

Ground state configuration of unitary fermions

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❖ Fermions at unitarity

- **Definition:** non-relativistic spin-1/2 fermions with an attractive interaction satisfying

$$r_0 \rightarrow 0 \quad \ll \quad n^{-\frac{1}{3}} \quad \ll \quad |a| \rightarrow \infty$$

Range of interaction

Interparticle spacing

s-wave scattering length



$$p \cot \delta_0 \simeq -\frac{1}{a} = 0 \quad (\text{or } \delta_0 = \pi/2)$$

$$\mathcal{A} = \frac{4\pi}{M} \frac{1}{p \cot \delta_0 - ip}$$

0

- The unitarity limit has no intrinsic scale except the density or fermi energy, i.e. strongly coupled non-relativistic conformal (scale invariant) system
- Exhibit *universal* features

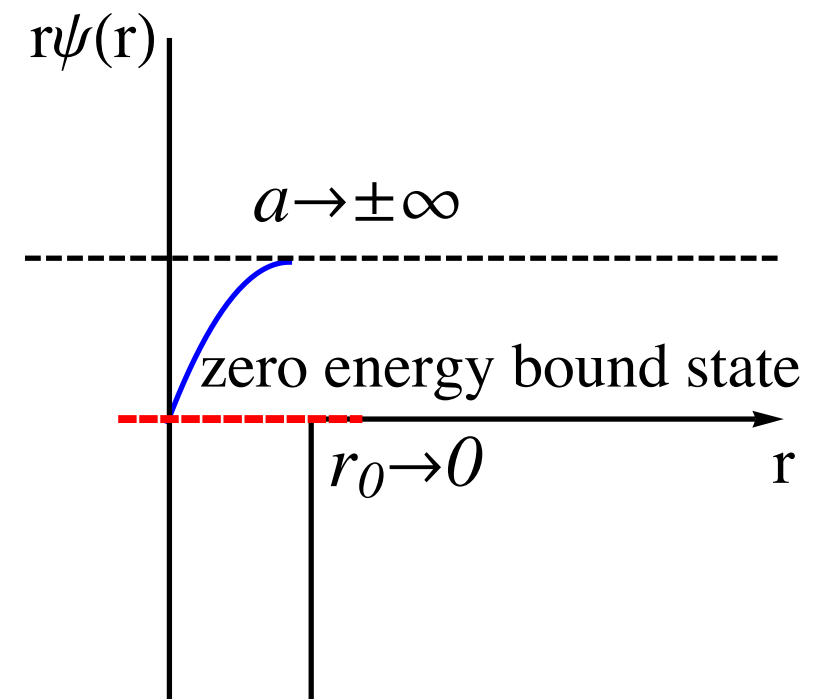
Physics at low energy or long distance is independent on the details of interaction

Bertsch parameter

$$E^{\text{unitary}}(n) = \xi E^{\text{free}}(n)$$

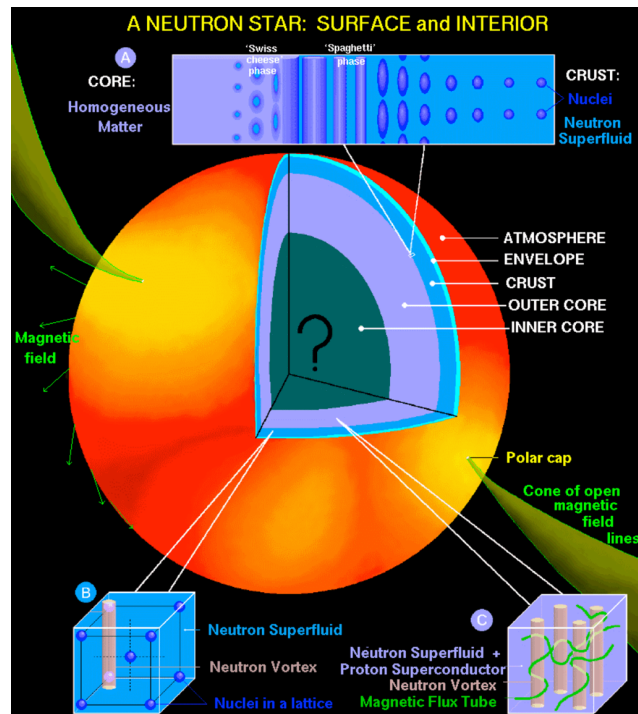
Pairing gap

$$\varepsilon^{\text{unitary}}(n) = \Delta \varepsilon_F^{\text{free}}(n)$$



❖ Applications in nuclear and atomic physics

- Approximate the low-density neutron matter in the crust of a neutron star

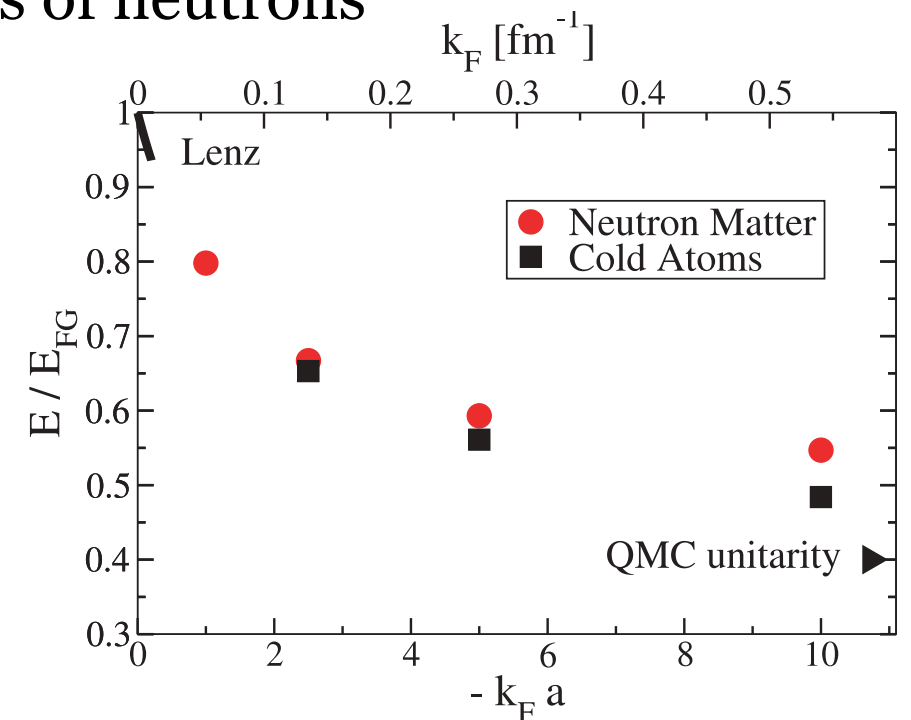


dilute, interacting fermi gas of neutrons

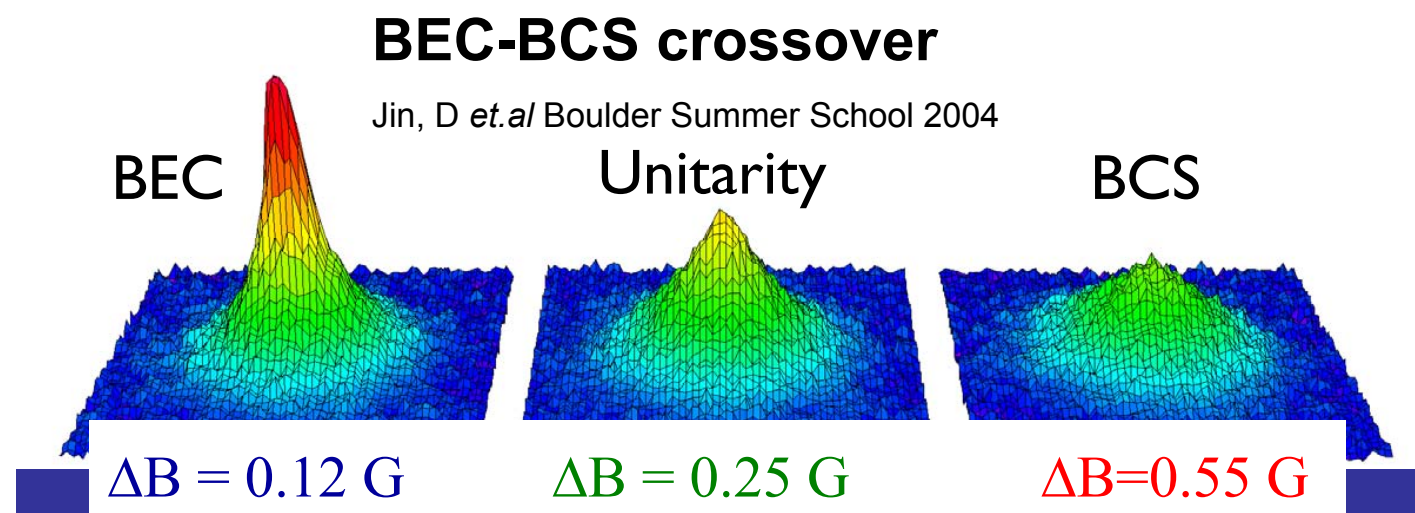
$$k_F a \sim -10, \quad a \sim -7r_e$$

A. Gezerlis &
J. Carlson (2008)

Credit: Dany P Page



- Realized in the laboratory experiments: ultra-cold atomic system tuned by strong magnetic field using Feshbach resonance



❖ Lattice models and the unitarity limit

- The unitary fermi gas (UFG) is a strongly coupled system and thus *its quantitative studies require numerical calculations*, e.g. Quantum Monte Carlo (QMC), based on the *lattice models* in either a Hamiltonian or a Lagrangian approach.
- **Requirement:** recover the universality of the zero-range limit, corresponding to the continuum limit of the lattice models
- **Question:** How do we guarantee the universality in the lattice models?

In the case of three unitary fermions at zero net momentum *L. Pricoupenko & Y. Castin (2007)*

- existence of non-negative solutions, i.e. no bound states
- rapid convergence in the zero lattice spacing limit
- compared to the zero-range model in the continuous space

In this work, we consider three unitary fermions at both zero and non-zero momenta

- ground state configurations are dominated by the zero-momentum pairs

The UFG energetically prefers the configuration that maximizes the overlap with the s-wave zero-energy scattering state.

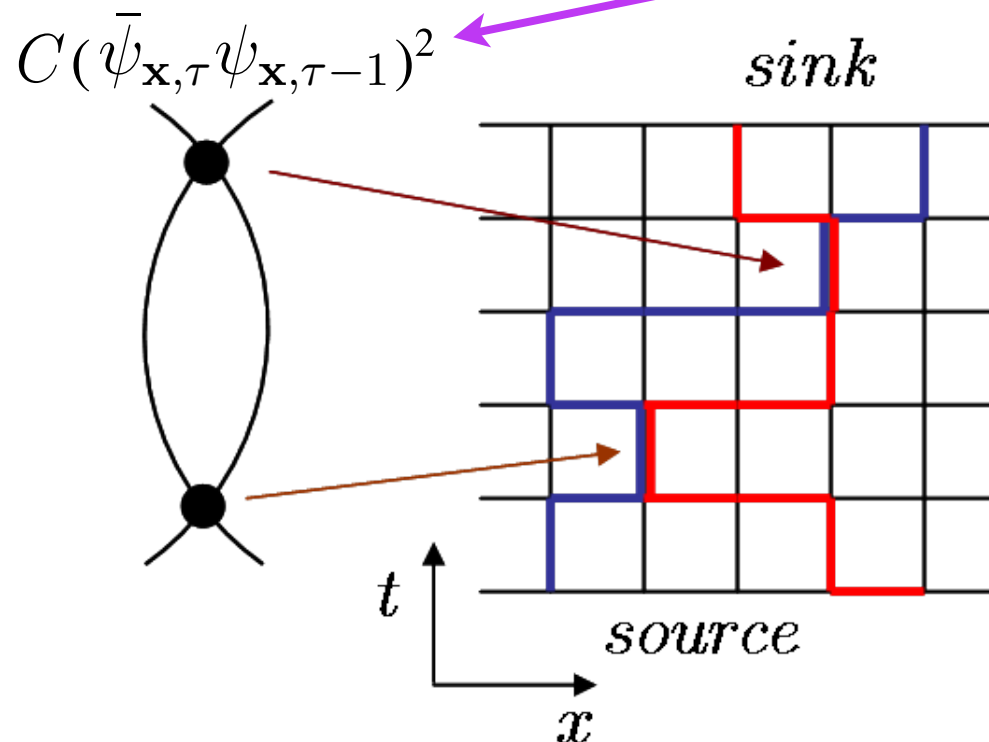
❖ Non-relativistic interacting fermions on the lattice

- Lattice action for non-relativistic 2-component fermions discretized on a 4-dim. Euclidean space-time, **no sign problem at finite chemical potential**

J. -W. Chen & D. B. Kaplan (2004)

$$S = b_\tau b_s^3 \sum_{\tau, \mathbf{x}} \left[\bar{\psi}_{\mathbf{x}, \tau} (\partial_\tau \psi)_{\mathbf{x}, \tau} - \frac{1}{2M} \bar{\psi}_{\mathbf{x}, \tau} (\nabla^2 \psi)_{\mathbf{x}, \tau} + \underbrace{(\sqrt{C} \phi)_{\mathbf{x}, \tau} \bar{\psi}_{\mathbf{x}, \tau} \psi_{\mathbf{x}, \tau-1}} \right]$$

Integrating out



$T \times L^3$ Euclidean Lattice

- (1) Four-Fermi interaction via auxiliary fields, Z_2 ($\phi = \pm 1$) or Gaussian, on time-links

Only fermion loop with forward propagators

$$\langle \phi_{\mathbf{x}, \tau} \rangle = 0, \quad \langle \phi_{\mathbf{x}, \tau} \phi_{\mathbf{x}', \tau'} \rangle = \delta_{\mathbf{x}, \mathbf{x}'} \delta_{\tau, \tau'}$$

- (2) Open B.C. in time and periodic B.C. in space

Restricted to zero temperature

- (3) Observables: N -body correlation functions

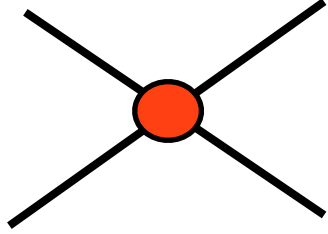
$$\mathcal{C}_N(\tau) = \langle \det S^{\downarrow \uparrow}(\tau) \rangle,$$

$$S_{i,j}^{\downarrow \uparrow}(\tau) = \sum_{\mathbf{q} \in BZ} \tilde{\Psi}(\mathbf{q}) \langle \mathbf{q} | K^{-1}(\tau, 0) | \mathbf{p}_i, \downarrow \rangle \langle -\mathbf{q} | K^{-1}(\tau, 0) | \mathbf{p}_j, \uparrow \rangle$$

M. Endres, D. B. Kaplan, JWL, A. Nicholson (2011)

❖ Tuning coupling for fermions at unitarity

- The coupling of four-fermi operator is tuned to reproduce the phase shift of s-wave scattering via Luscher's finite volume analysis



$$C(\mathbf{p}) = \frac{4\pi}{M} \sum_{n=0}^{N_{\mathcal{O}}-1} C_{2n} \mathcal{O}_{2n}(\mathbf{p})$$

↔

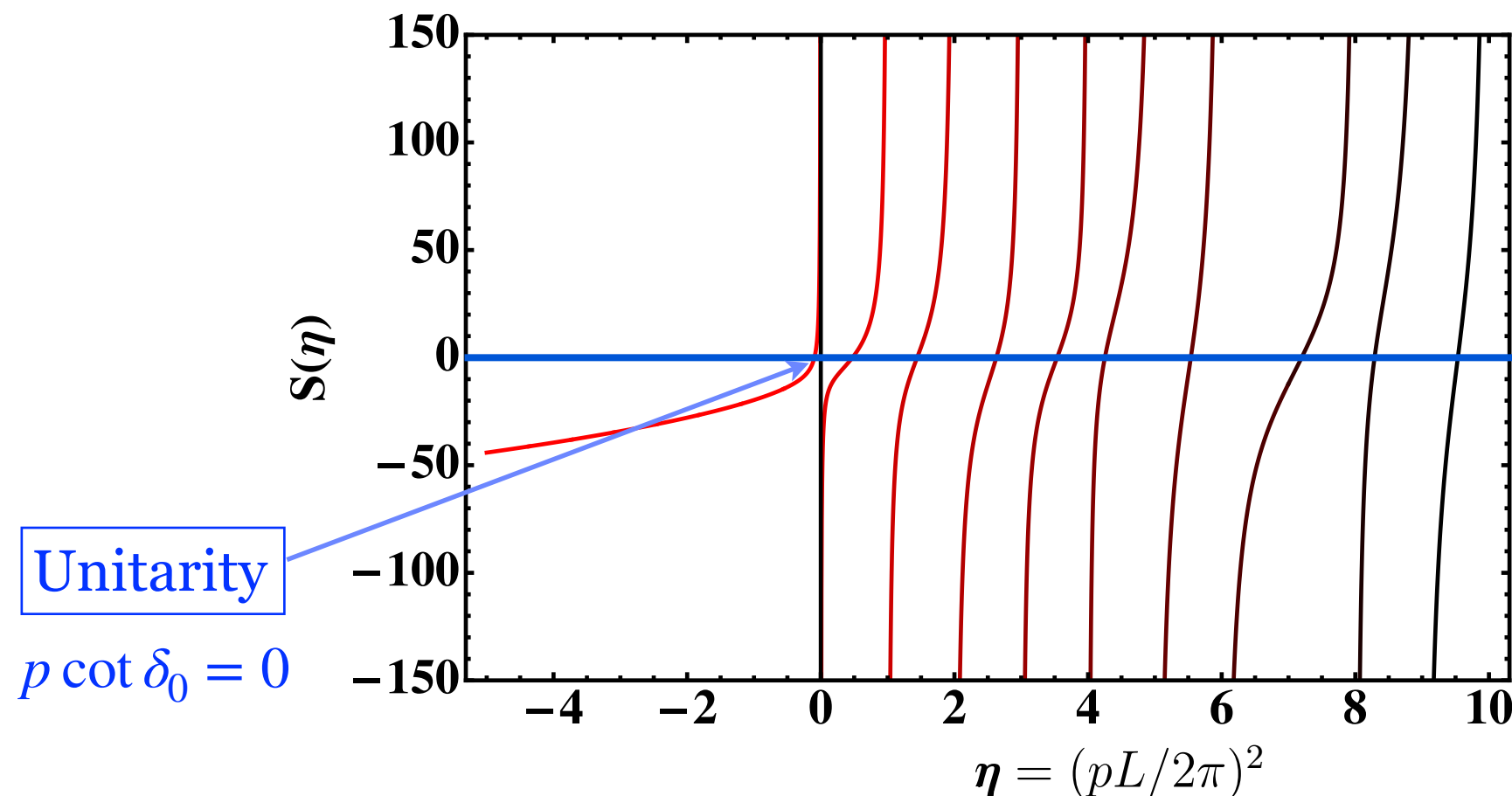
$p \cot \delta_0 = \frac{1}{\pi L} S(\eta)$

Continuum &
infinite volume

confined in a box

S. Beane, P. Bedaque, A. Parreno & M. Savage (2004)

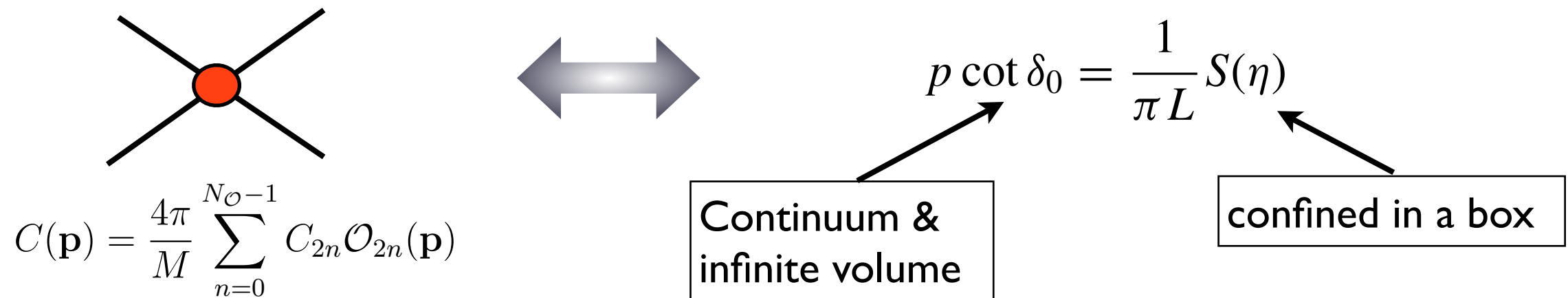
M. Luscher (1986, 1991)



$$S(\eta) = \lim_{\Lambda \rightarrow \infty} \left[\sum_{|\mathbf{j}| < \Lambda} \frac{1}{\mathbf{j}^2 - \eta} - 4\pi \Lambda \right]$$

❖ Tuning coupling for fermions at unitarity

- The coupling of four-fermi operator is tuned to reproduce the phase shift of s-wave scattering via Luscher's finite volume analysis.

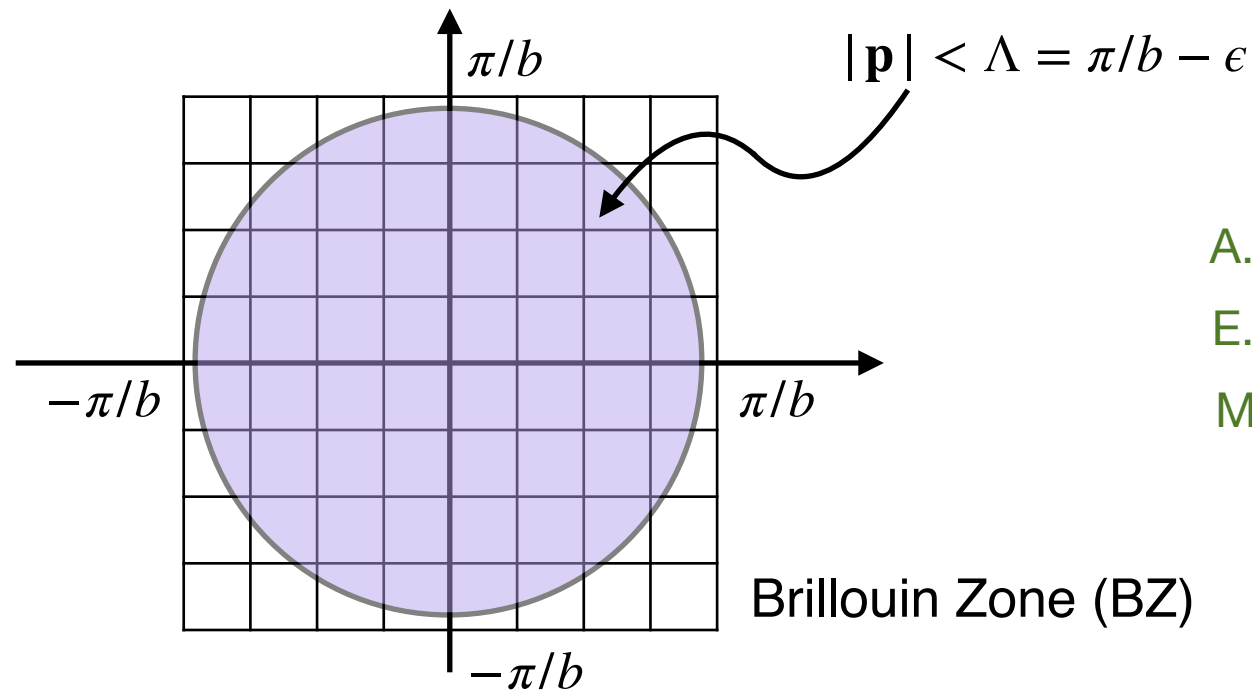


- Matching the lowest $N_{\mathcal{O}}$ eigenstates effectively tunes away the lowest $N_{\mathcal{O}}$ terms in the effective range expansion, and thus highly suppresses finite volume corrections.

$$p \cos \delta_0 = -\frac{1}{a} + \frac{1}{2} \sum_{n=1} r_{n-1} p^{2n} \quad \xrightarrow[\substack{\text{Tuned to unitarity} \\ a \rightarrow 0}]{\text{blue arrow}} \quad p \cos \delta_0 = 0 + \mathcal{O}(1/L^{2N_{\mathcal{O}}-1})$$

❖ Single particle momentum cut-off

- A (hard) spherical momentum cut-off has been widely used in numerical simulations: simple analysis & reduced computational cost, yet, the continuum limit can be reached by $\Lambda \rightarrow \infty$.



A. Bulgac, J. E. Drut & P. Magrieski (2006, 2008)

E. Burovski, E. Kozik, N. Prokof'ev, B. Svistunov, (2008)

M. Endres, D. B. Kaplan, JWL, A. Nicholson (2011)

- However, Werner and Castin pointed out that the unitarity (tuned in the center-of-momentum frame) is violated when pairs of fermions have a non-zero net-momentum P (due to a violation of Galilean invariance).

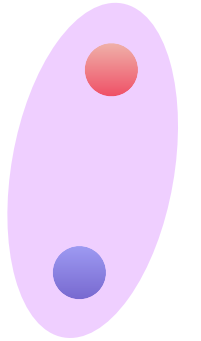
F. Werner & Y. Castin (2012)

$$p \cos \delta_0 = -\frac{1}{a} + \frac{P}{2\pi} + \frac{1}{2} \sum_{n=1} r_{n-1} p^{2n}$$

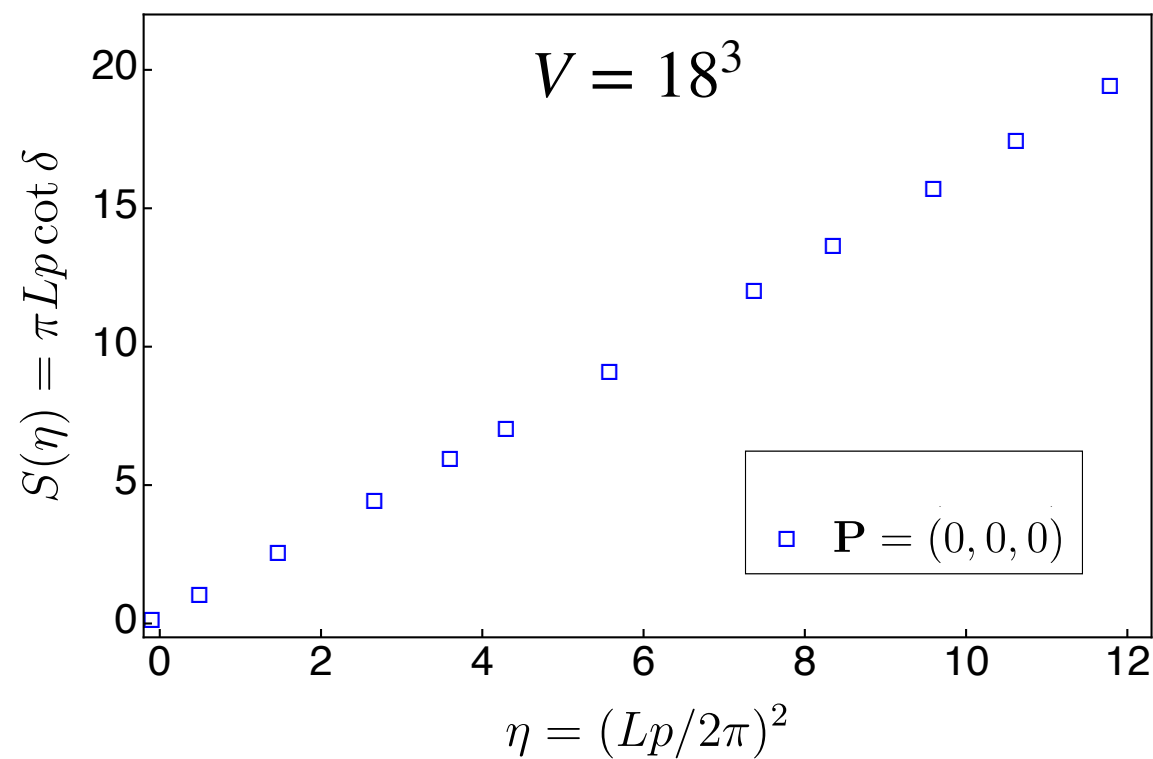
❖ A pair of unitary fermions in a moving frame

$\mathbf{P} = 0$

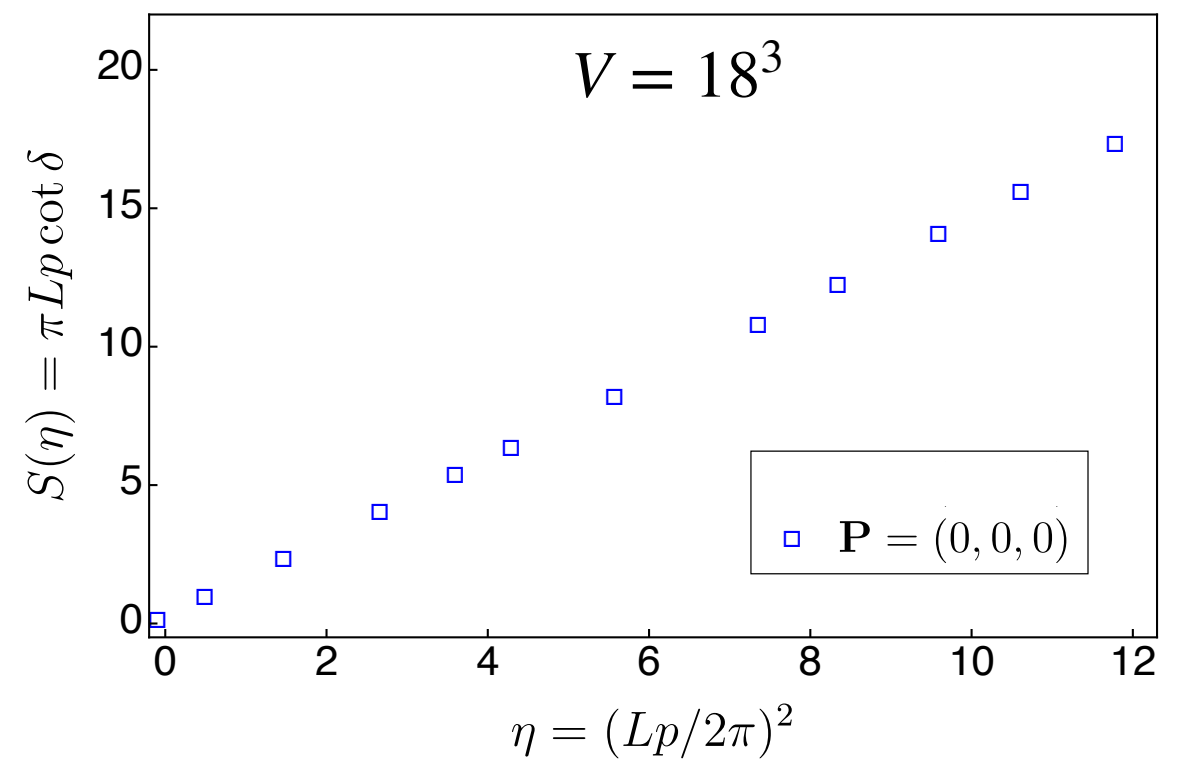
- The coupling with $N_{\mathcal{O}} = 1$ operator tuned to infinite s-wave scattering length with and without a spherical momentum cut-off in the CoM frame



momentum cut-off Λ



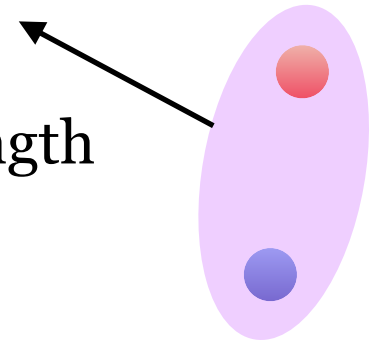
Full Brillouin Zone



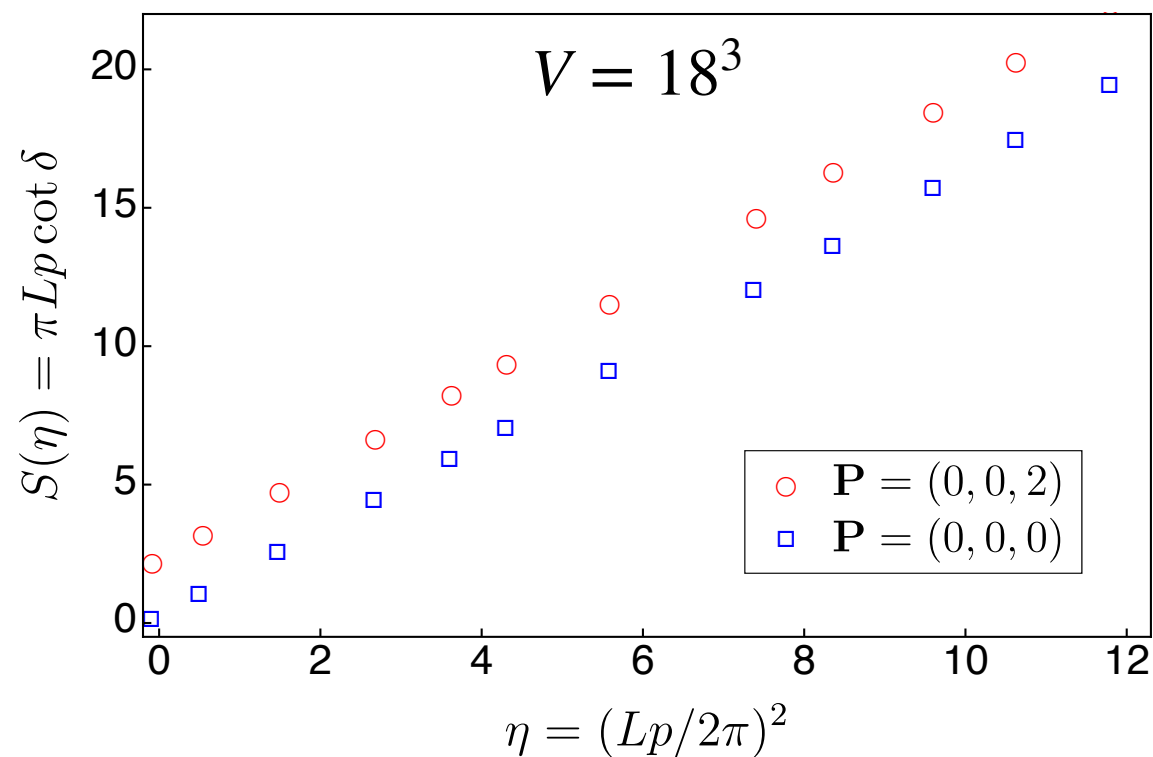
❖ A pair of unitary fermions in a moving frame

- The coupling with $N_{\mathcal{O}} = 1$ operator tuned to infinite s-wave scattering length with and without a spherical momentum cut-off in the CoM frame

$$\mathbf{P} = \frac{2\pi}{L}(0,0,2)$$

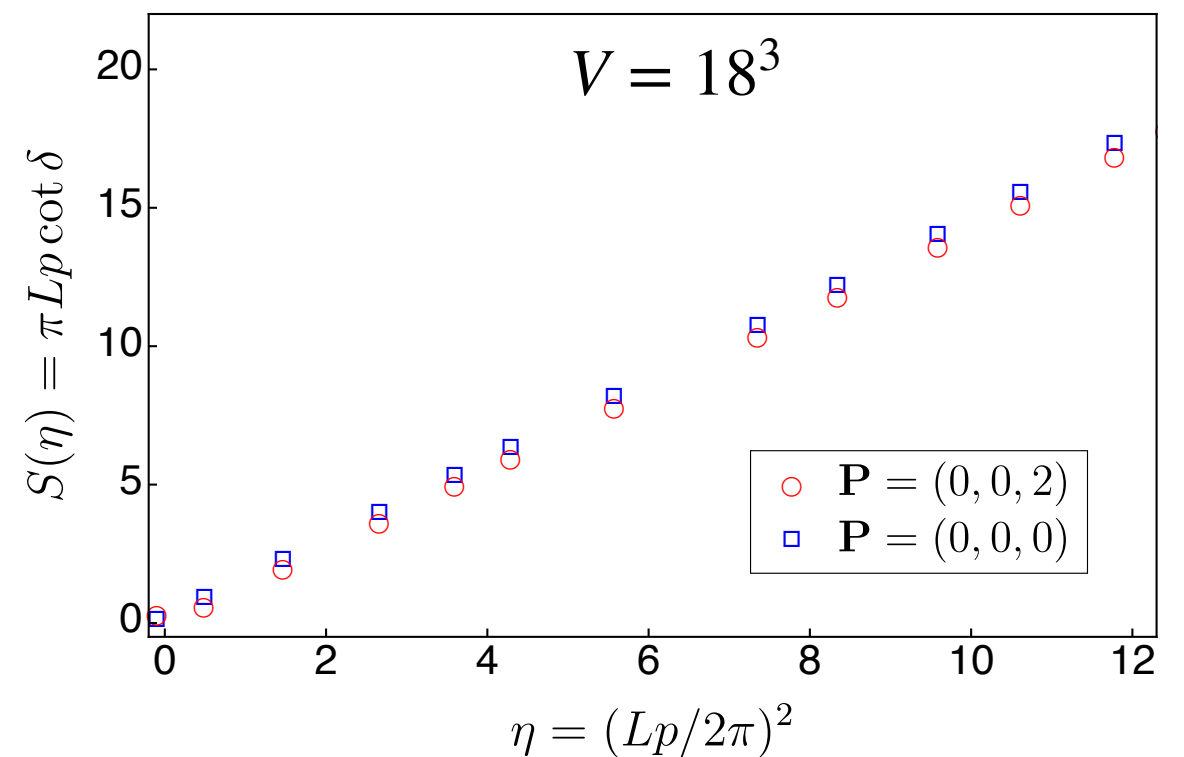


momentum cut-off Λ



deviates from the unitarity

Full Brillouin Zone



remains at the unitarity

- The deviation persists even in the infinite volume limit, suggesting that the existence of the cut-off Λ violates the unitarity unless the pair is at zero CoM.

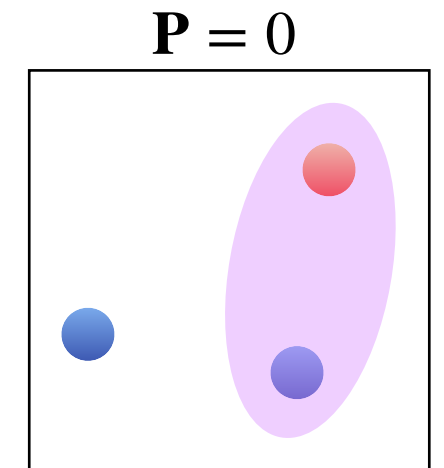
See also S. Jensen, C. N. Gilbreth & Y. Alhassid (2020)

❖ Three unitary fermions at zero net total momentum

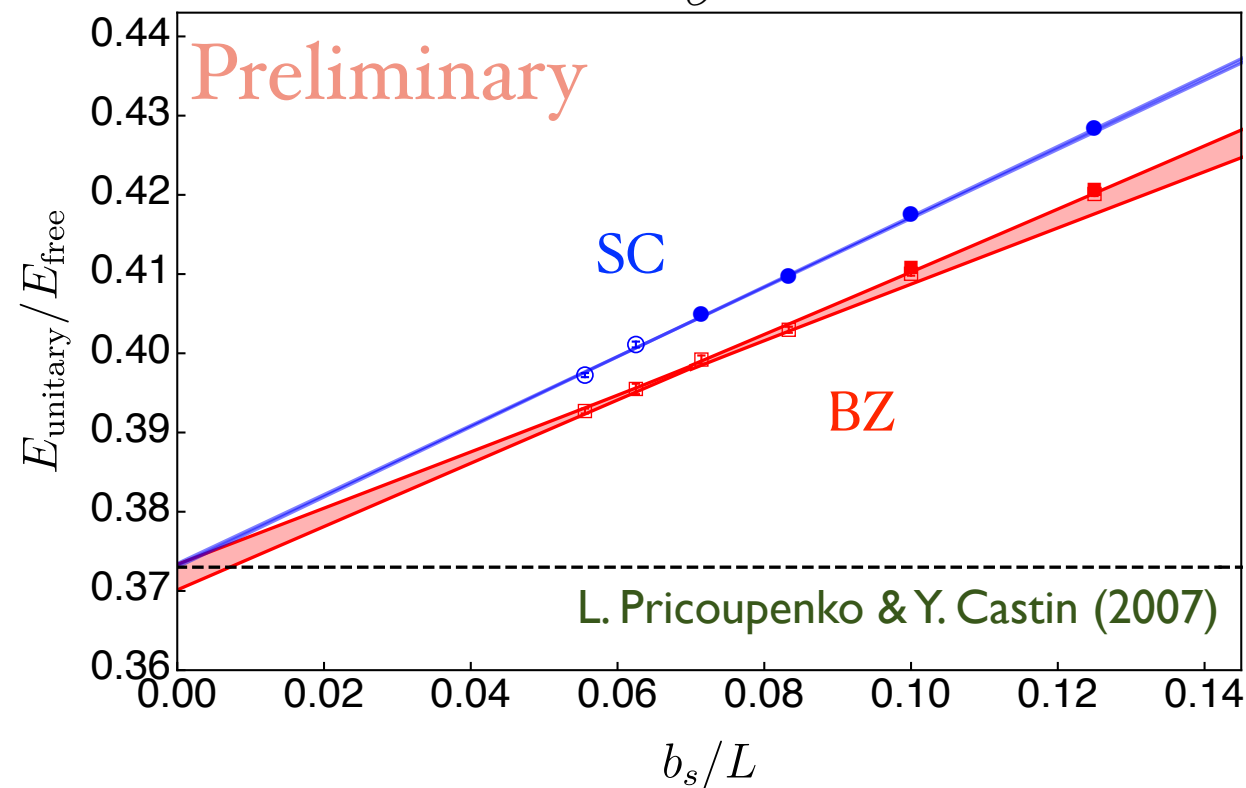
- Compute the ground state energies at various volumes using lattice simulations, complemented by exact solutions via the matrix diagonalizations at small lattices

SC: a spherical momentum cut-off

BZ: full Brillouin zone



$$N_{\mathcal{O}} = 1$$

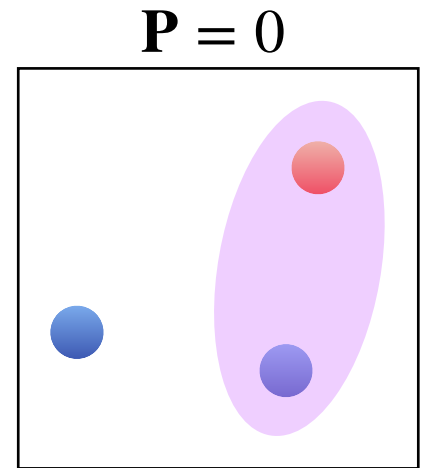


- In the continuum limit, both results are in good agreement within a 1 % error.

Pair of unitary fermions at zero momentum

❖ Three unitary fermions at zero net total momentum

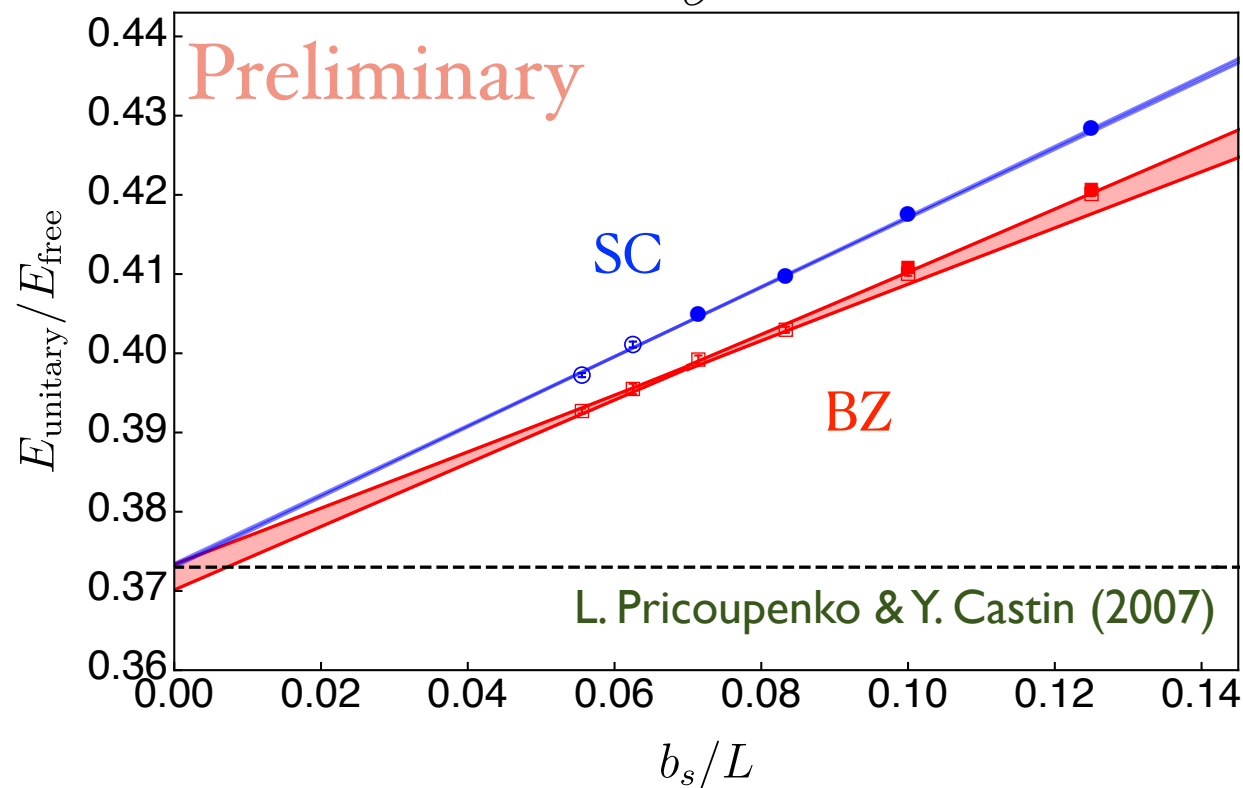
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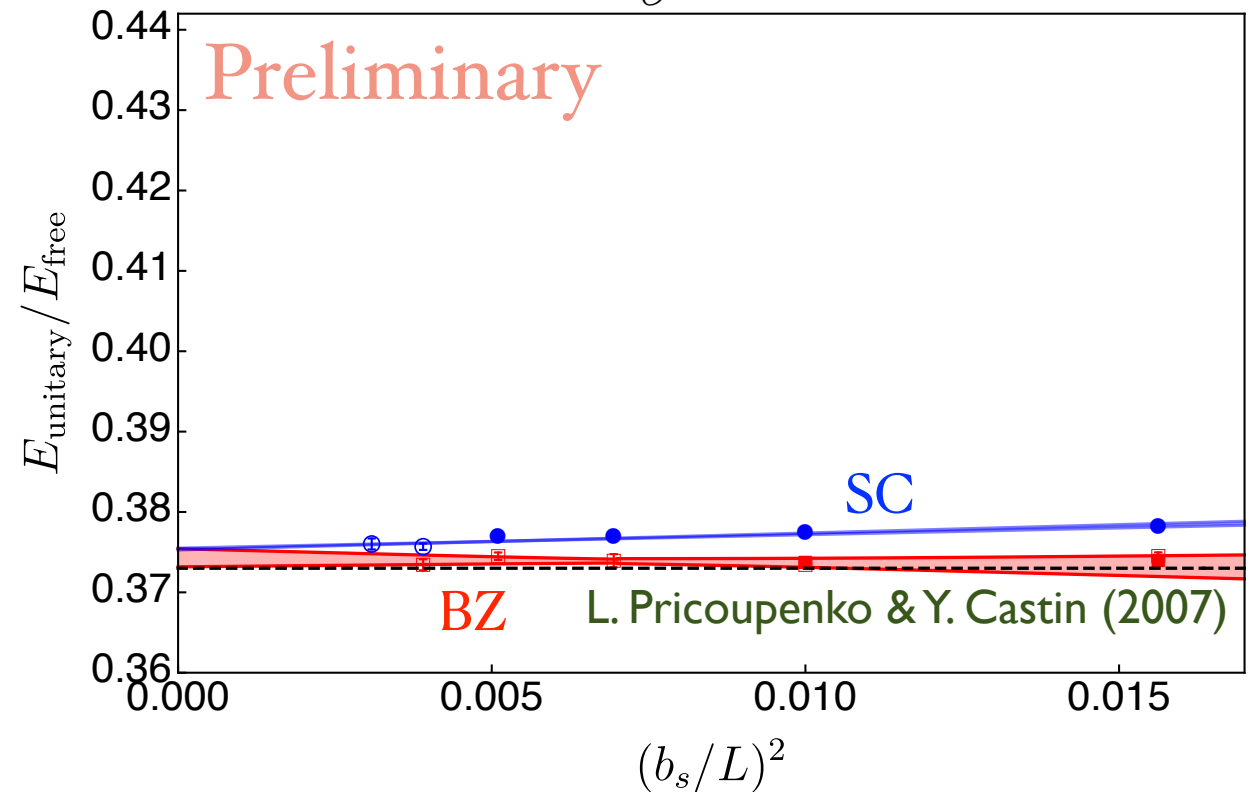
SC: a spherical momentum cut-off

BZ: full Brillouin zone

$N_{\mathcal{O}} = 1$



$N_{\mathcal{O}} = 2$



- In the continuum limit, both results are in good agreement within a 1 % error.

Pair of unitary fermions at zero momentum

- Coupling tuning with $N_{\mathcal{O}} = 2$ operators significantly improves the finite volume corrections in both cases.

❖ Three unitary fermions at non-zero net total momentum

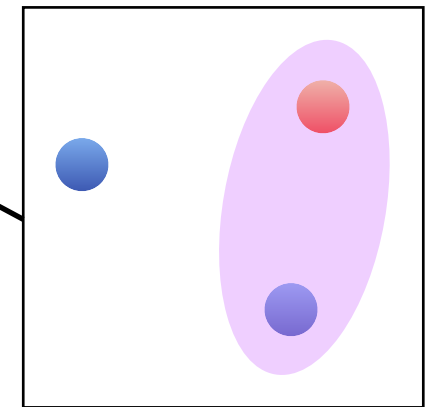
- Compute the ground state energies at various volumes using lattice simulations, complemented by exact solutions via the matrix diagonalizations at small lattices

SC: a spherical momentum cut-off

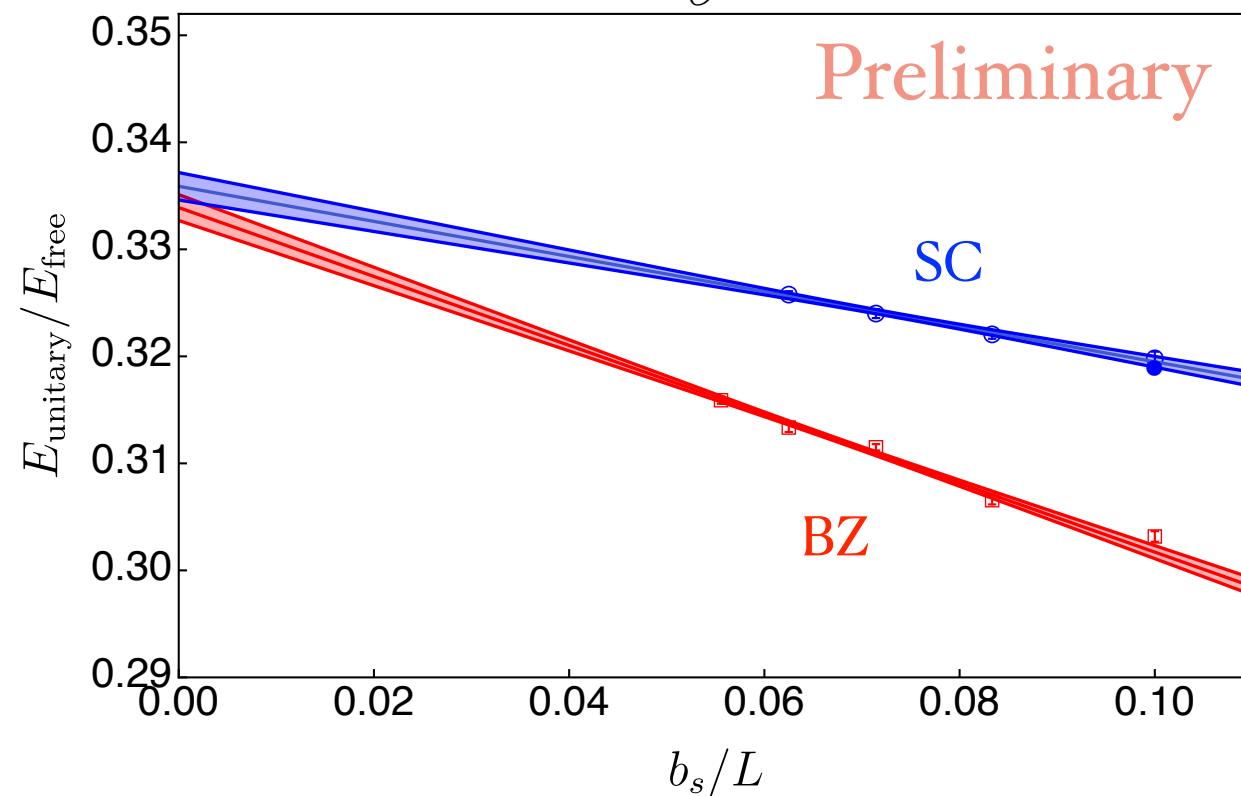
$$E_{\text{unitary}} = E_{\text{total}} - E_{\text{CM}}$$

BZ: full Brillouin zone

$$\mathbf{P} = \frac{2\pi}{L}(0,0,1)$$



$$N_{\mathcal{O}} = 1$$



- In the continuum limit, both results are in good agreement within a 1 % error.

Pair of unitary fermions at zero momentum

❖ Three unitary fermions at non-zero net total momentum

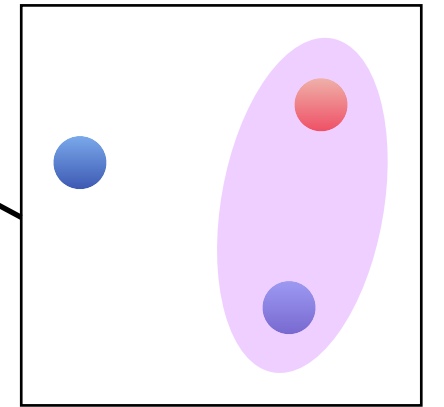
- Compute the ground state energies at various volumes using lattice simulations, complemented by exact solutions via the matrix diagonalizations at small lattices

$$E_{\text{unitary}} = E_{\text{total}} - E_{\text{CM}}$$

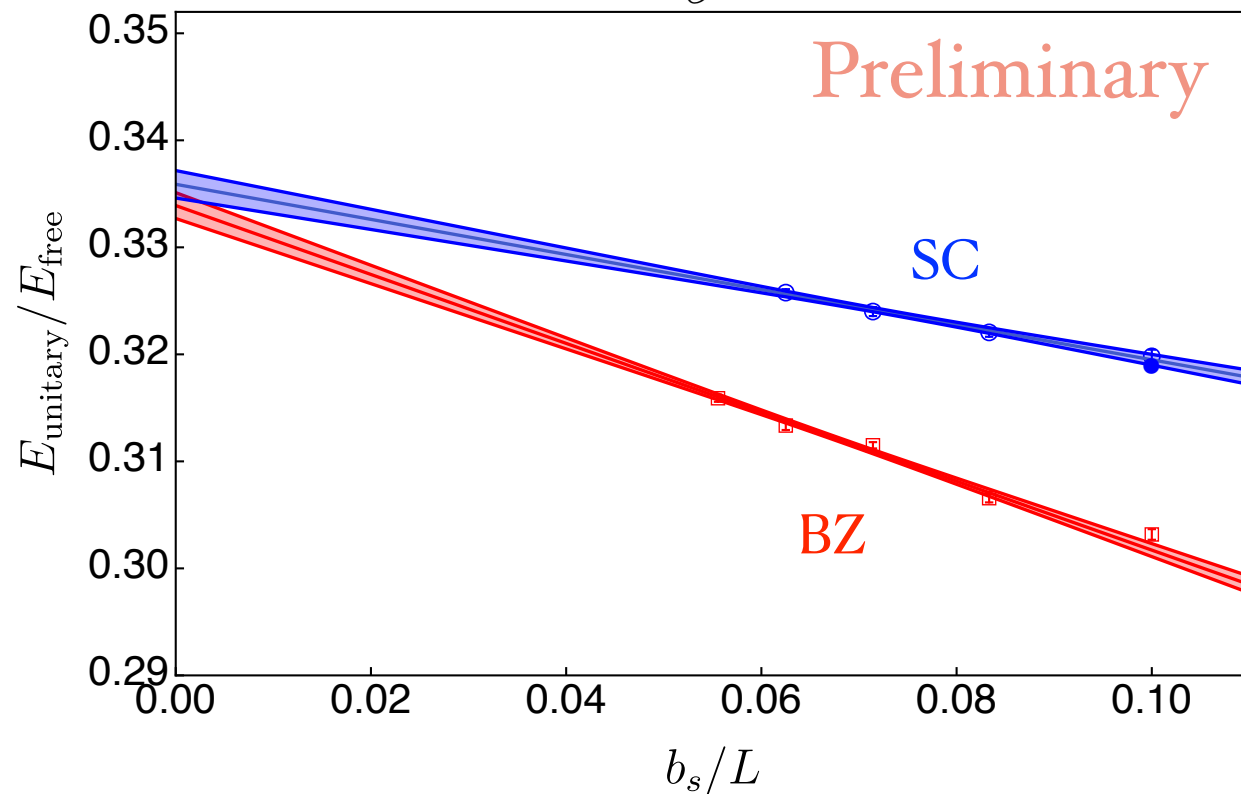
SC: a spherical momentum cut-off

BZ: full Brillouin zone

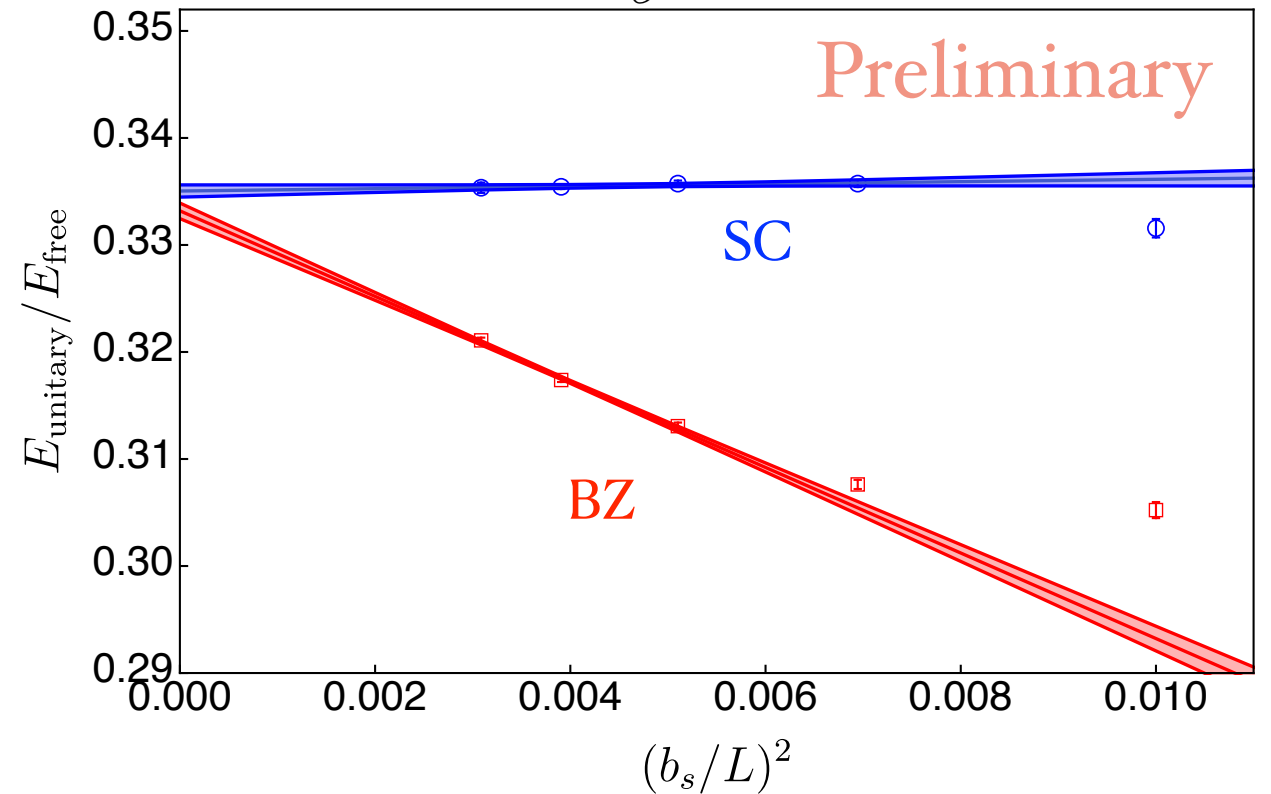
$$\mathbf{P} = \frac{2\pi}{L}(0,0,1)$$



$N_{\mathcal{O}} = 1$



$N_{\mathcal{O}} = 2$



- In the continuum limit, both results are again in good agreement within a 1 % error.

Pair of unitary fermions at zero momentum

- The ground-state energy is lower than the one for three unitary fermions at zero net momentum.

absolute ground state (?)

❖ Conclusion & outlook

- A spherical momentum cut-off in the lattice model of unitary fermions, tuned at the center-of-momentum, violates the unitarity if the pair of fermions has non-zero net momentum.
- Numerical calculations of three unitary fermions with and without a spherical momentum cut-off find that the ground-state energy is consistent to each other regardless of the total momentum of the system.

The ground state favors the configuration with a zero-momentum pair and a spectator which solely carries the total momentum of the system, consistent with what expected from the universality of the unitary fermi gas.

- Lattice model with a spherical momentum cut-off is still valid for the calculations of physical quantities at zero temperature in the continuum limit

Bertsch parameter, pairing gap & contact

M. Endres, D. B. Kaplan, JWL, A. Nicholson (2013)

- Finite-temperature lattice studies, such as the pseudo-gap near the transition, might require the full-BZ calculations.

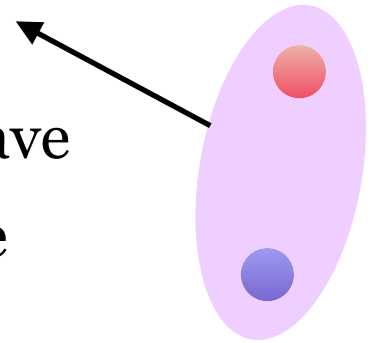
S. Jensen, C. N. Gilbreth & Y. Alhassid (2020, 2024)

Thank you for your attention.

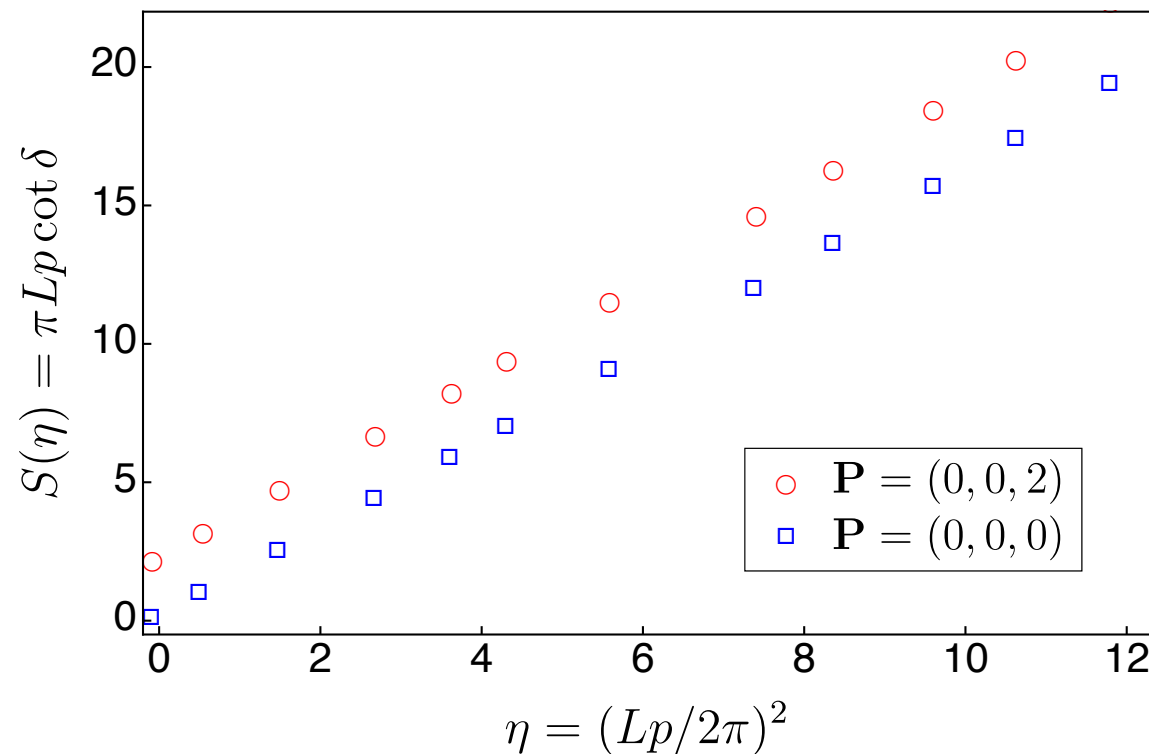
❖ A pair of unitary fermions in a moving frame

- Comparison between $N_{\mathcal{O}} = 1$ and $N_{\mathcal{O}} = 4$ operators tuned to infinite s-wave scattering length with a **spherical momentum cut-off Λ** in the CoM frame

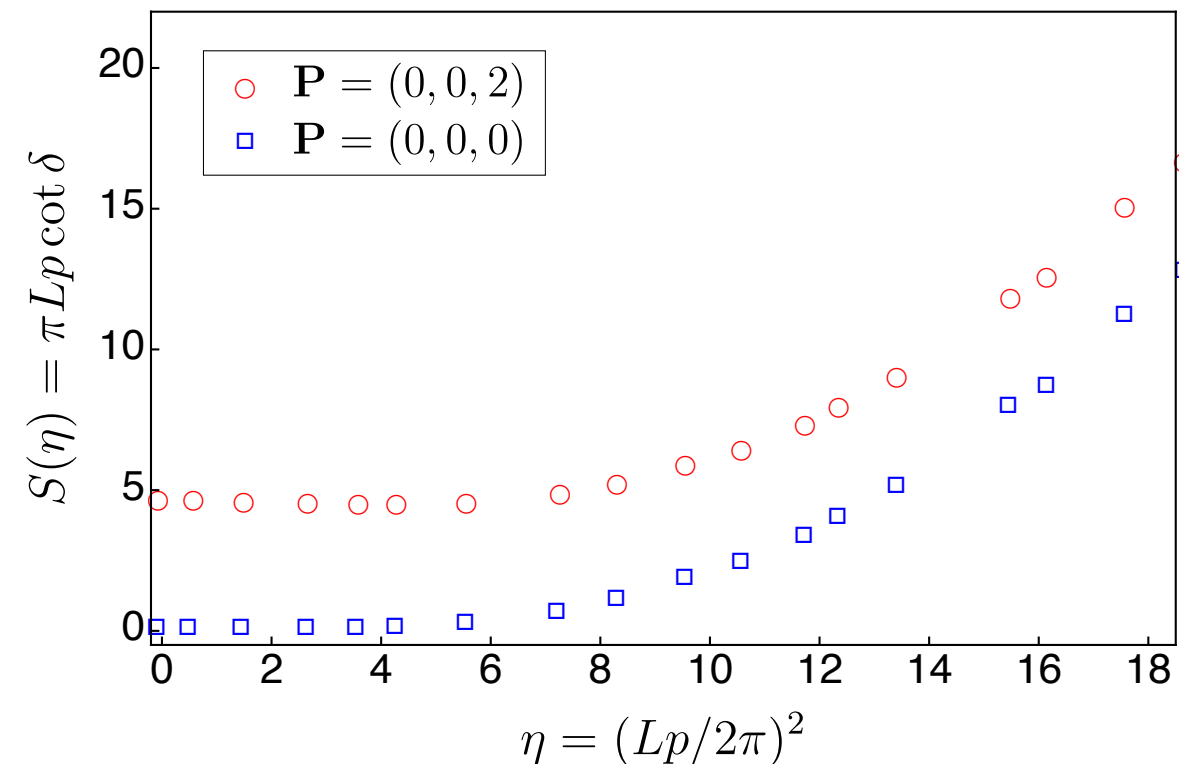
$$\mathbf{P} = \frac{2\pi}{L}(0,0,2)$$



$$N_{\mathcal{O}} = 1 \quad V = 18^3$$



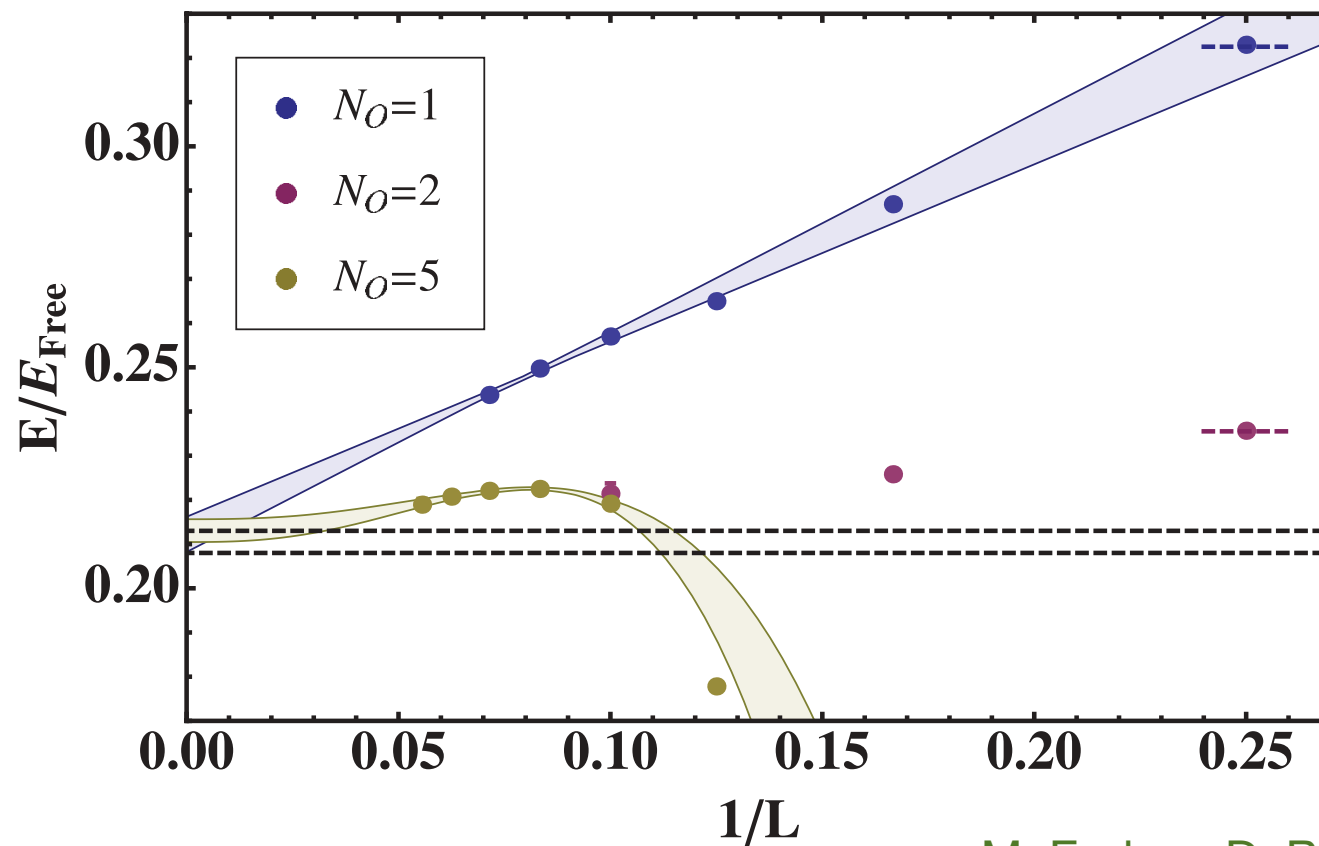
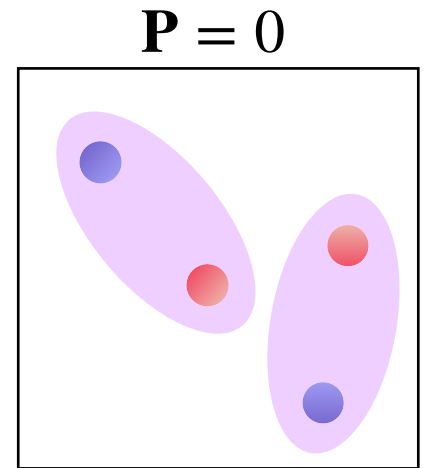
$$N_{\mathcal{O}} = 4 \quad V = 18^3$$



- The deviation persists even in the infinite volume limit, suggesting that the existence of the cut-off Λ violates the unitarity unless the pair is at zero CoM.

❖ Four unitary fermions at zero net total momentum

- Compute the ground state energies at various volumes using lattice simulations, and make a comparison between different numbers of tuned operators.



← S. Bour, X. Li, D. Lee, U.-G. Meißner & L. Mitas (2011)

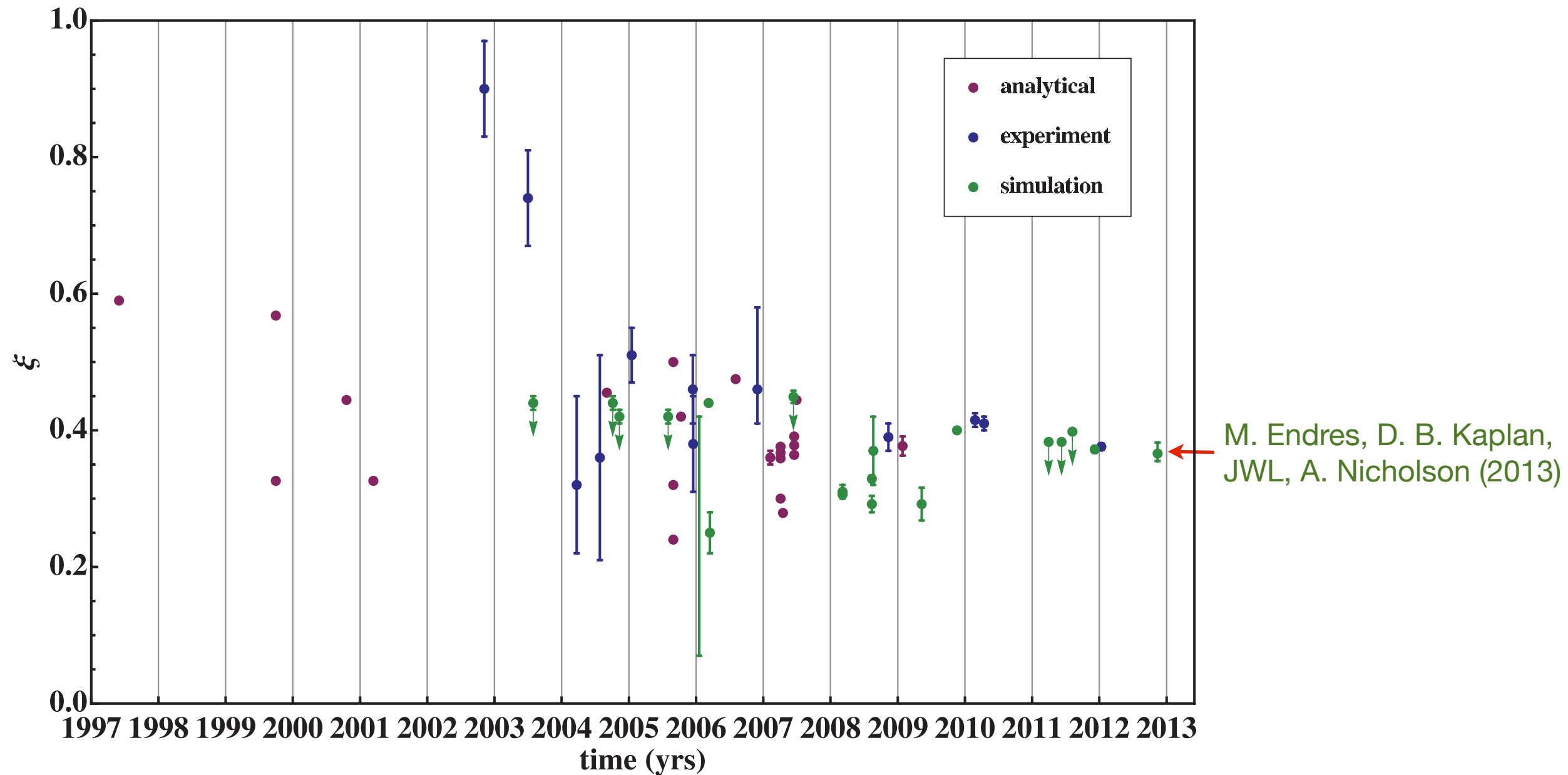
M. Endres, D. B. Kaplan, JWL, A. Nicholson (2013)

- In the continuum limit, both results are in good agreement within a $1 \sim 2\%$ error.

Pair of unitary fermions at zero momentum

- Coupling tuning with $N_{\mathcal{O}} = 2$ operators significantly improves the finite volume corrections in both cases.

❖ Chronology of the Bertsch parameter at unitarity

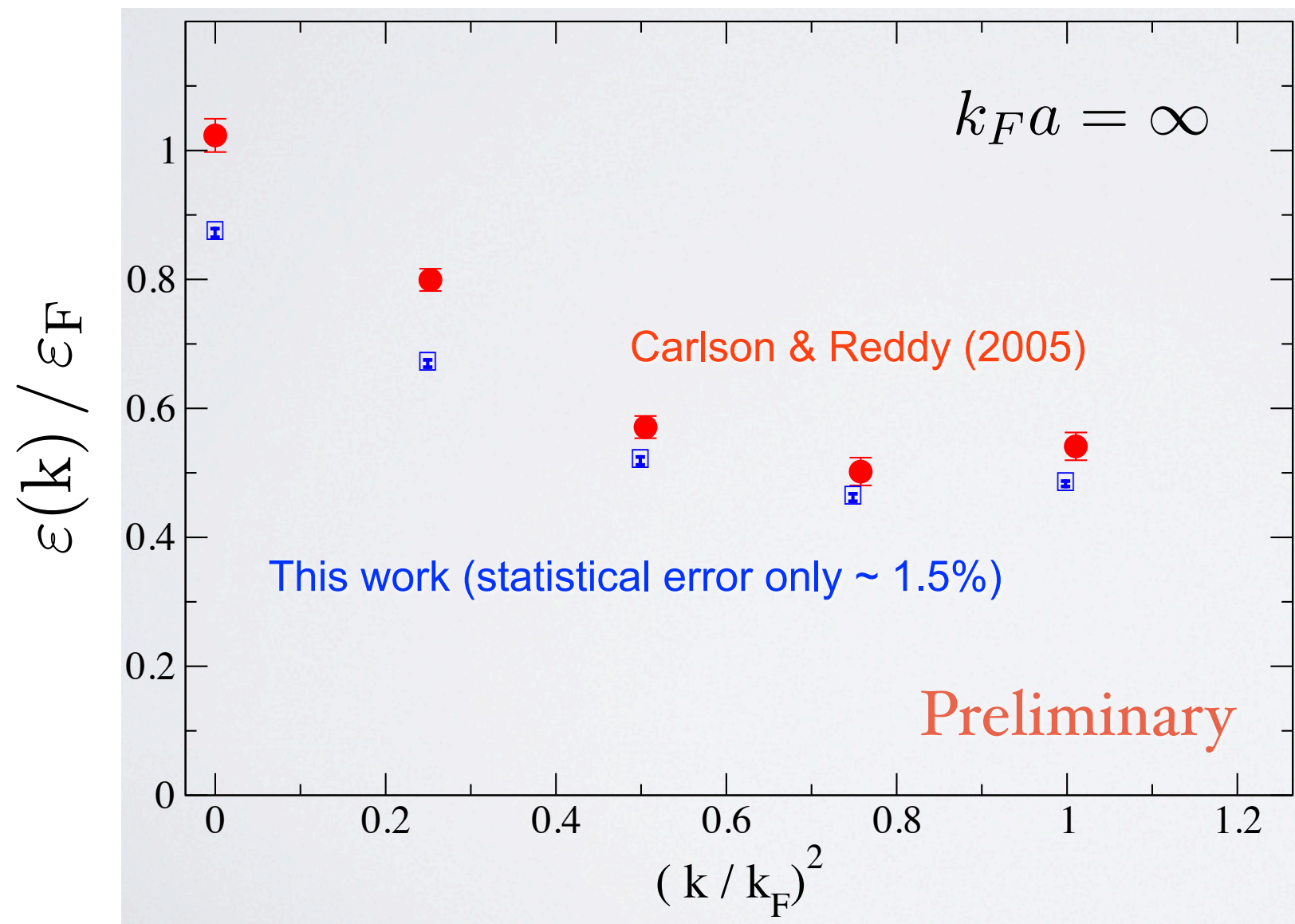


$\xi = 0.367(7)$ S. Jensen, C. N. Gilbreth & Y. Alhassid (2020)

The Bertsch parameter is approaching 0.37 at a few percent level.

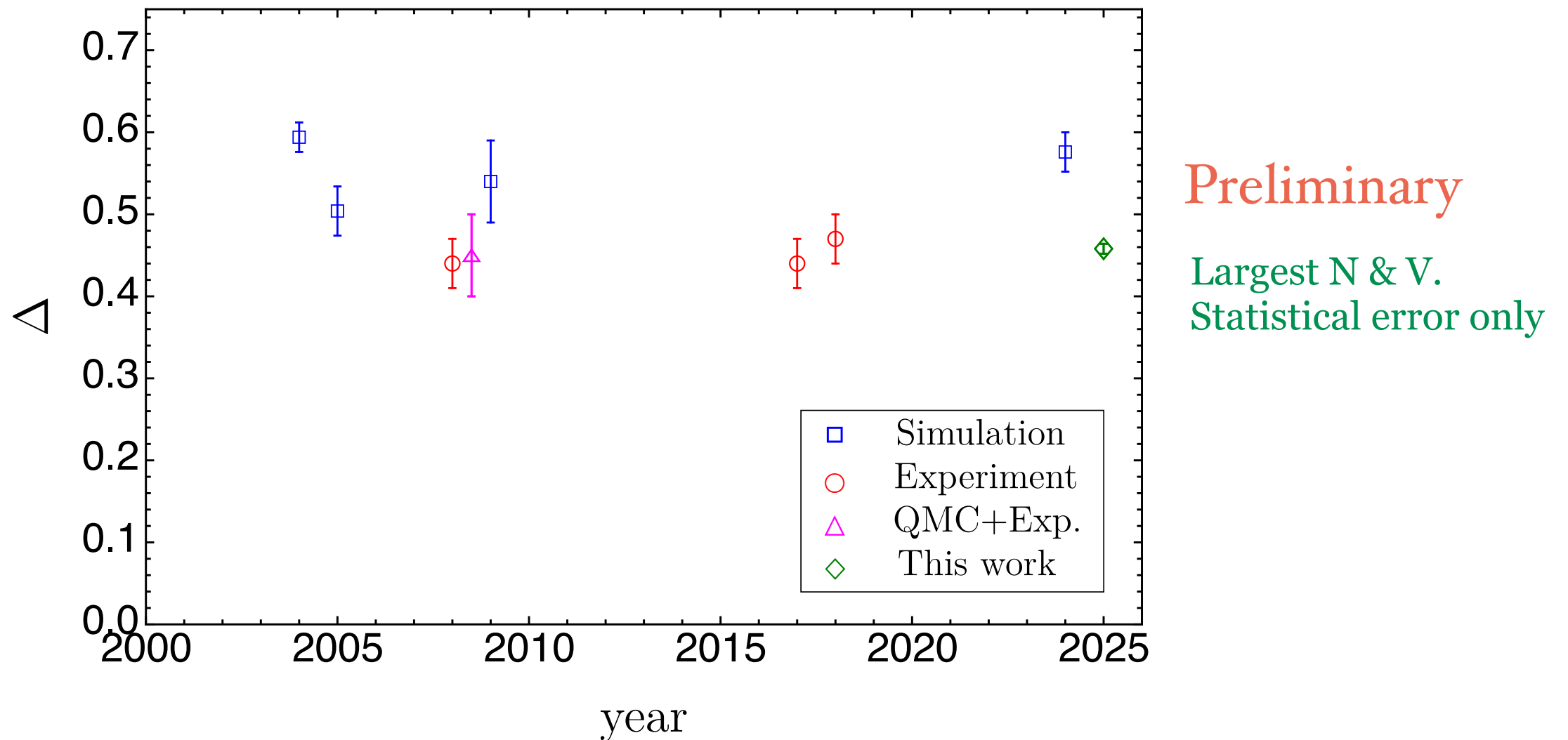
❖ Single particle dispersion relation at unitarity

$$N = 65, V = 16^3$$



Preliminary results of the ground state energies from the ensemble with largest N and V .

❖ Chronology of the pairing gap at unitarity ($T = 0$)



- Carlson, Chang, Pandharipande & Schmidt, Phys. Rev. Lett. 91, 050401 (2003)
- Carlson & Reddy, Phys. Rev. Lett. 95, 060401 (2005)
- Bulgac, Drut, Magierski, & Wlazlowski, Phys. Rev. Lett. 103, 210403 (2009)
- Jensen, Gilbreth & Alhassid, Phys. Rev. Lett. 124, 090604 (2020)

- Carlson & Reddy, Phys. Rev. Lett. 100, 150403 (2008)
- Ketterle et al, Phys. Rev. Lett. 101, 140403 (2008)
- Horikoshi et al, Phys. Rev. X 7, 041004 (2017)
- Hoinka et al, Nature 13, 943-946 (2018)