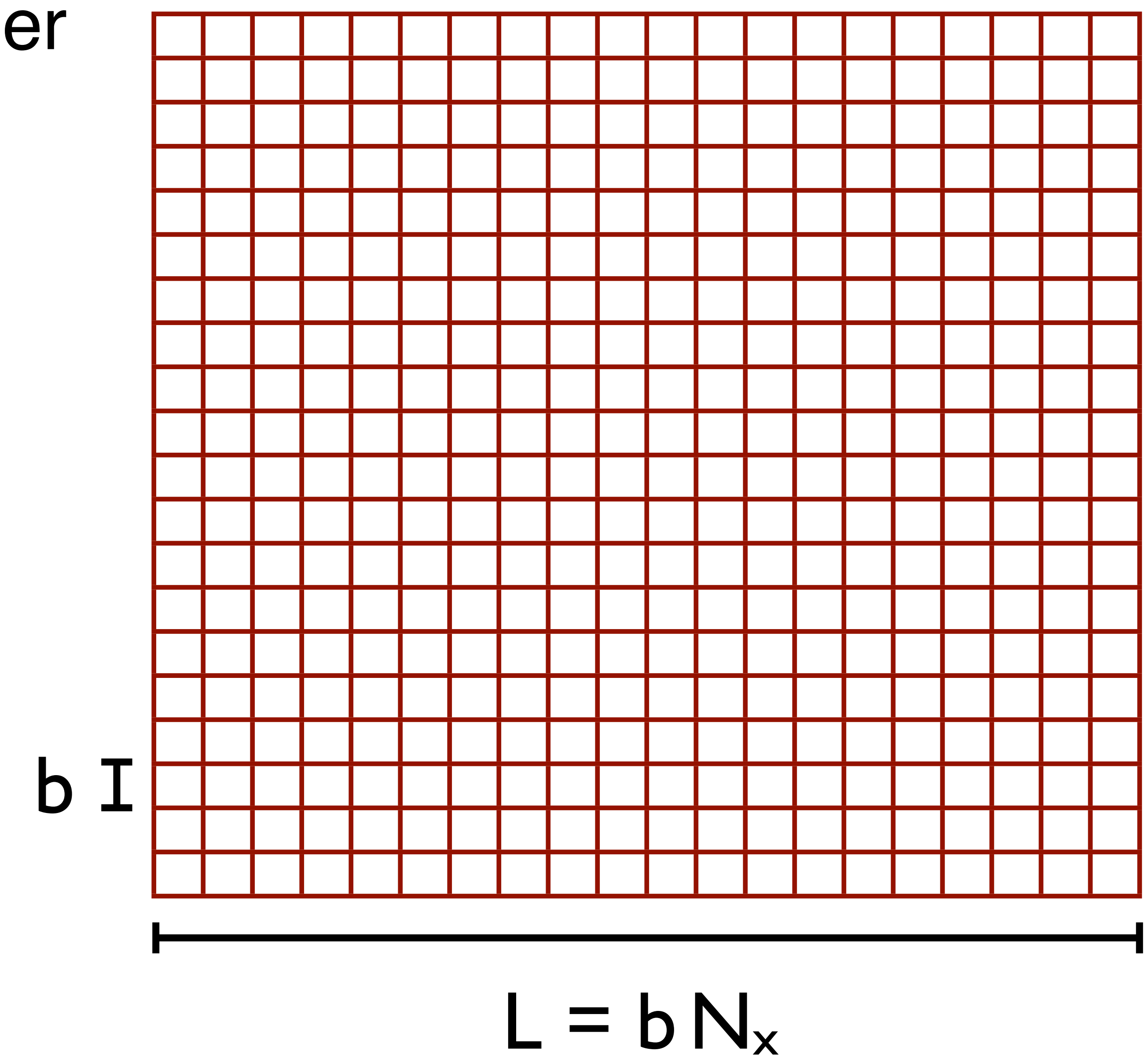
The lattice gives us a finite number of degrees of freedom.

Signal-to-noise issues aside, we can treat **any** problem *fully non-perturbatively*, taking complete account of fluctuations, quantum and thermal.

We pay the price in terms of systematic effects:

- Lattice spacing
- Lattice volume

(These are of course related!)



Only systematic uncertainties left!

In particular...

The unitary limit

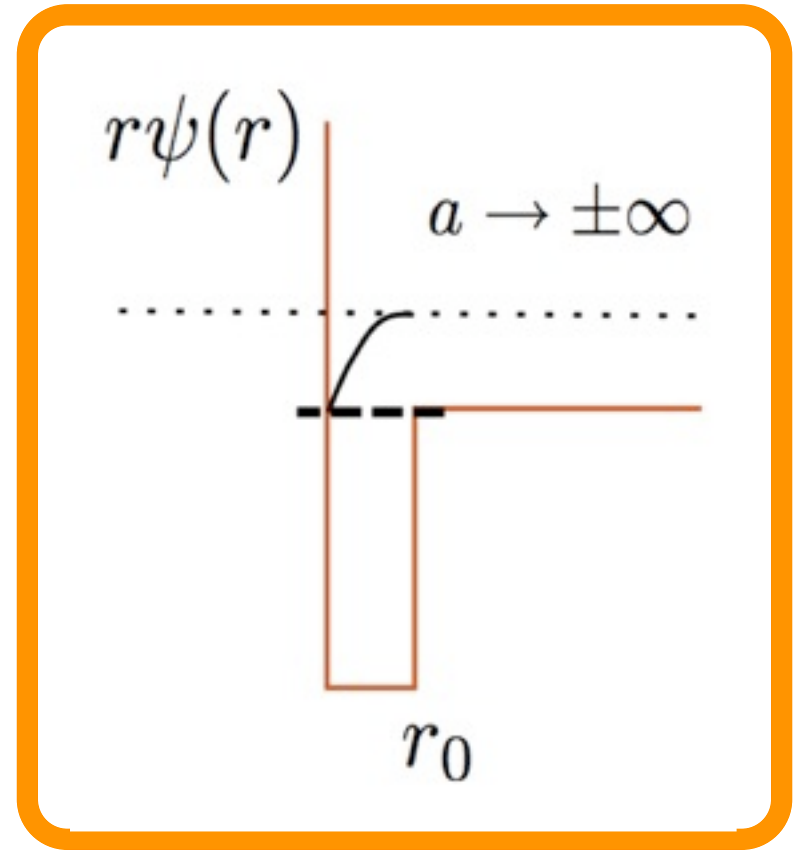
- Spin 1/2 fermions, at unitarity

$$r_0 \to 0 \ll n^{-1/3} \ll |a| \to \infty$$

Range of the interaction

Inter-particle distance

S-wave scattering length



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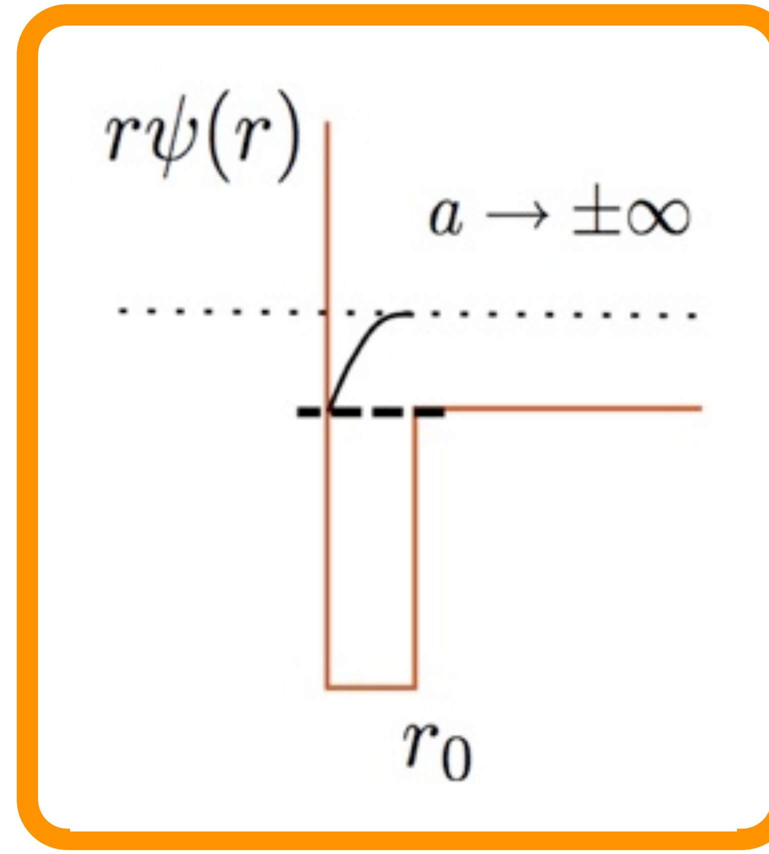

- As many scales as a free gas!

$$k_F = \hbar(3\pi^2 n)^{1/3} \qquad \varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

- Qualitatively

Every dimensionful quantity should come as a power of ε_F times a **universal** constant/function.

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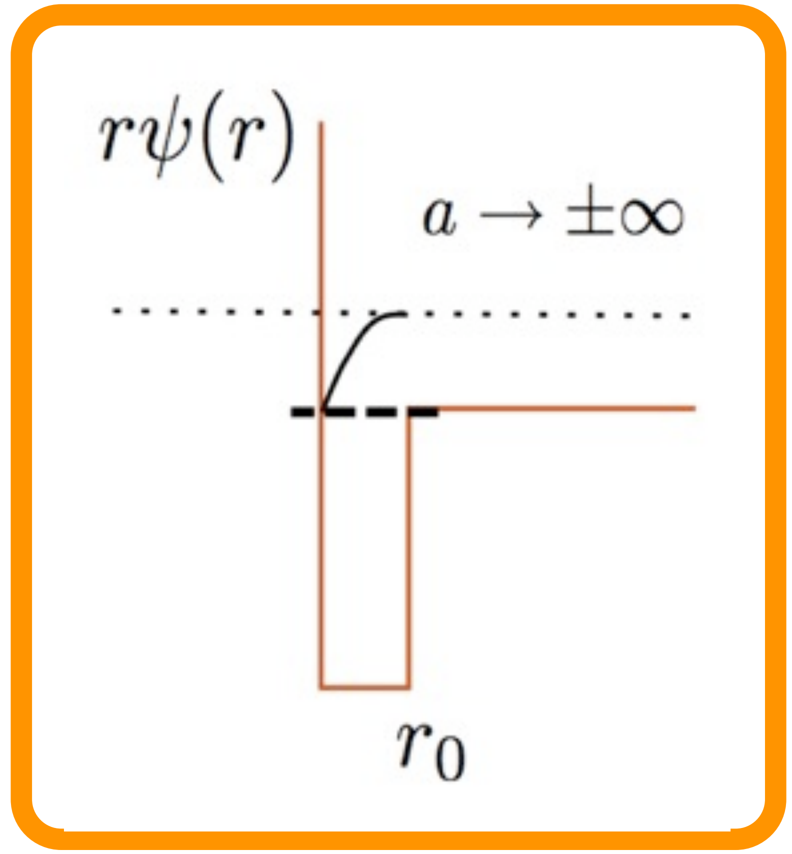

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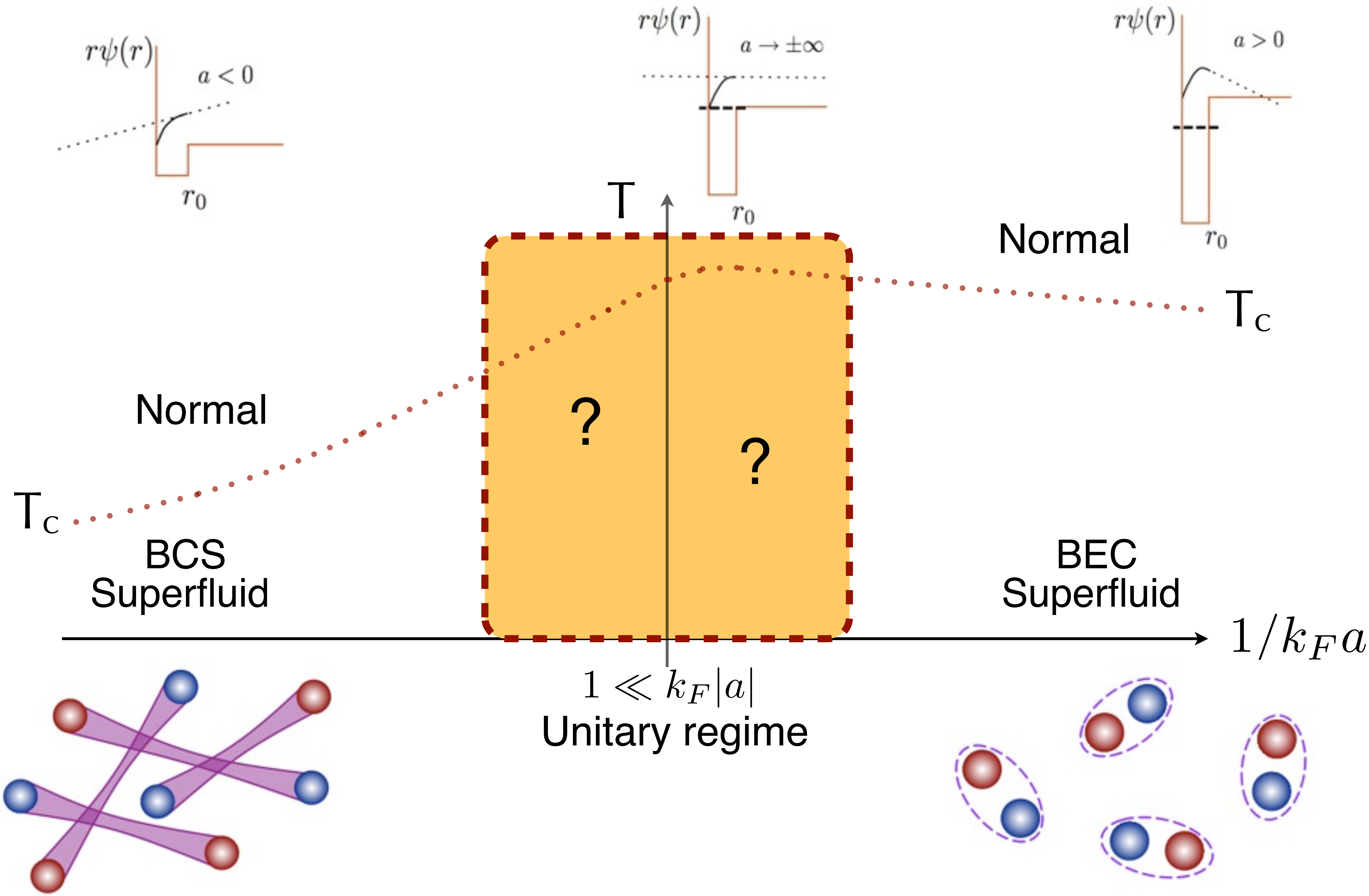
- Quantitatively **?**

The BCS-BEC Crossover



In the last few years...

- Advances in theory and experiment

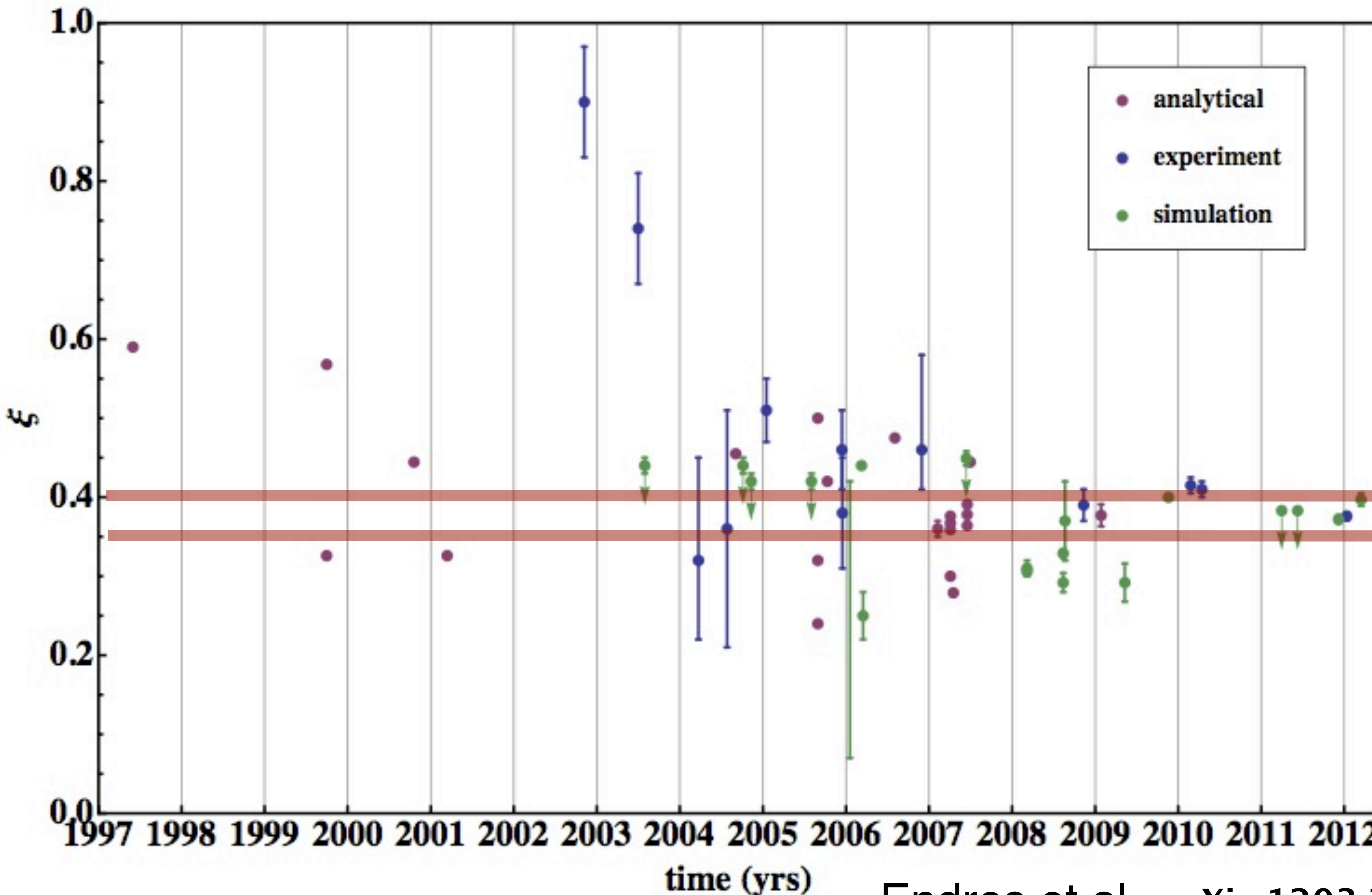
  ↙ ↘

  Analytic & numerical

  - Energy & chemical potential (zero and finite T)
  - Momentum distribution & contact
  - Critical temperature
  - Quasiparticle spectral properties
  - Structure factor (static & dynamic)
  - Virial coefficients
  - Various susceptibilities
  - ...

Energy (ground state)

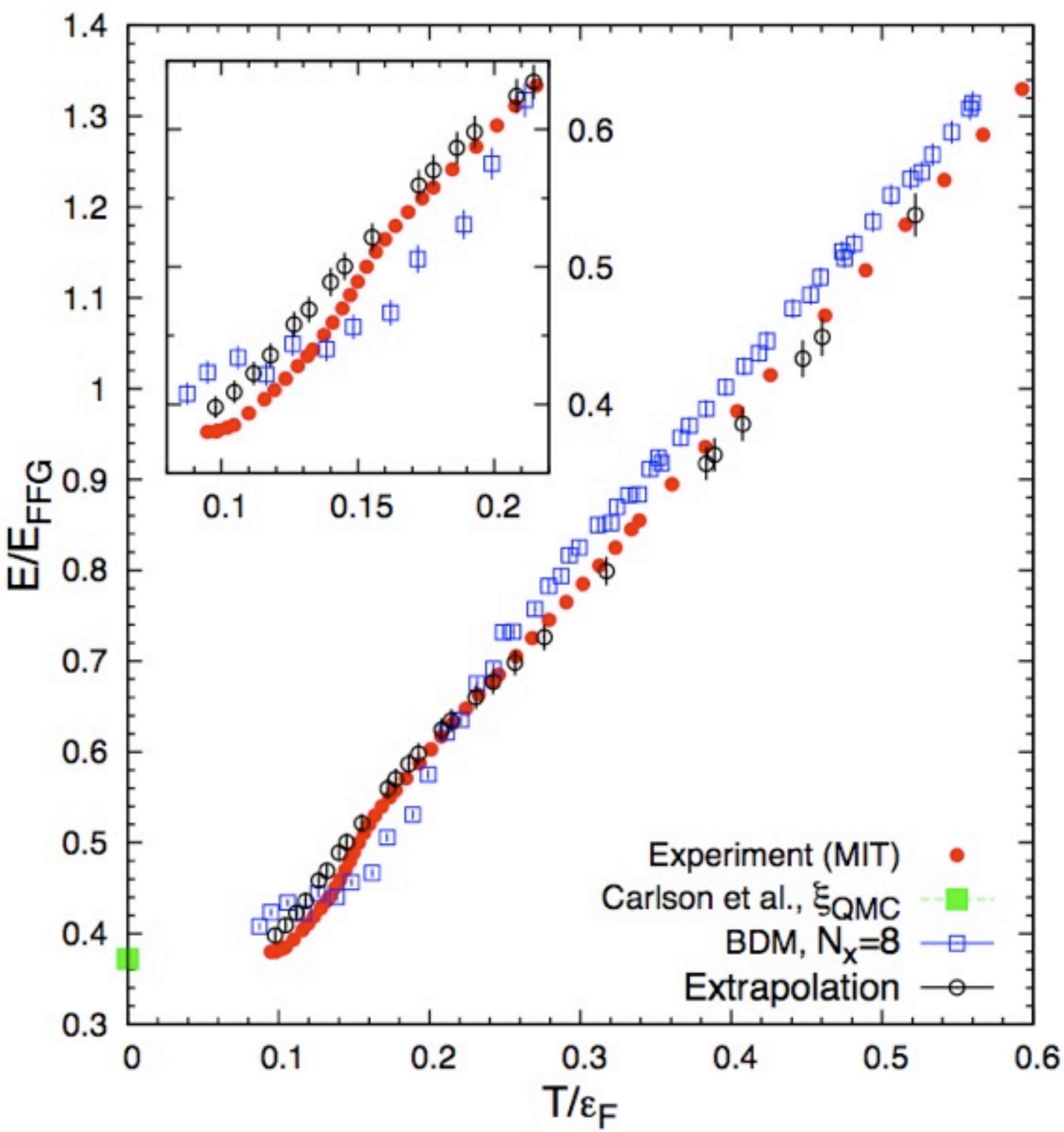
- Ground state energy per particle



Endres et al. arXiv:1203.3169

Energy (finite temperature)

- Finite T equation of state (theory & experiment)



$N_x = 8, 10, 12, 14, 16$

$k_F r_{\text{eff}} \simeq 0.3 - 0.5$

Experiment: Zwierlein et al. (MIT)

Drut, Lähde, Wlazlowski, Magierski, PRA **85**, 051601(R) (2012)

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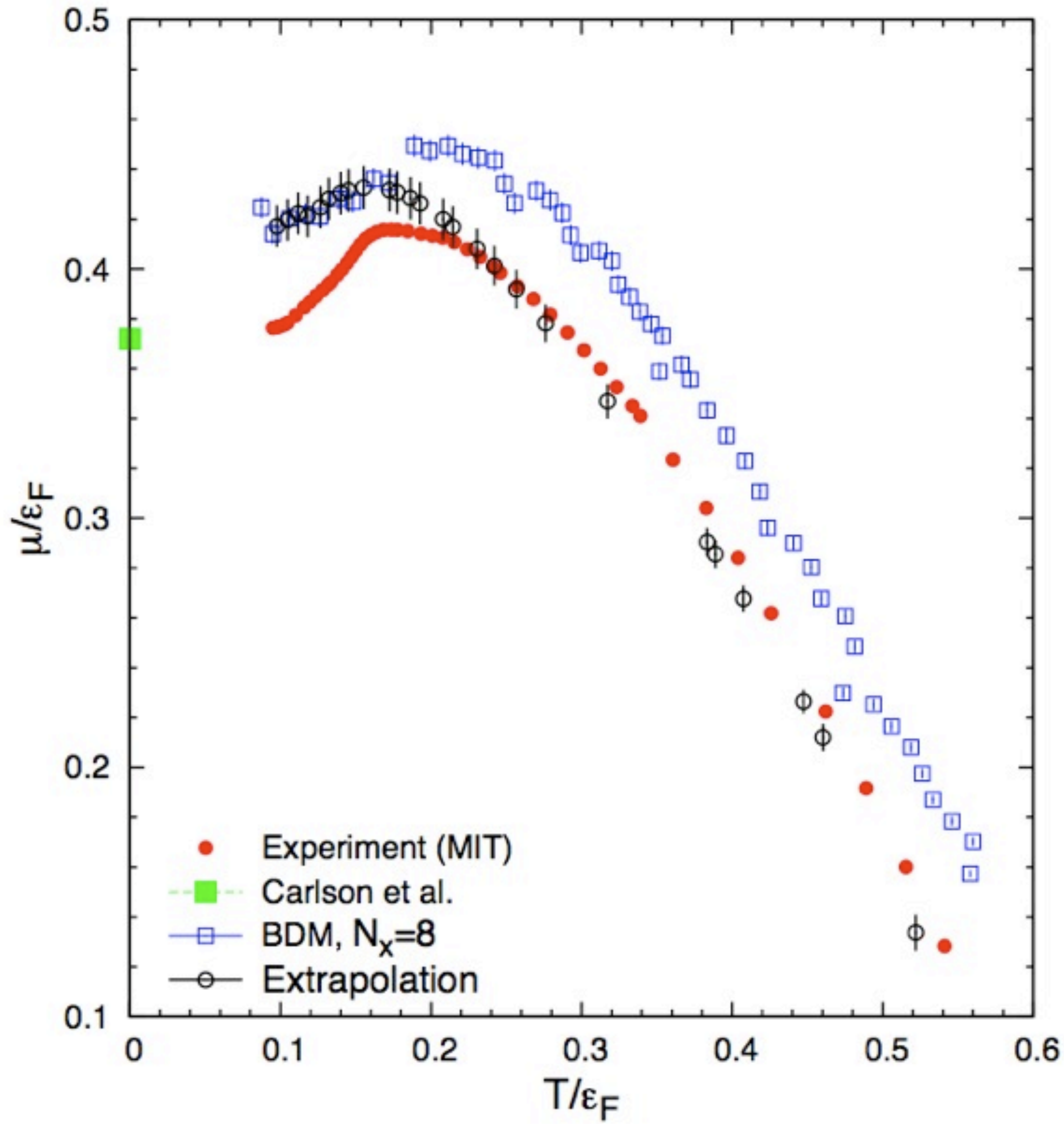

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The Tan relations and the "contact"

- Momentum distribution tail

$$n_k \underset{k \to \infty}{\longrightarrow} C/k^4$$

S. Tan, Annals of Physics **323**, 2952 (2008).

E. Braaten and L. Platter,
Phys. Rev. Lett. **100**, 205301 (2008).

- Energy relation

$$T + U = \sum_\sigma \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left(n_\sigma(\boldsymbol{k}) - \frac{C}{k^4} \right) + \frac{\hbar^2}{4\pi m a} C$$

- Short distance density-density correlator

$$\langle n_1(\boldsymbol{R} + \tfrac{1}{2}\boldsymbol{r})\, n_2(\boldsymbol{R} - \tfrac{1}{2}\boldsymbol{r}) \rangle \longrightarrow \frac{1}{16\pi^2} \left(\frac{1}{r^2} - \frac{2}{ar} \right) \mathcal{C}(\boldsymbol{R})$$

- Adiabatic relation

$$\mathcal{C} = \frac{4\pi m a^2}{\hbar^2} \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}a}$$

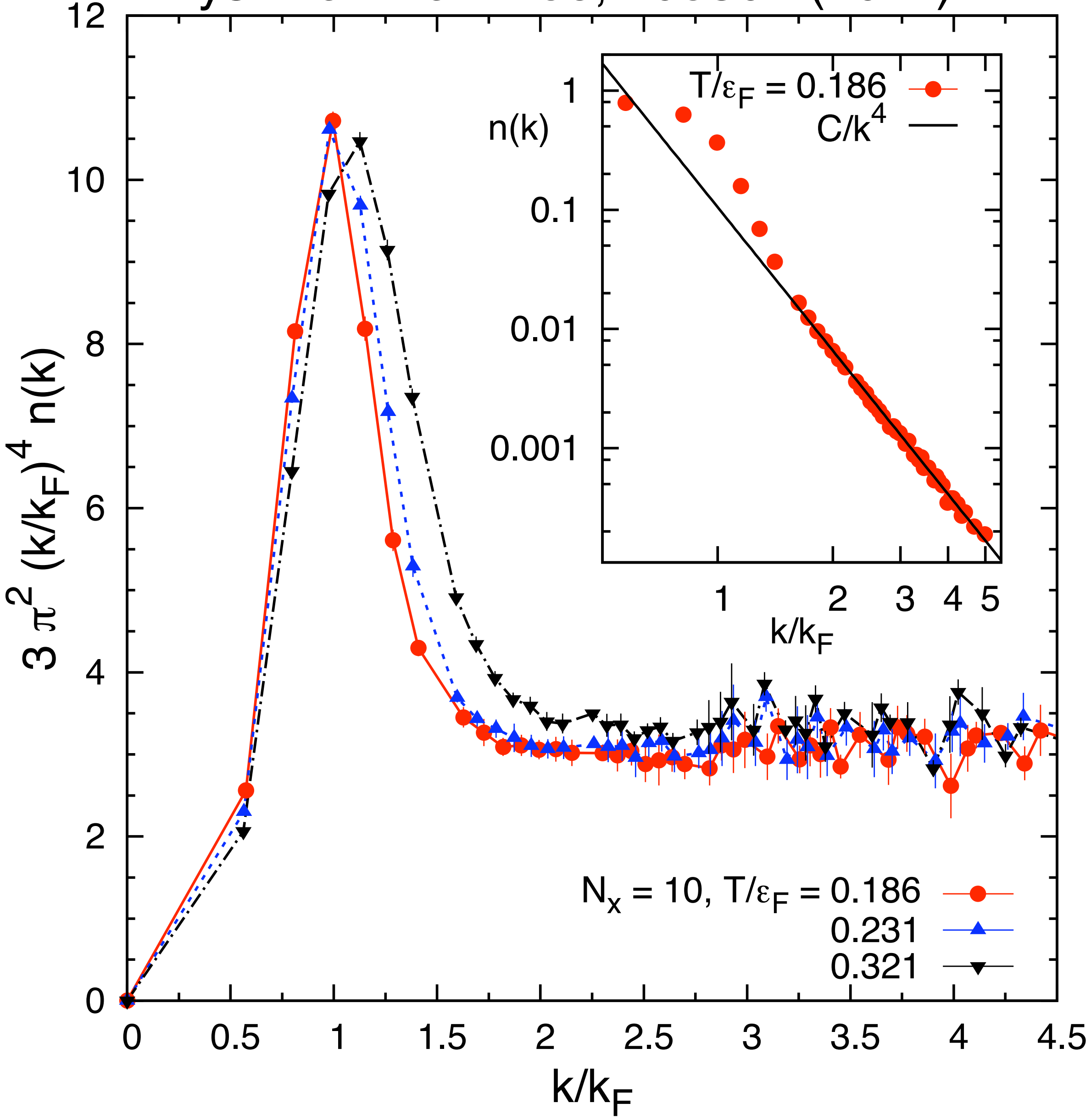
- Pressure relation

$$P = \frac{2\varepsilon}{3} + \frac{\mathcal{C}}{12\pi m a}$$

Momentum distribution & Contact

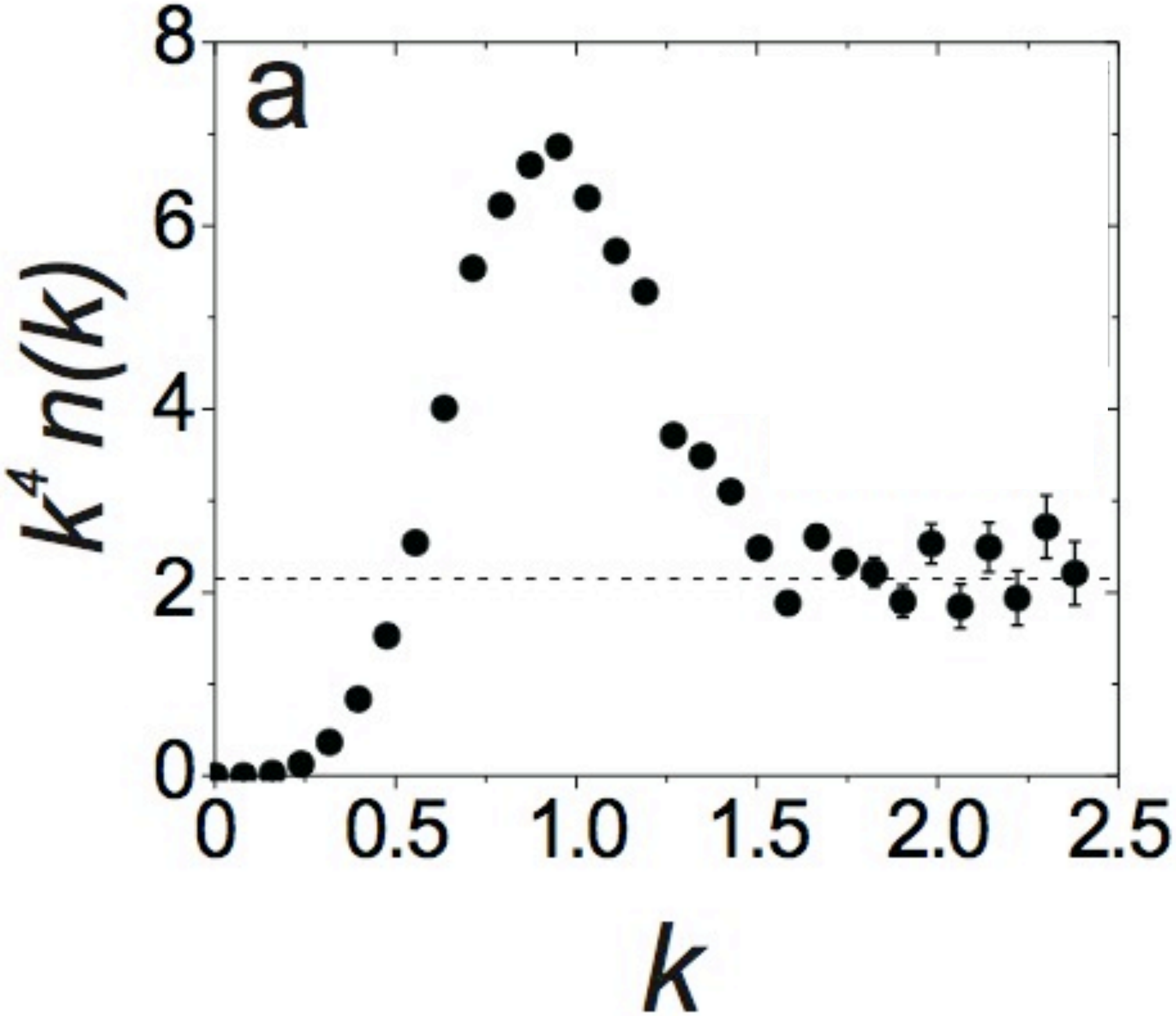
Theory (lattice)

J. E. Drut, T. A. Lähde, T. Ten
Phys. Rev. Lett. **106**, 205302 (2011)



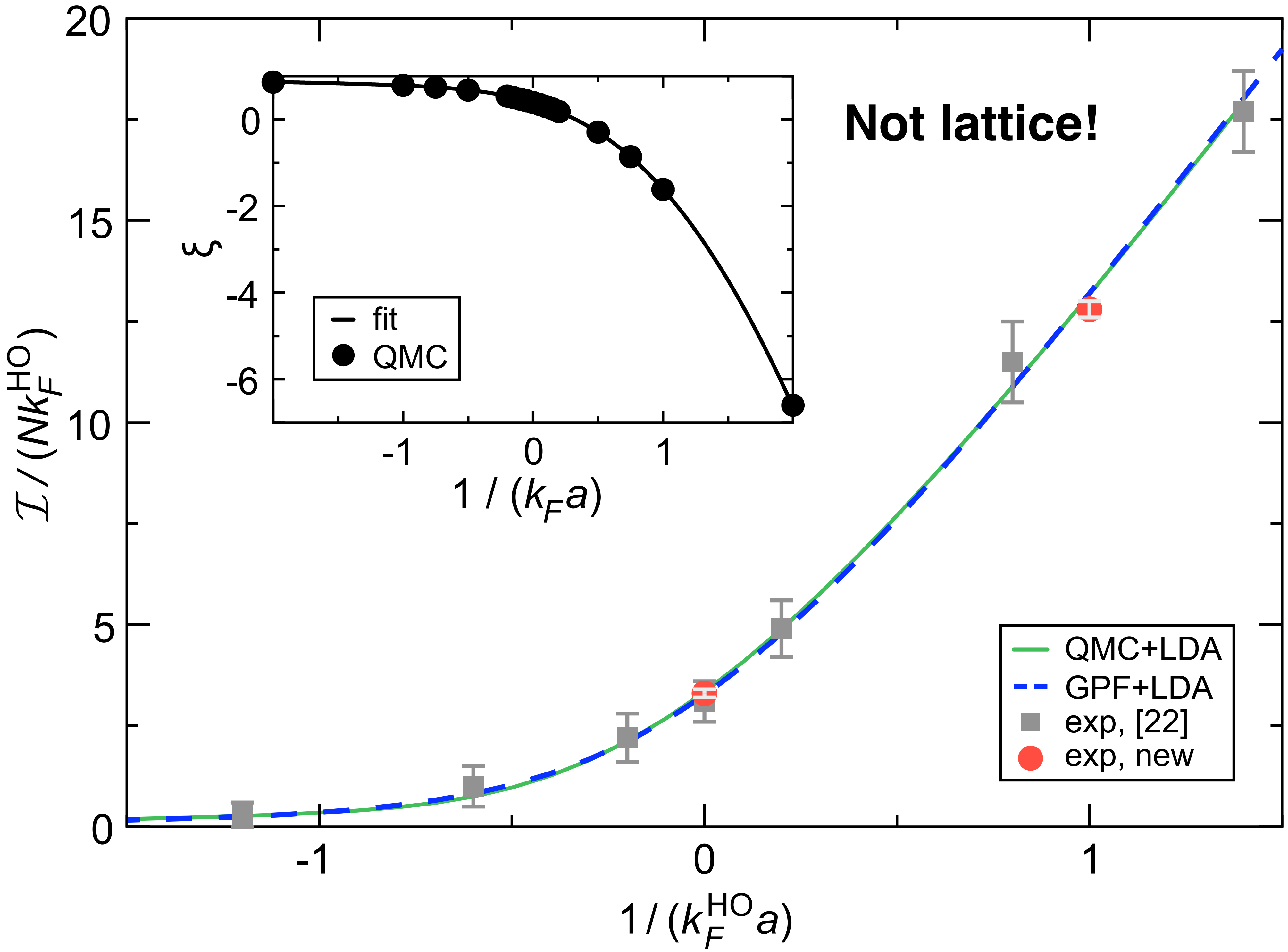
Experiment

J. T. Stewart et al
PRL **104**, 235301 (2010)



- T/T_F = 0 - 0.5 $\quad k_F r_{\text{eff}} \simeq 0.3 - 0.5$
- Plateau seen both in **theory** and **experiment**!

Contact (ground state, in a trap)



S. Hoinka, M. Lingham, K. Fenech, H. Hu, C. J. Vale, **JED**, S. Gandolfi
[arXiv:1209.3830]

How...
(...to deal with finite-range effects)

Dealing with systematic effects

Finite volume

Finite lattice spacing

→ Related to each other

Induce finite-range effects

In general we have...
$$p \cot \delta(p) = -\frac{1}{a} + \frac{1}{2} r_{\text{eff}} p^2 + O(p^4).$$

But we want...
$$p \cot \delta(p) \equiv 0$$
... at unitarity

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... at unitarity

→ **Can't do that with only one parameter!**

Effective range remains finite!

Point-like interaction

$$\hat{V} \equiv -g \sum_{\boldsymbol{i}} \hat{n}_{\uparrow,\boldsymbol{i}} \hat{n}_{\downarrow,\boldsymbol{i}}$$

Transfer matrix

$$\mathcal{T} \equiv e^{-\tau \hat{H}} \simeq e^{-\frac{\tau \hat{T}}{2}} e^{-\tau \hat{V}} e^{-\frac{\tau \hat{T}}{2}} + O(\tau^2)$$

Dealing with systematic effects

→ **We need a "richer" HS transformation**

Endres et al. multiple papers.

Typically...

$$\mathcal{T} = \int \mathcal{D}\sigma \; \mathcal{T}_\uparrow[\sigma]\mathcal{T}_\downarrow[\sigma]$$

$$\mathcal{T}_s[\sigma] = e^{-\frac{\tau \hat{T}_s}{2}} \prod_{\boldsymbol{i}} \left(1 + \sqrt{A}\,\hat{n}_{s,\boldsymbol{i}} \sin\sigma_{\boldsymbol{i}}\right) e^{-\frac{\tau \hat{T}_s}{2}}$$

Now...

$$A(\mathbf{p}) = \sum_{n=0}^{N_{\mathcal{O}}-1} C_n \mathcal{O}_n(\mathbf{p})$$

$$\mathcal{O}_n(\mathbf{p}) = \left(1 - e^{-\mathbf{p}^2}\right)^n$$

$$\mathcal{O}_n(\mathbf{p}) = \left[2\sin(p/2)\right]^{2n}$$

How do we tune these coefficients?

Dealing with systematic effects

- **Highly improved actions**
  (transfer matrices, actually)

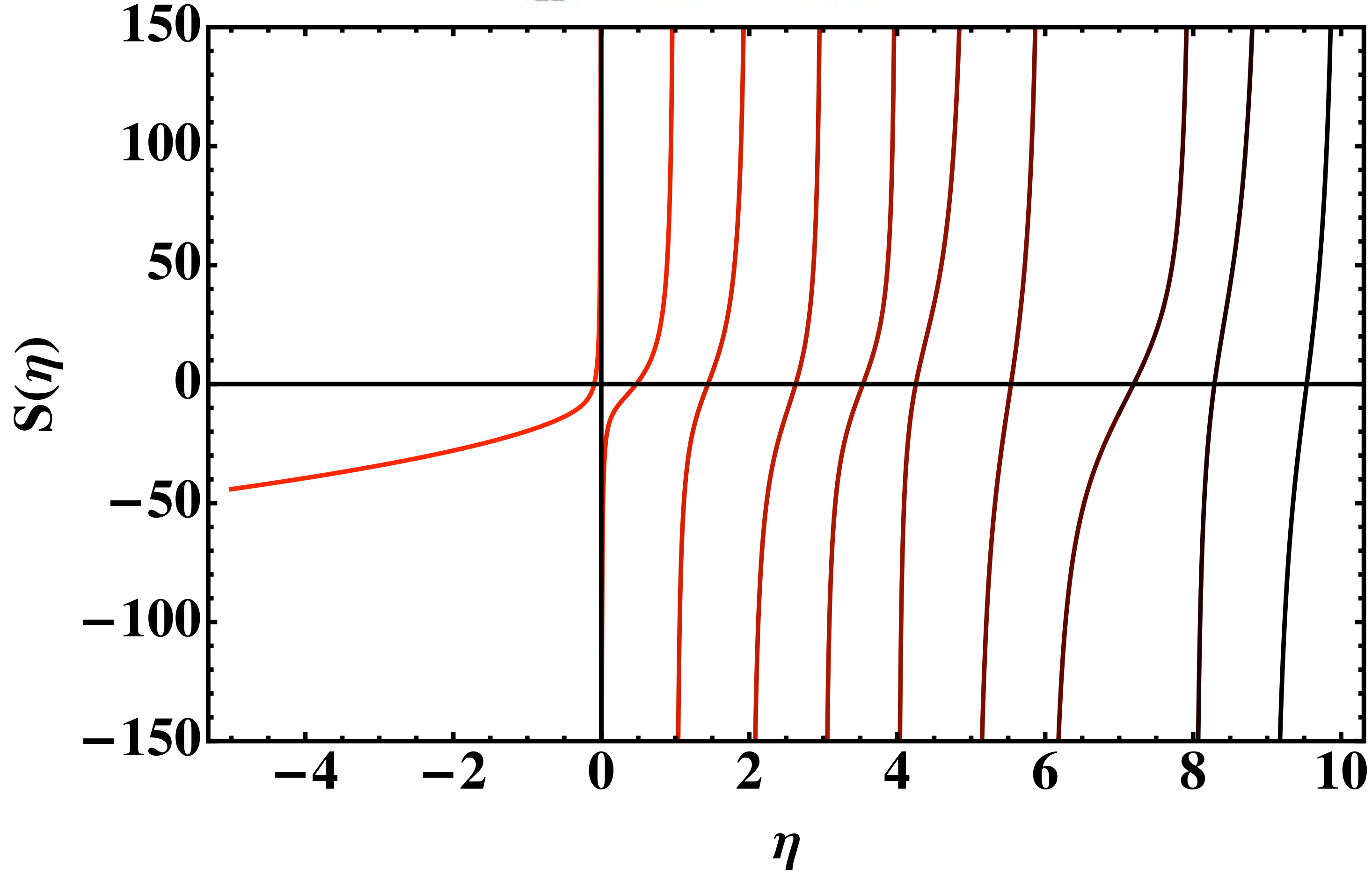
  e.g. using Lüscher's formula

$$p \cot \delta = \frac{\mathcal{S}(E)}{\pi L}$$

s-wave phase shift

Energy eigenvalues
in a box (no lattice)

$$\mathcal{S}(\eta) \equiv \lim_{\Lambda \to \infty} \sum_{\mathbf{n}} \frac{\Theta(\Lambda^2 - \mathbf{n}^2)}{\mathbf{n}^2 - \eta^2} - 4\pi\Lambda$$



$$\eta = \frac{pL}{2\pi}$$

$$E = p^2/m$$

Dealing with systematic effects

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(scattering experiment information)

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→ Decide what scattering parameters you need

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s-wave phase shift
(scattering experiment information)

Energy eigenvalues
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(theory information)

→ Decide what scattering parameters you need

→ Tune your Hamiltonian accordingly

$$\eta = \frac{pL}{2\pi}$$

$$E = p^2/m$$

Dealing with systematic effects

- **Highly improved actions**
  (transfer matrices, actually)

  e.g. using Lüscher's formula
  $$p \cot \delta = \frac{\mathcal{S}(E)}{\pi L}$$

  s-wave phase shift
  (scattering experiment information)

  Energy eigenvalues
  in a box (no lattice)
  (theory information)

→ Decide what scattering parameters you need

→ Tune your Hamiltonian accordingly

→ **Profit!**

$$\eta = \frac{pL}{2\pi}$$
$$E = p^2/m$$

Dealing with systematic effects

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e.g. using Lüscher's formula

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s-wave phase shift
(scattering experiment information)

Energy eigenvalues
in a box (no lattice)
(theory information)

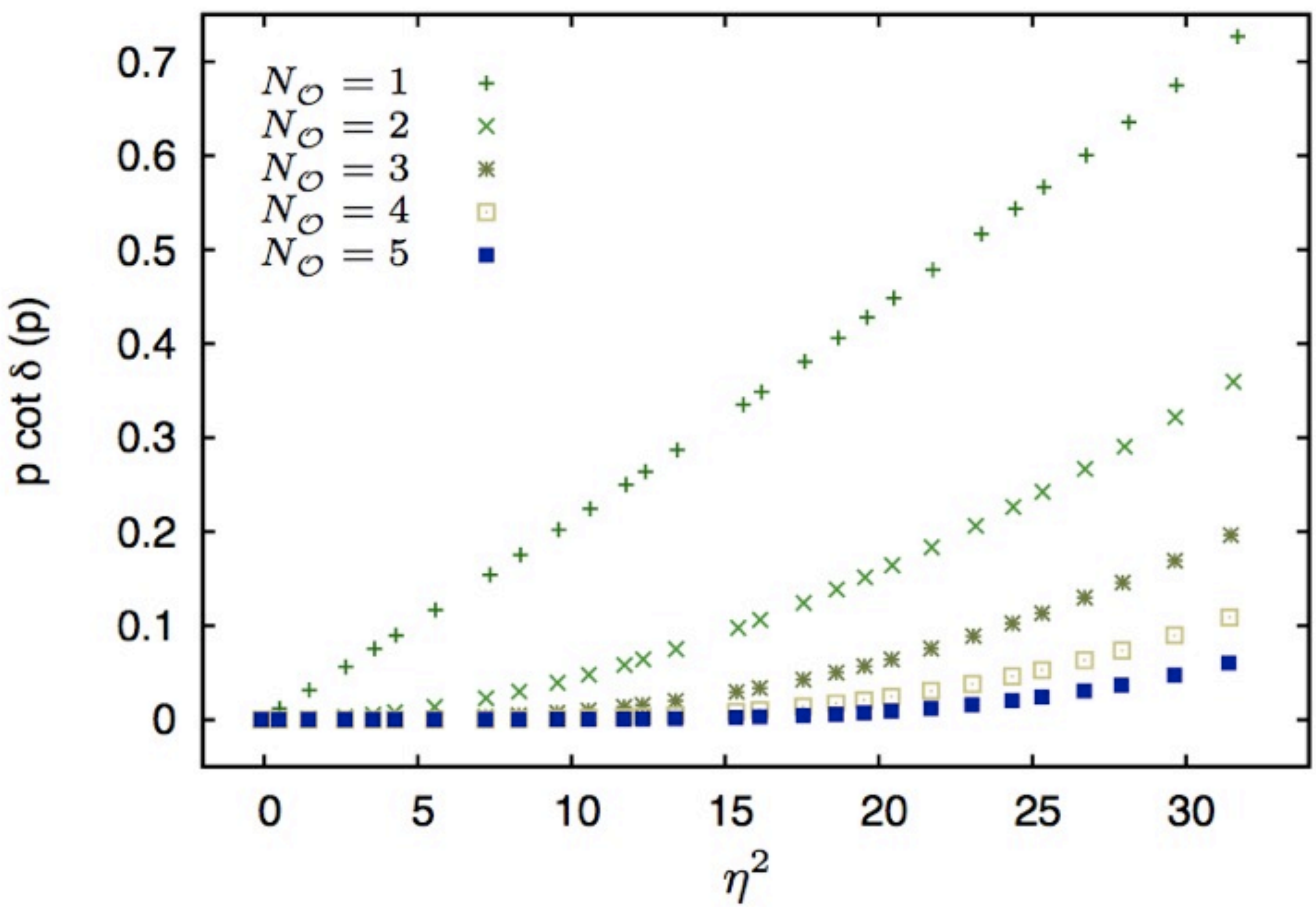
Tuning for unitarity

$N_{\mathcal{O}}$	C_0	C_1	C_2	C_3	C_4
1	0.68419	–	–	–	–
2	0.53153	0.07896	–	–	–
3	0.49278	0.04366	0.01807	–	–
4	0.47217	0.03711	0.00784	0.00467	–
5	0.45853	0.03331	0.00718	0.00132	0.00129

Dealing with systematic effects

- **Highly improved actions**

  Adding more parameters to the transfer matrix and tuning via Lüscher's formula...



Improved transfer matrix

Endres et al. multiple papers.

JED

PRA **86**, 013604 (2012)

How about operators?

Dealing with systematic effects: energy

- **Highly improved actions & operators**

$$-\frac{\partial \log \mathcal{Z}}{\partial \beta} = E - \mu N.$$

$$-\frac{\partial \langle E|\mathcal{T}_2|E\rangle}{\partial \tau} = \langle E|e^{-\frac{\tau p_r^2}{2m}}\left[K_2 + U_2\right]e^{-\frac{\tau q_r^2}{2m}}|E\rangle \;= E_2 \exp\left(-\tau E_2\right)$$

$$K_2 \equiv \left[\frac{p_r^2}{2m} + \frac{q_r^2}{2m}\right]\left[\delta_{\boldsymbol{p}_r \boldsymbol{q}_r} + \frac{A(\boldsymbol{p}_r)}{2V}\right]$$

$$U_2 \equiv -\frac{1}{2V}\frac{\partial A(\boldsymbol{p}_r)}{\partial \tau} = \frac{1}{2V}\sum_{n=0}^{N_{\max}-1} D_n \mathcal{O}_n(\boldsymbol{p}_r)$$

We need these for an improved Hamiltonian operator!

Dealing with systematic effects: energy

- **Highly improved actions & operators**

$$-\frac{\partial \log \mathcal{Z}}{\partial \beta} = E - \mu N.$$

$$-\frac{\partial \langle E|\mathcal{T}_2|E\rangle}{\partial \tau} = \langle E|e^{-\frac{\tau p_r^2}{2m}}\left[K_2 + U_2\right]e^{-\frac{\tau q_r^2}{2m}}|E\rangle \; = E_2 \exp\left(-\tau E_2\right)$$

Tuning for unitarity

$N_{\mathcal{O}}$	D_0	D_1	D_2	D_3	D_4
1	-14.76869	–	–	–	–
2	-11.54894	-1.74519	–	–	–
3	-10.74506	-0.96946	-0.40164	–	–
4	-10.31974	-0.82605	-0.17494	-0.10404	–
5	-10.03874	-0.74266	-0.16064	0.02948	-0.02878

Dealing with systematic effects: energy

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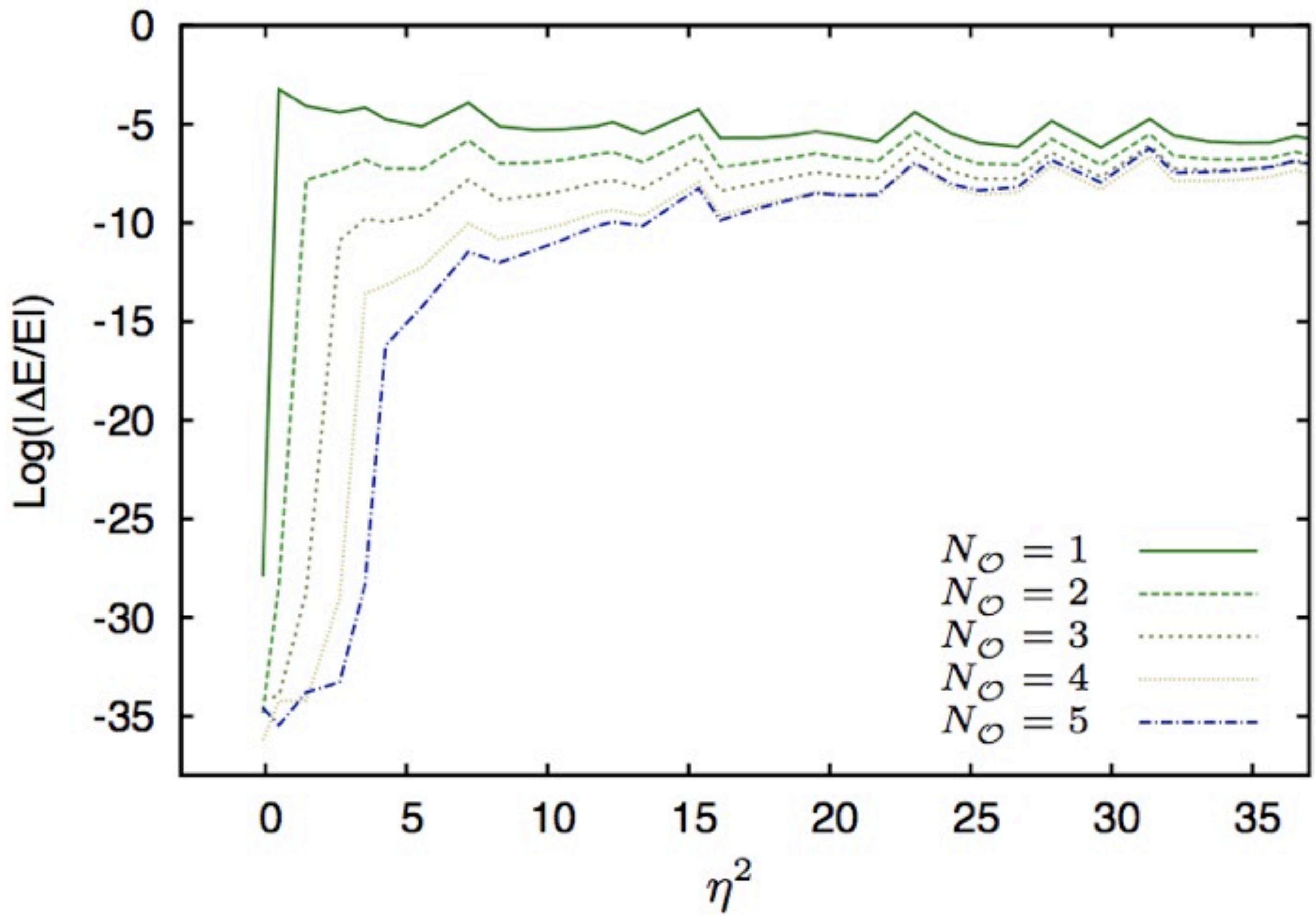
Adding more parameters to the transfer matrix and tuning via Lüscher's formula...



Energy

JED

PRA **86**, 013604 (2012)

A more direct way to the contact...

At T=0...

$$\frac{\partial E}{\partial a^{-1}} = -\frac{\hbar^2}{4\pi m} C$$

At finite T...

$$\left(\frac{\partial \Omega}{\partial a^{-1}}\right)_{T,\mu} = -\frac{1}{\beta}\left(\frac{\partial \log \mathcal{Z}}{\partial a^{-1}}\right)_{T,\mu} = -\frac{\hbar^2}{4\pi m} C$$

In both cases we need

$$\frac{\partial T_2^{\text{exact}}}{\partial a^{-1}} = -\tau \frac{\partial E_2}{\partial a^{-1}} \exp\left(-\tau E_2\right)$$

$$\frac{\partial E_2}{\partial a^{-1}} = -\frac{4\pi^3}{L}\left(\frac{d\mathcal{S}}{d\eta^2}\right)^{-1}$$

Roots, etc...

TABLE IV. First 30 roots of $\mathcal{S}(\eta)$, and $d\mathcal{S}/d\eta^2$ evaluated at those roots.

k	η_k^2	$d\mathcal{S}/d\eta_k^2$
1	-0.0959007	123.82387
2	0.4728943	39.75514
3	1.4415913	82.36519
4	2.6270076	106.24712
5	3.5366199	84.23133
6	4.2517060	161.88763
7	5.5377008	212.49220
8	7.1962632	62.95336
9	8.2879537	231.79580
10	9.5345314	247.82611
11	10.5505341	233.82976
12	11.7014957	185.61411
13	12.3102392	183.65019
14	13.3831152	316.68684
15	15.3537375	82.86757
16	16.1218253	506.59914
17	17.5325415	371.40245
18	18.6053932	308.00372
19	19.5186394	255.97969
20	20.4033187	329.98905
21	21.6944179	394.81924
22	23.0194727	94.98929
23	24.3306210	342.25749
24	25.3016129	526.27127
25	26.6803600	514.90705
26	27.8780019	150.20773
27	29.6156511	548.38017
28	31.3536974	114.02114

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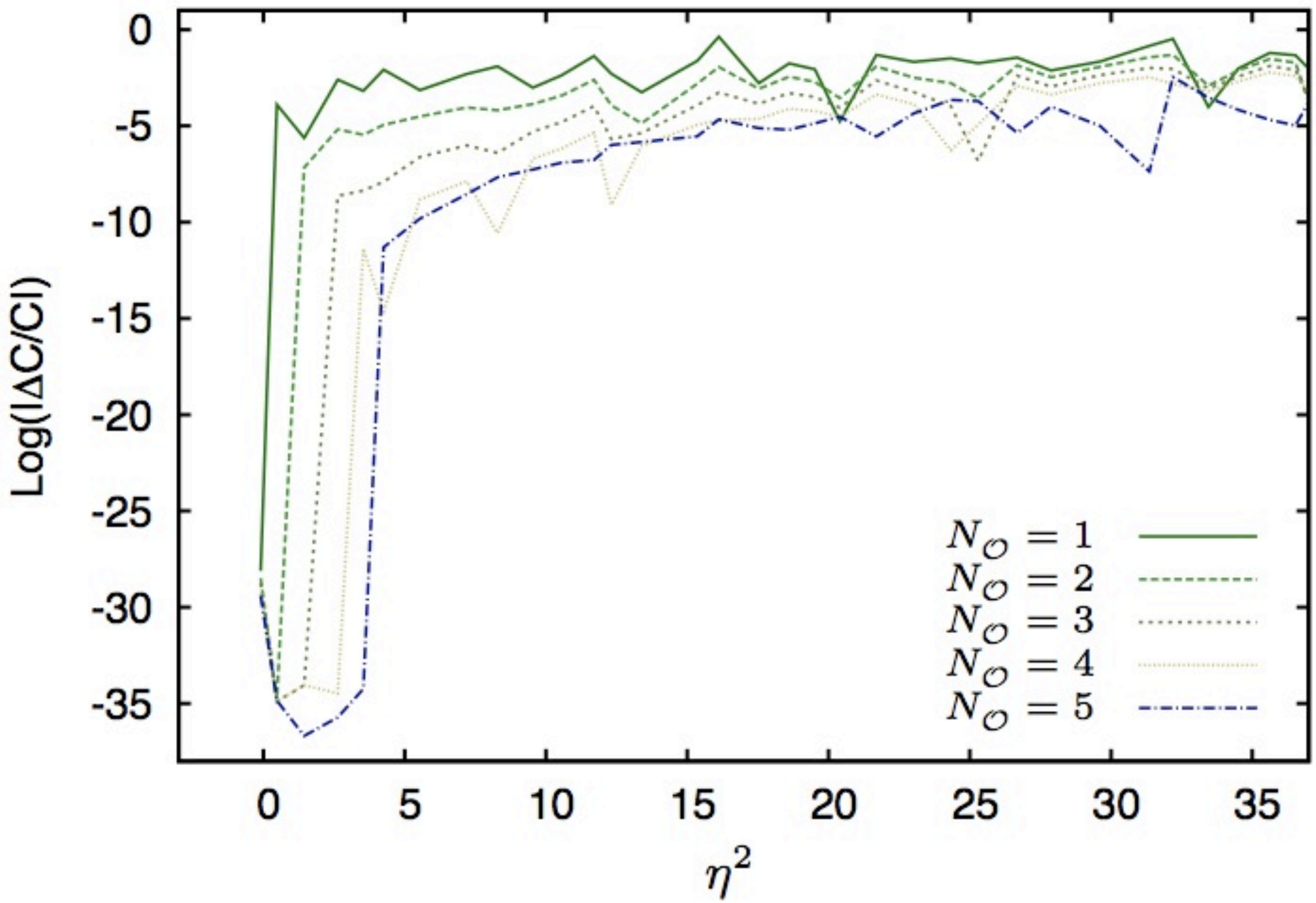
Tuning for unitarity

$N_{\mathcal{O}}$	F_0	F_1	F_2	F_3	F_4
1	0.36773	–	–	–	–
2	0.14532	0.07568	–	–	–
3	0.11370	0.02220	0.01957	–	–
4	0.09659	0.01695	0.00415	0.00538	–
5	0.08205	0.01278	0.00406	-0.00023	0.00180

Dealing with systematic effects: contact

- **Highly improved actions & operators**

  Adding more parameters to the transfer matrix and tuning via Lüscher's formula...



Contact

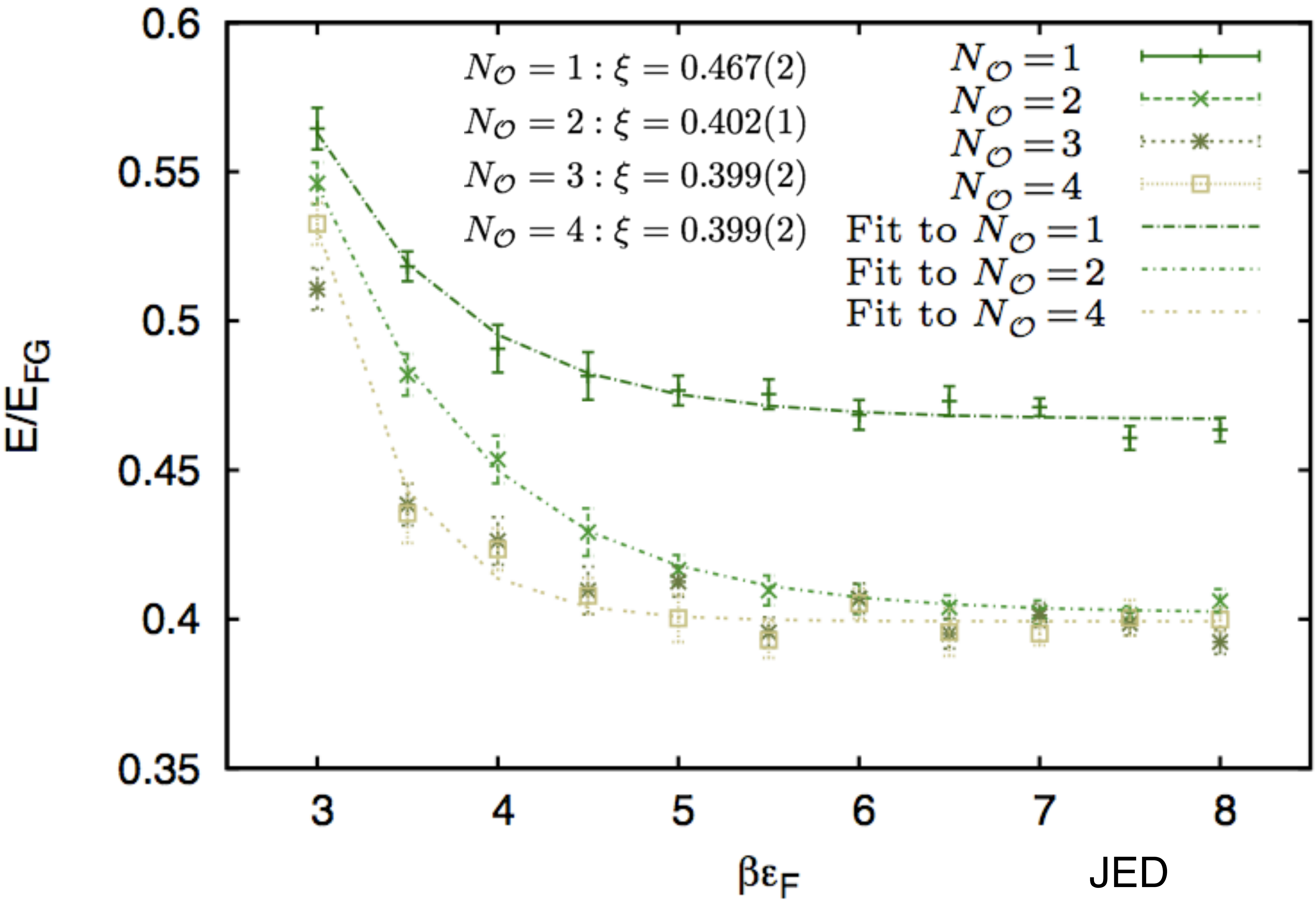
JED

PRA **86**, 013604 (2012)

Illustrative results

- Lattice transfer-matrix approach for ground-state calculations
- Only use one lattice size: $N_x = 10$
- Starting wavefunction: single free-particle Slater determinant.
- Sampling via Hybrid Monte Carlo (about 500 field configurations)

Illustrative results: Energy (ground state)



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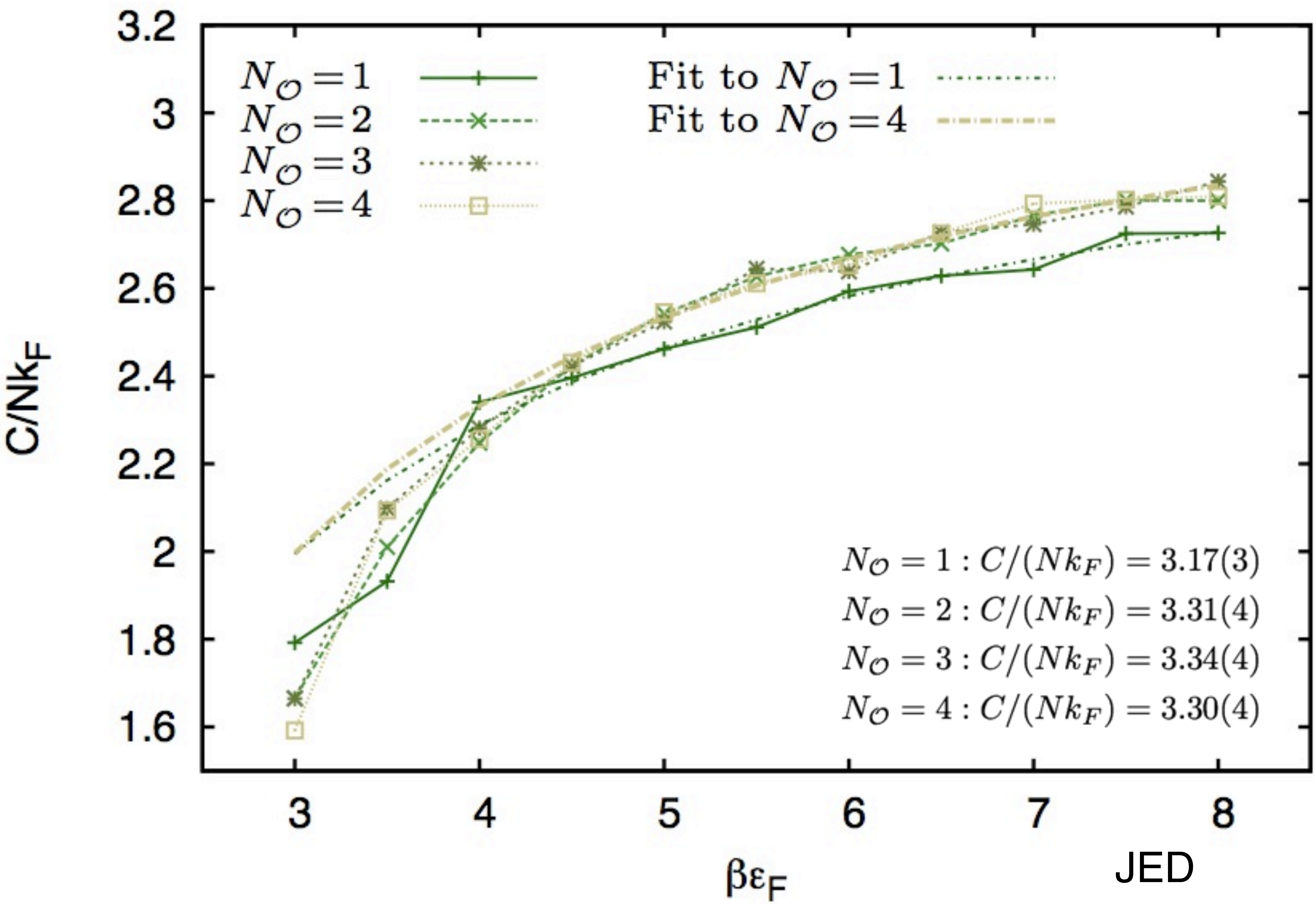
PRA **86**, 013604 (2012)

Illustrative results: Contact (ground state)



JED

PRA **86**, 013604 (2012)

Extrapolations

$$\mathcal{Z}_0(\beta) = \sum_k A_k e^{-\beta E_k} \qquad A_k \equiv |\langle \psi_0 | E_k \rangle|^2$$

- Energy

$$E(\beta) \equiv -\frac{\partial \log \mathcal{Z}_0(\beta)}{\partial \beta} \to E_0 + b_E e^{-\beta\delta}$$

$$b_E = \frac{A_1}{A_0}(E_1 - E_0) \qquad \delta = E_1 - E_0$$

- Contact

$$C(\beta) \equiv \frac{4\pi m}{\hbar^2 \beta} \frac{\partial \log \mathcal{Z}_0(\beta)}{\partial a^{-1}} \to C_0 + b_{C1}\beta^{-1} + b_{C2} e^{-\beta\delta}$$

$$b_{C1} = \frac{4\pi m}{\hbar^2} \frac{\partial \log A_0}{\partial a^{-1}},$$

$$b_{C2} = -\frac{4\pi m}{\hbar^2} \frac{A_1}{A_0} \left(\frac{\partial E_1}{\partial a^{-1}} - \frac{\partial E_0}{\partial a^{-1}} \right)$$

Summary & Conclusions

- There is a natural way to extend the improvement of actions to improve also operators.
- It seems clear that using improved actions **and** operators does help in bringing lattice calculations closer to the continuum limit.
- Not unexpected: the impact of improvement is observable-dependent.
- The next step is to use all this at finite temperature. However, some testing remains to be done:
  - Does it help to tune **every other** Lüscher eigenvalue?
  - How about tuning using **virial coefficients**? (à la Lee-Schäfer)
- We are reassessing our previous calculations in the light of new ones done with these new tools.
- We are simultaneously pursuing the calculation of response functions (specific heat, compressibility, susceptibility, viscosities).

Thank you!

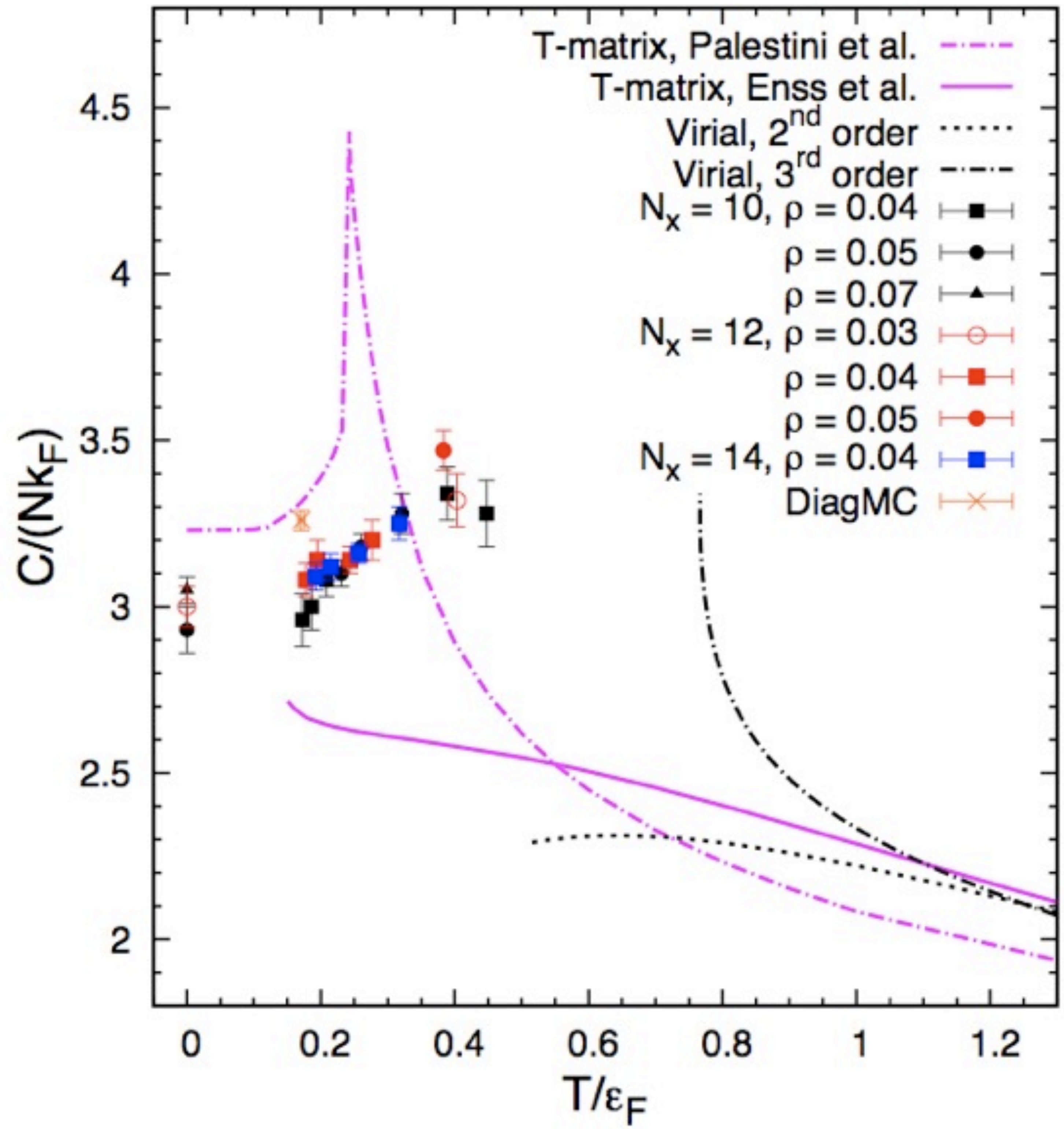
What do we know so far?

- Growth at low T
- Decrease at high T
- Maximum around $T \cong 0.4 T_F$
- Finite density effects?
- What happens in the crossover?

Virial expansion:
Yu, Bruun & Baym PRA **80**, 023615 (2009)
Hu, Liu, & Drummond, arXiv:1011.3845

T-matrix: Palestini et al.
PRA **82**, 021605 (2010)

Improved T-matrix: Enss et al.
`doi 10.1016/j.aop.2010.10.002`



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