# Universal Fermi gases on the lattice

Michael G. Endres

Computational approaches to nuclear many-body problems and related quantum systems

Feb 13, 2013

# Outline

- Motivation
  - "unitary" Fermi gas in 3D
  - universal four-component Fermi gas in 1D
- Solution to the sign problem for nonrelativistic fermions in 1D
  - Mean-field results
  - Numerical results for universal Fermi gas
    - few-body results: energy spectrum
    - many-body results: evidence for a "universality" between conformal theories in *different* spatial dimensions
- Summary & Outlook

# Unitary Fermi gas (three dimensions)

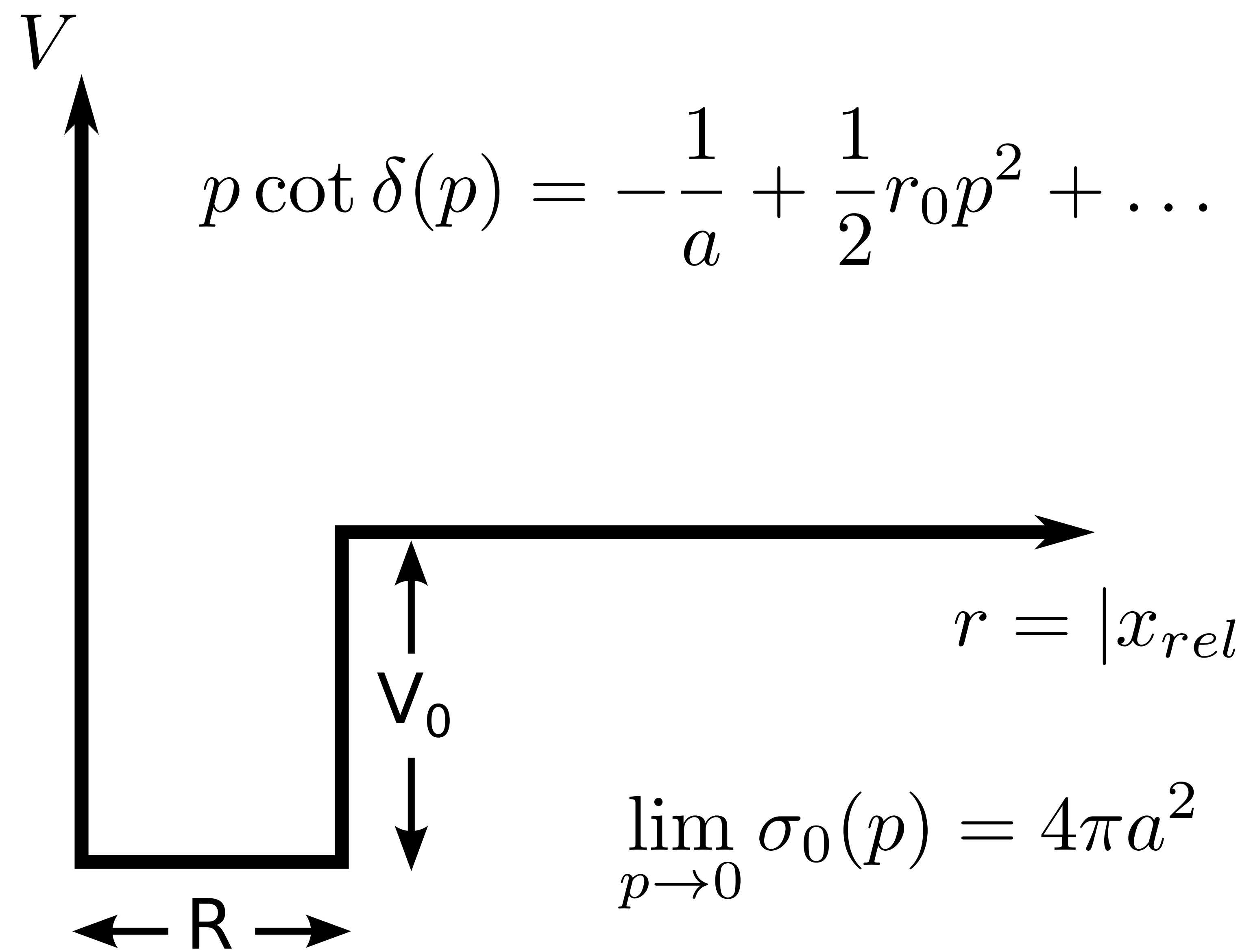
*A dilute mixture of spin 1/2 fermions at infinite scattering length*

# 2-particle scattering from a short-range potential

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

$$p = \sqrt{EM}$$

scattering phase shift




$$p\cot\delta(p) = -\frac{1}{a} + \frac{1}{2}r_0 p^2 + \dots$$

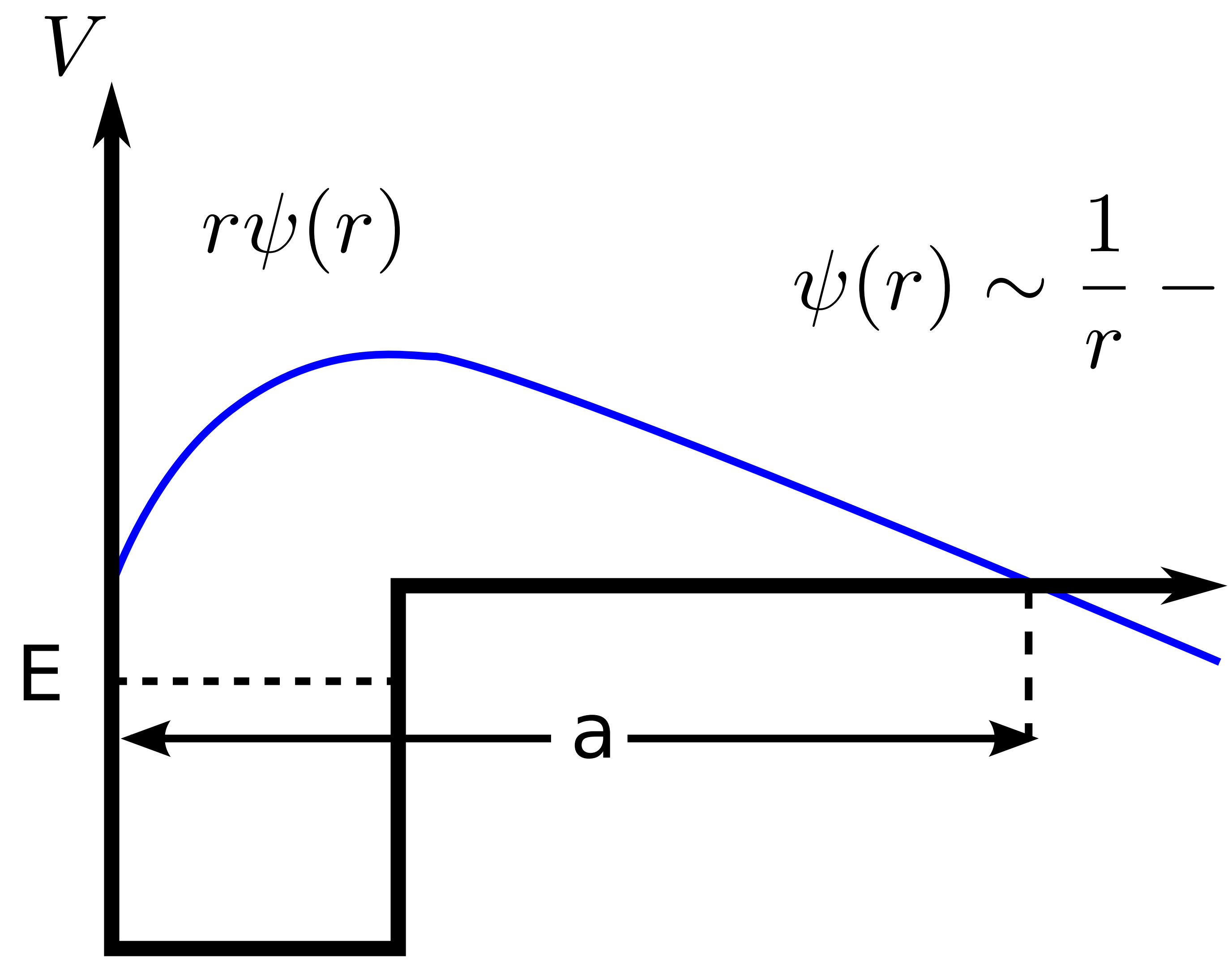
$$\lim_{p\to 0}\sigma_0(p) = 4\pi a^2$$

radial profile of spherically symmetric potential

# 2-particle scattering from a short-range potential

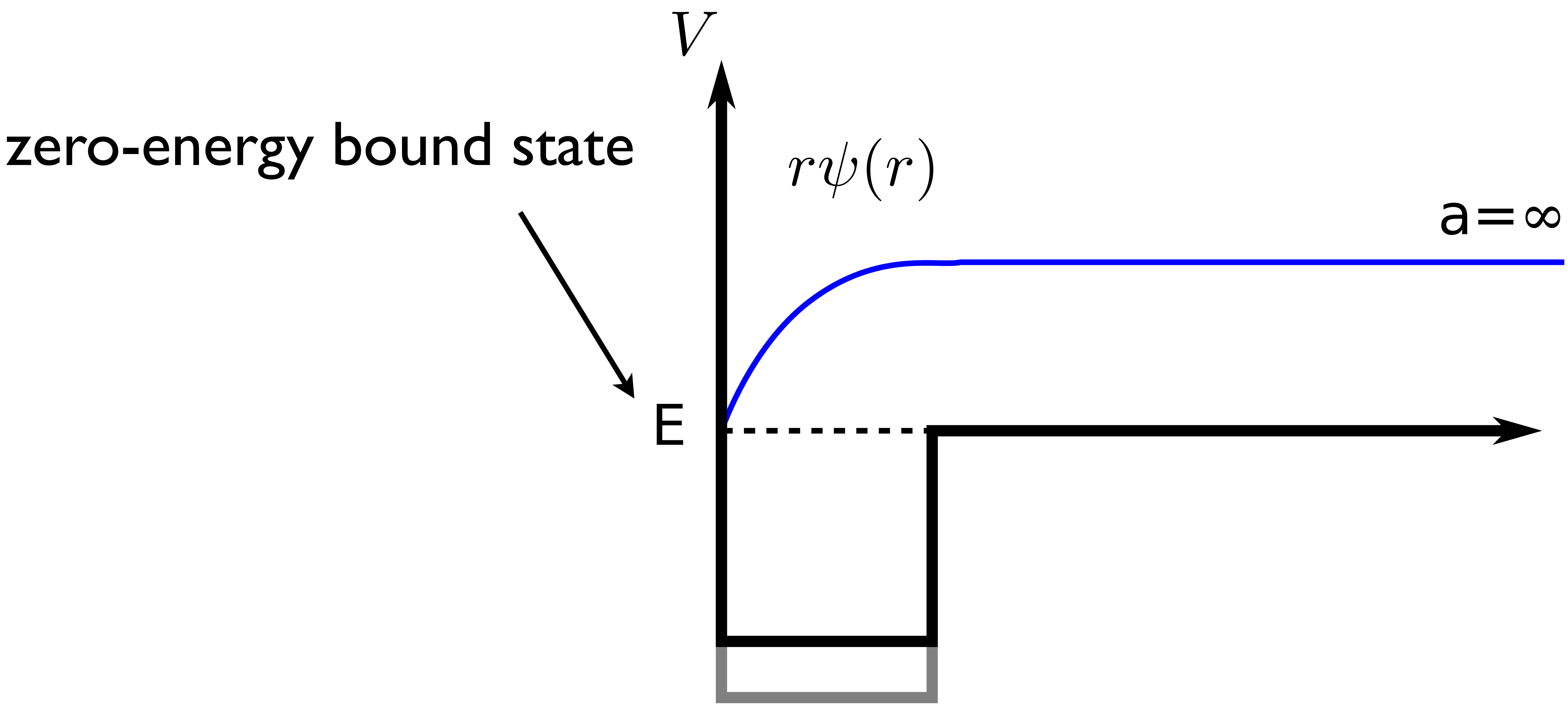
weakly bound state

$$E \sim \frac{1}{Ma^2}$$

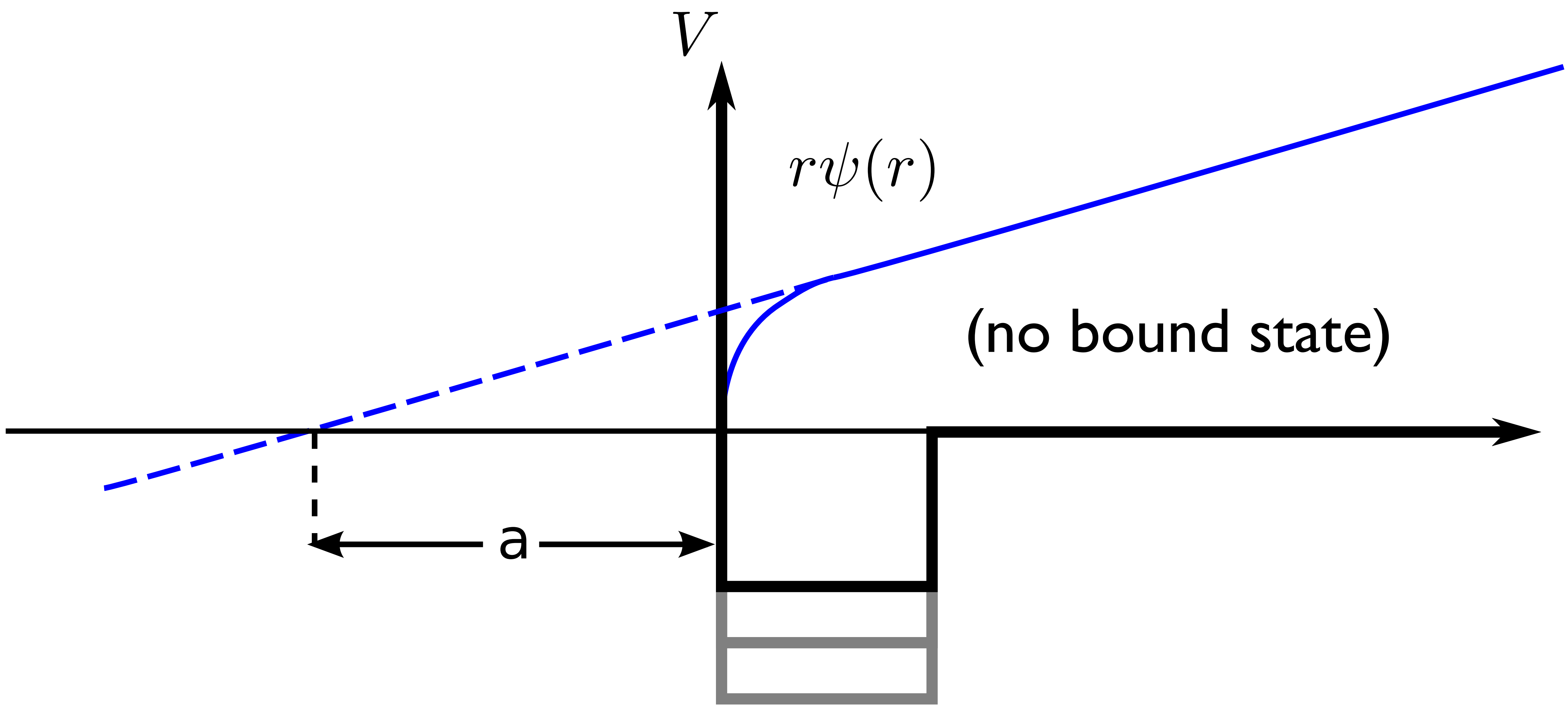



$$\psi(r) \sim \frac{1}{r} - \frac{1}{a}$$

# 2-particle scattering from a short-range potential



# 2-particle scattering from a short-range potential



# 2-particle scattering from a short-range potential

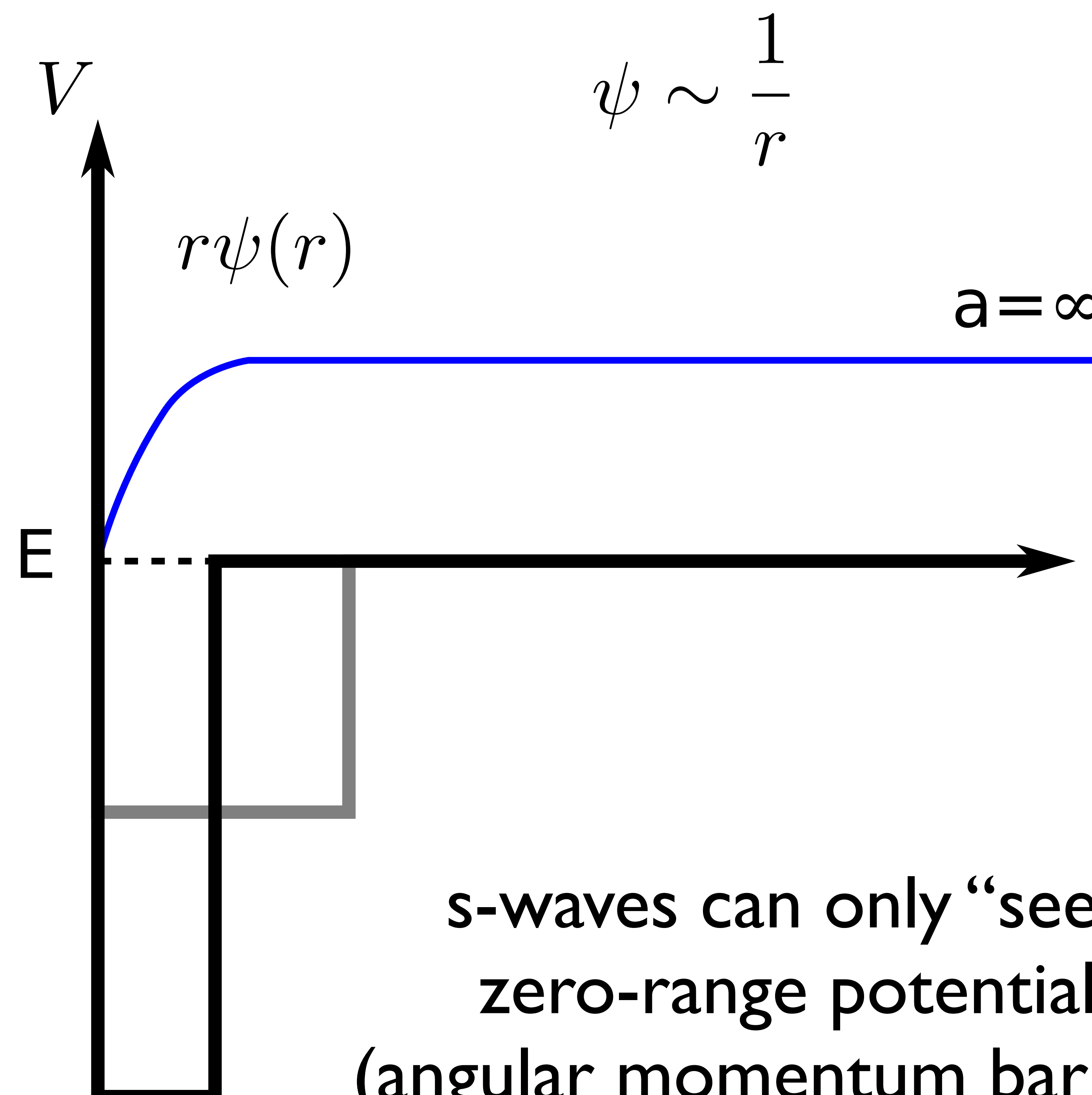
$$p \cot \delta = 0$$

$$a \to \infty$$

$$R \to 0$$

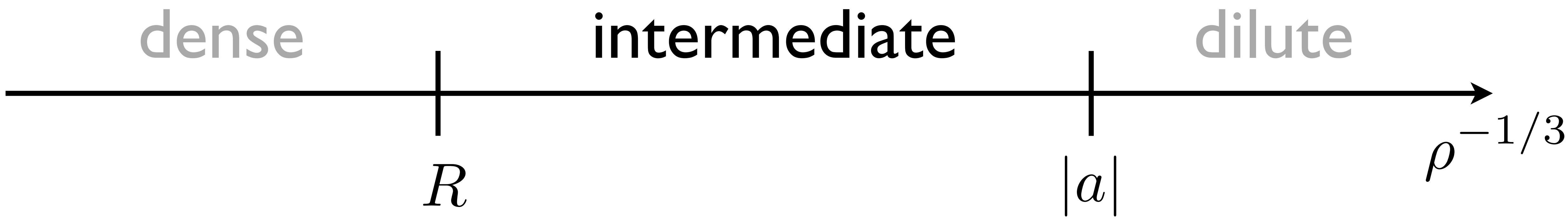
$$\sigma_0 \leq \frac{4\pi}{p^2}$$

"unitarity bound"
is saturated!

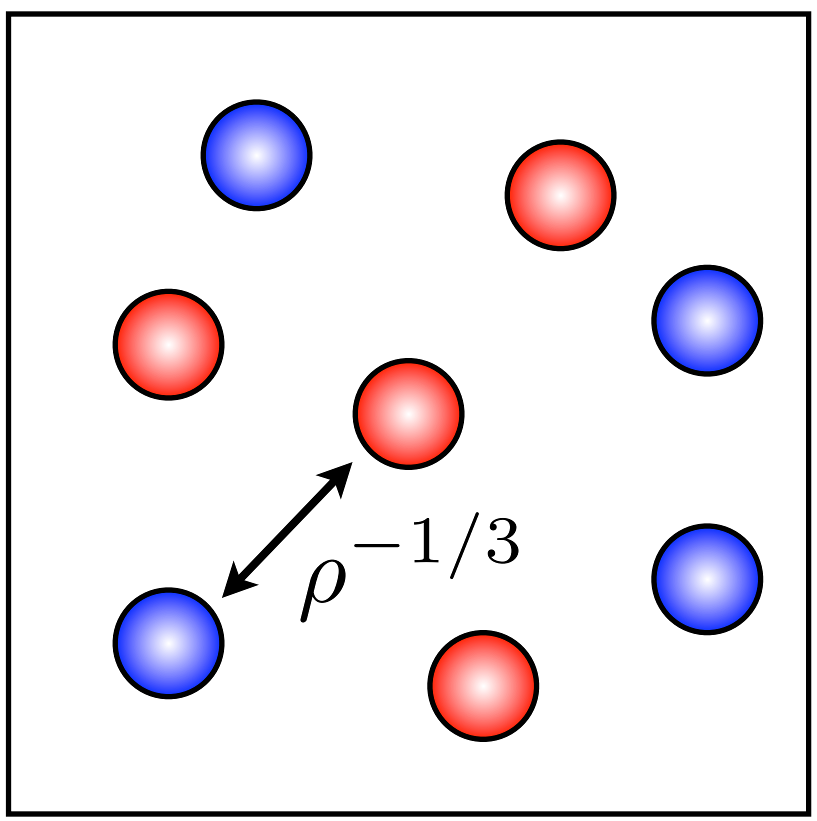



s-waves can only "see"
zero-range potential
(angular momentum barrier)

# Interacting Fermi gas



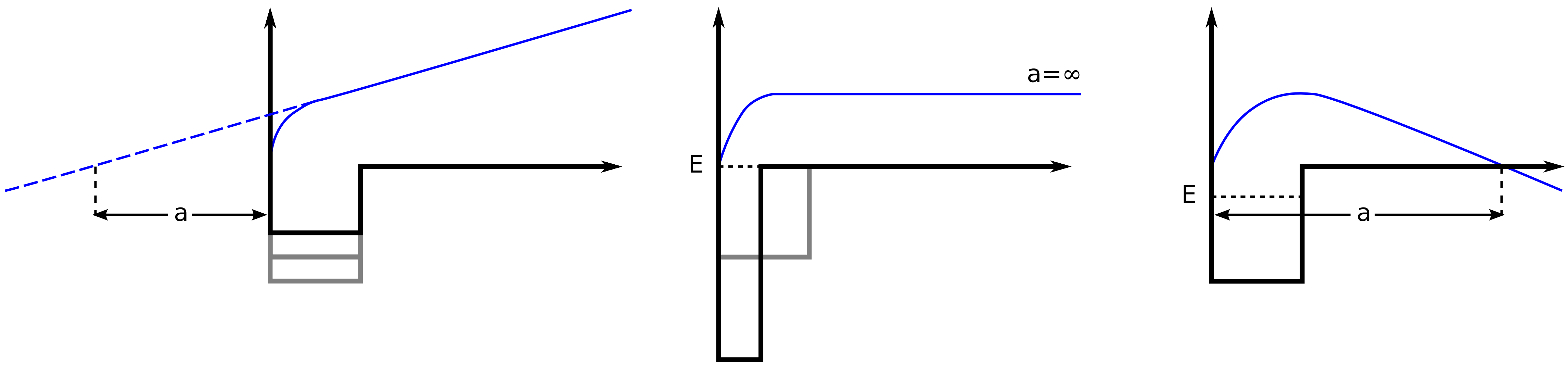

$\rho = N/V$




$$R \ll \rho^{-1/3} \ll a$$

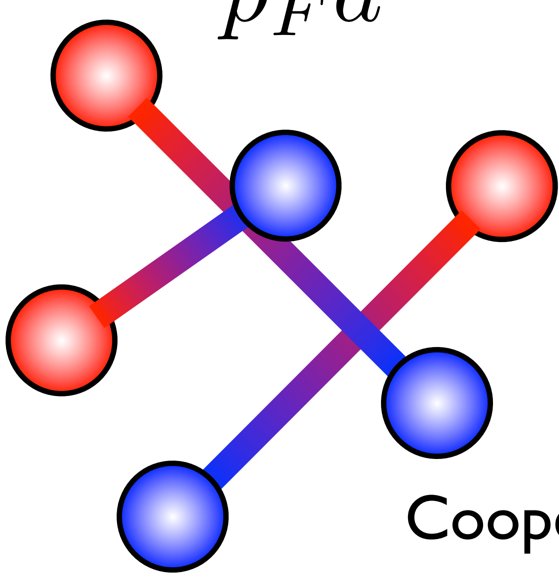
$$\psi \sim \frac{1}{r_{ij}} - \frac{1}{a}\,, \qquad r_{ij} = x_i^{\uparrow} - x_j^{\downarrow}$$

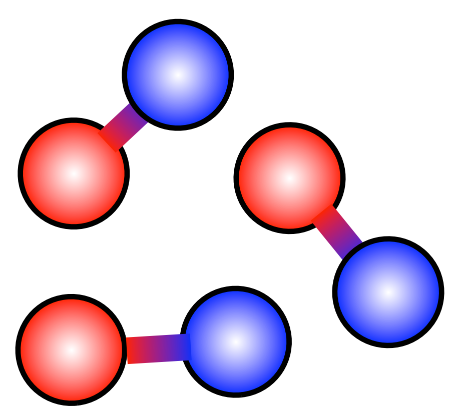
# Interacting Fermi gas

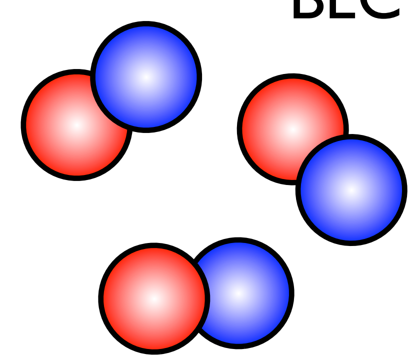



BCS | cross-over | BEC

$$\frac{1}{p_F a} < 0 \qquad \frac{1}{p_F a} = 0 \qquad \frac{1}{p_F a} > 0$$

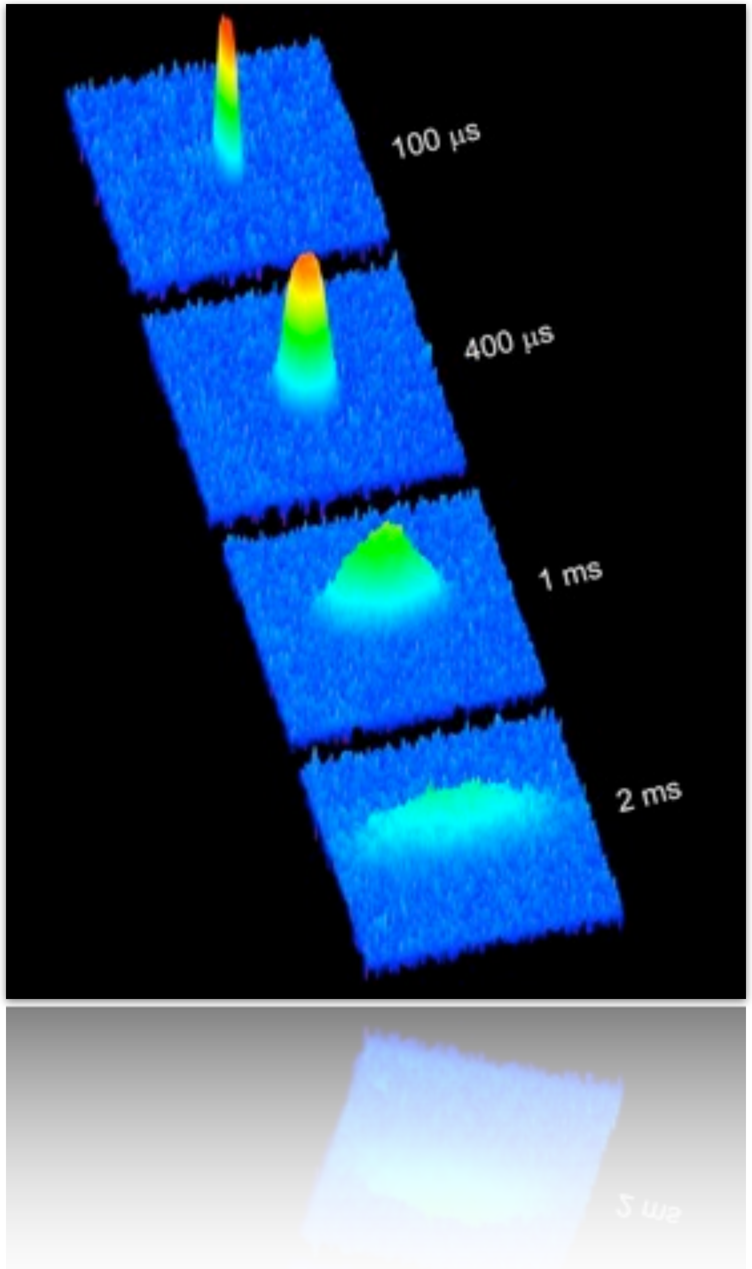




# Physical realization: ultra-cold atoms

*Science*, **298**, pp. 2179-2182 (2002)




$$r_0(^{40}K) \sim 60 a_0$$

Bohr radius

$$r_0(^{6}Li) \sim 30 a_0$$

$$\rho^{-1/3} \sim 5000 - 10000 a_0$$

interacting gas of fermions
($^6$Li or $^{40}$K atoms often used)

# Physical realization: ultra-cold atoms

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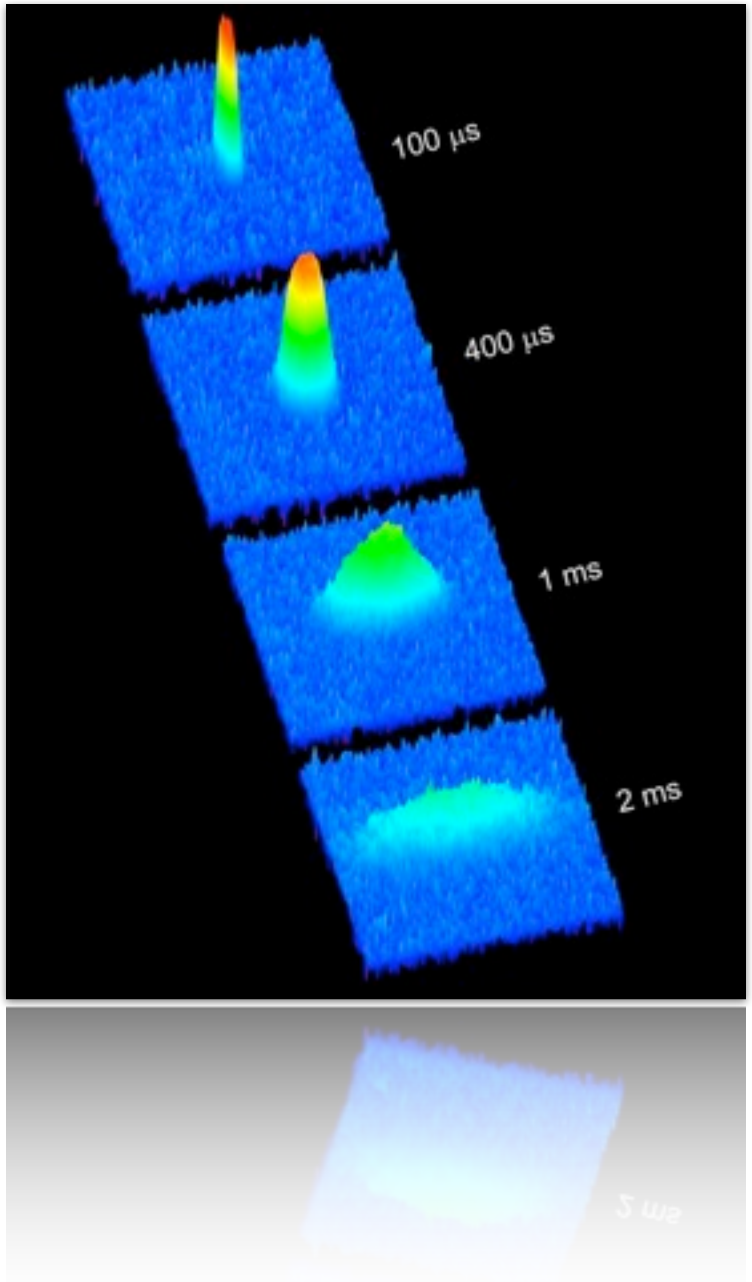


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Bohr radius

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Scattering length tuned by exploiting properties of a Feshbach resonance

# Effective field theory description

$$S_{cont}(\mu) = \int d^4x \left[\psi^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\psi - C_0(\psi^\dagger\psi)^2\right]$$

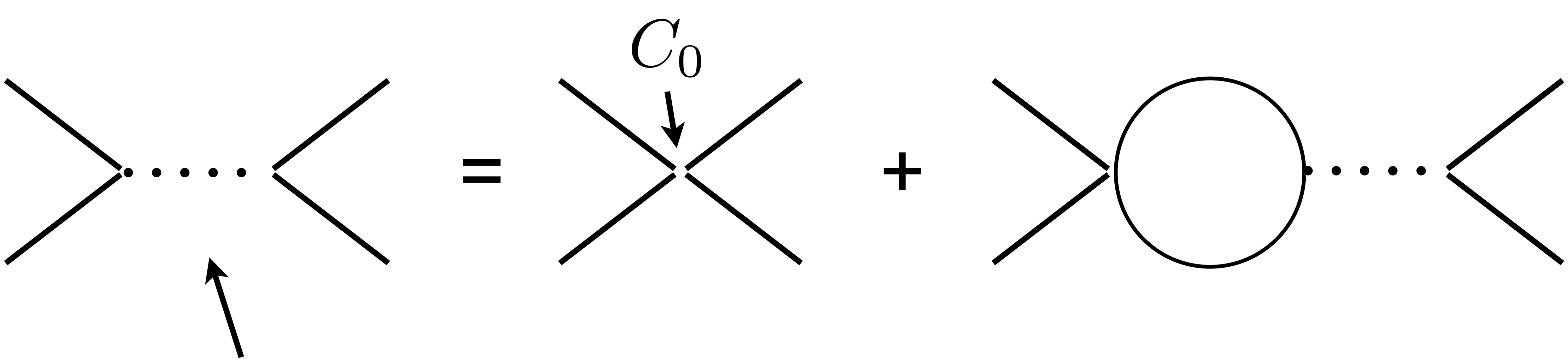
$$\psi = (\psi_\uparrow, \psi_\downarrow)$$

zero-range contact interaction

# Effective field theory description

$$S_{cont}(\mu) = \int d^4x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - C_0 (\psi^\dagger \psi)^2 \right]$$

## Relationship between coupling ($C_0$) and scattering length:




two-particle
scattering amplitude

$$\mathcal{A}^{-1}(p)\Big|_{p\to 0} = \frac{m}{4\pi a}$$

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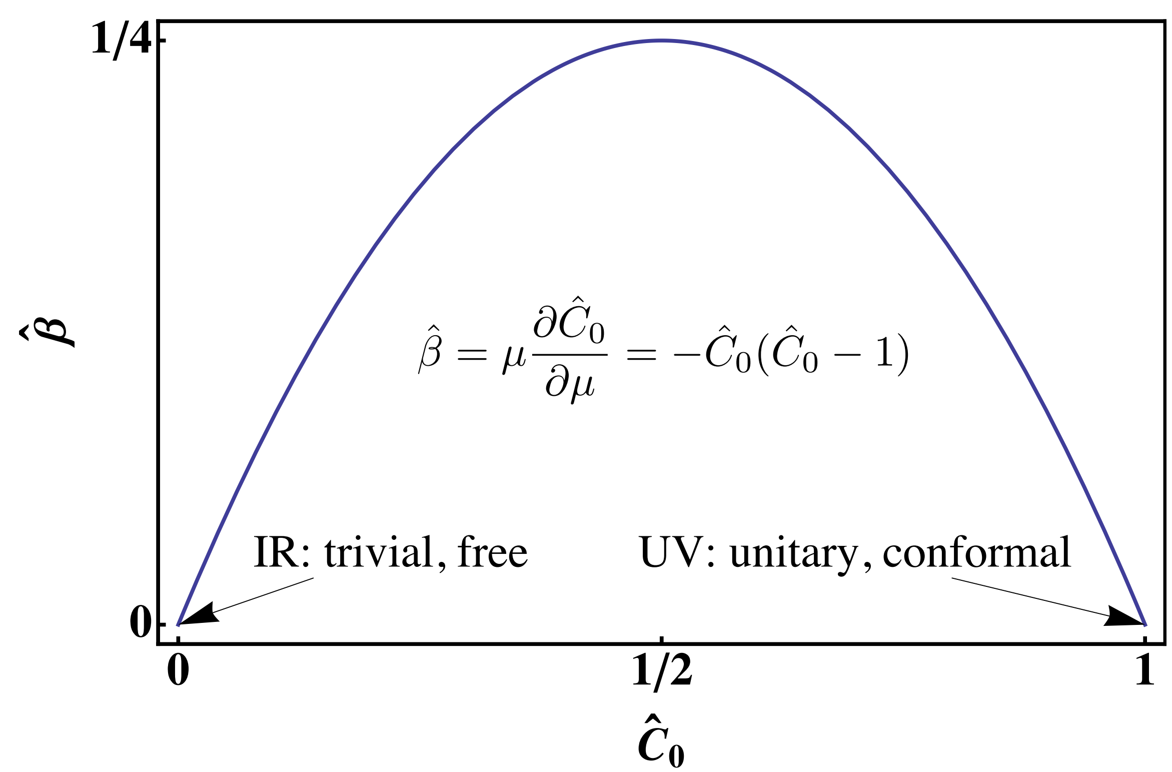
## Relationship between coupling ($C_0$) and scattering length:

$$\hat{C}_0(\mu) = -\frac{m\mu}{4\pi} C_0(\mu)$$

Renormalization scale
(not chemical potential)

Kaplan-Savage-Wise



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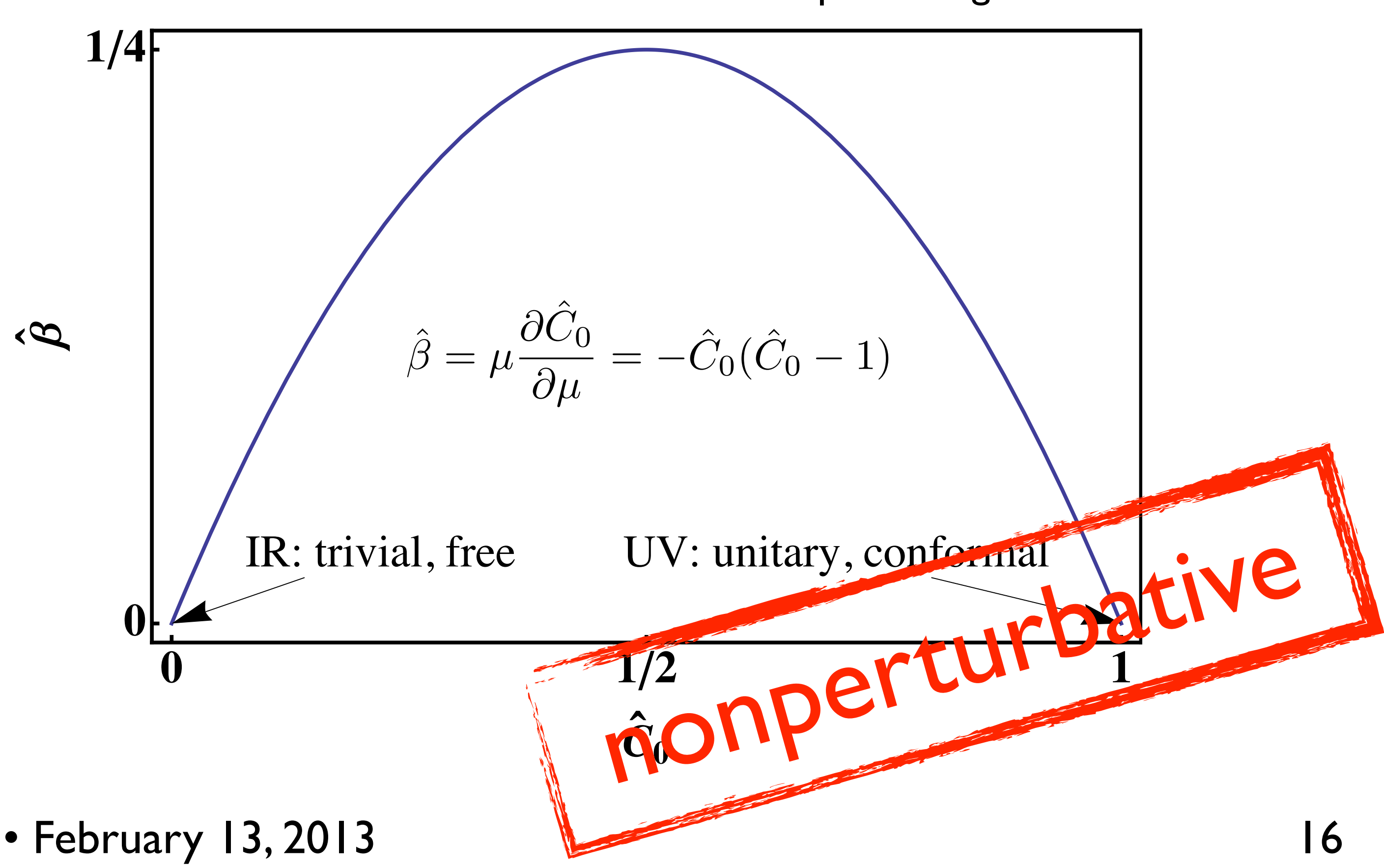
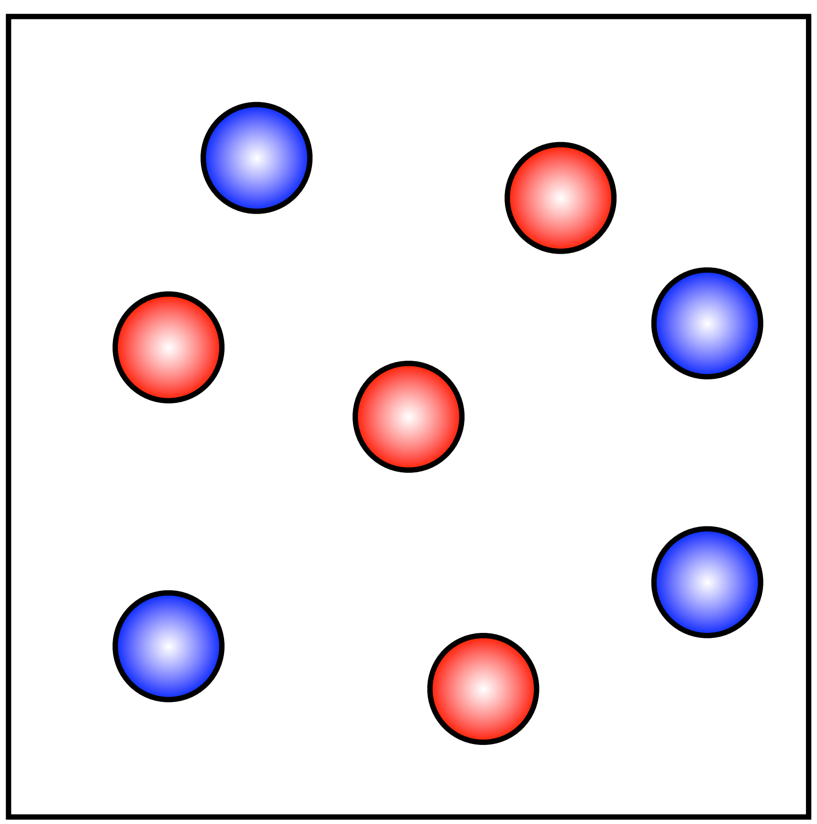


# Unitary fermions: in a box and in a trap



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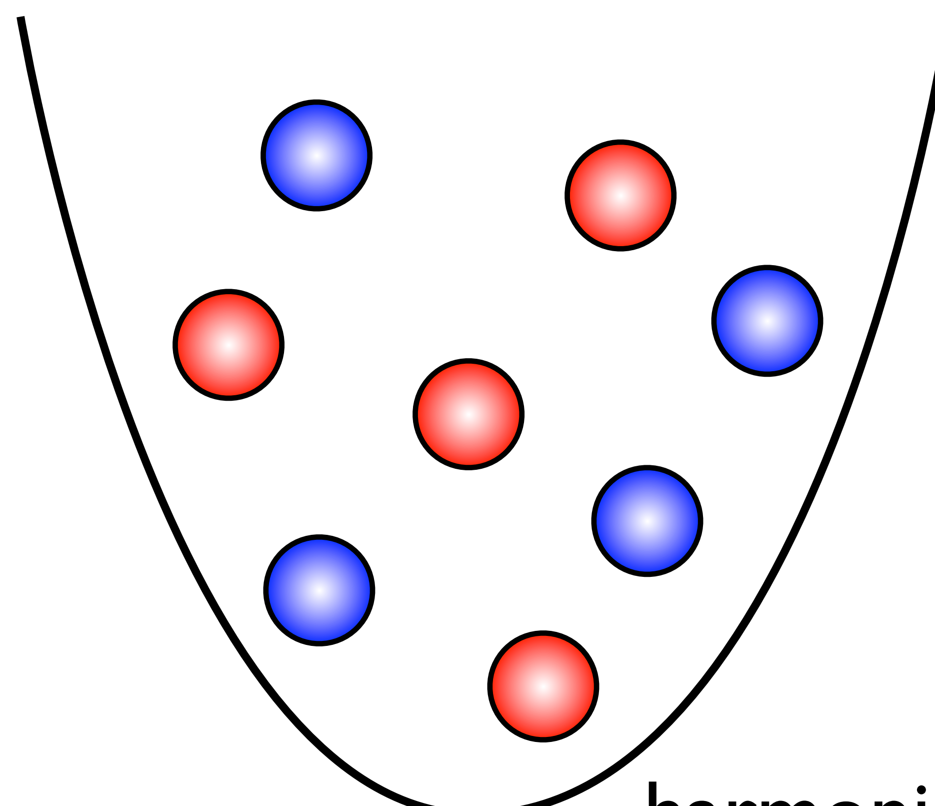

harmonic trap

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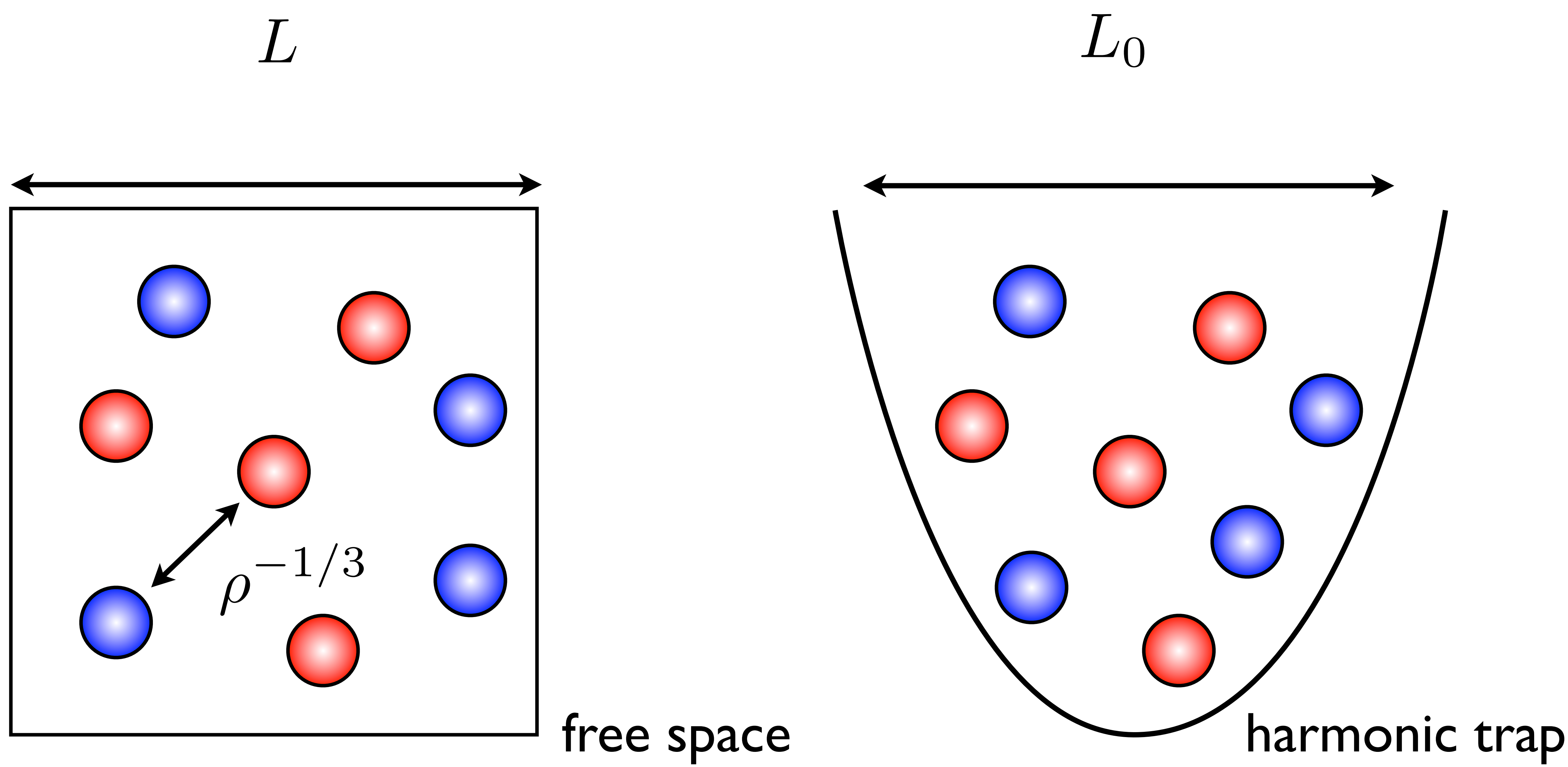

# Properties of unitary fermions

- Operator state correspondence
- Virial theorems
- Rich and fascinating physics!
    - universal few- and many-body physics
    - universal (Tan) relations
    - Efimov physics

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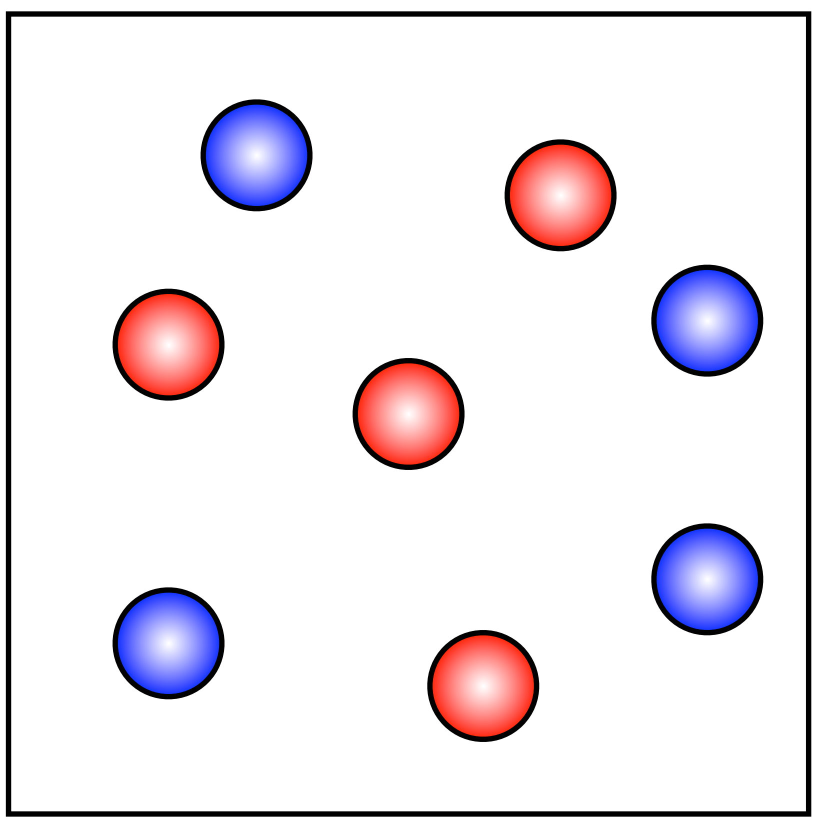
# Example: energy of many-body system

Bertsch parameter

$$\frac{E}{E_{FG}} = \xi$$

*same* Bertsch parameter

$$\frac{E}{E_{FG}} = \sqrt{\xi}$$



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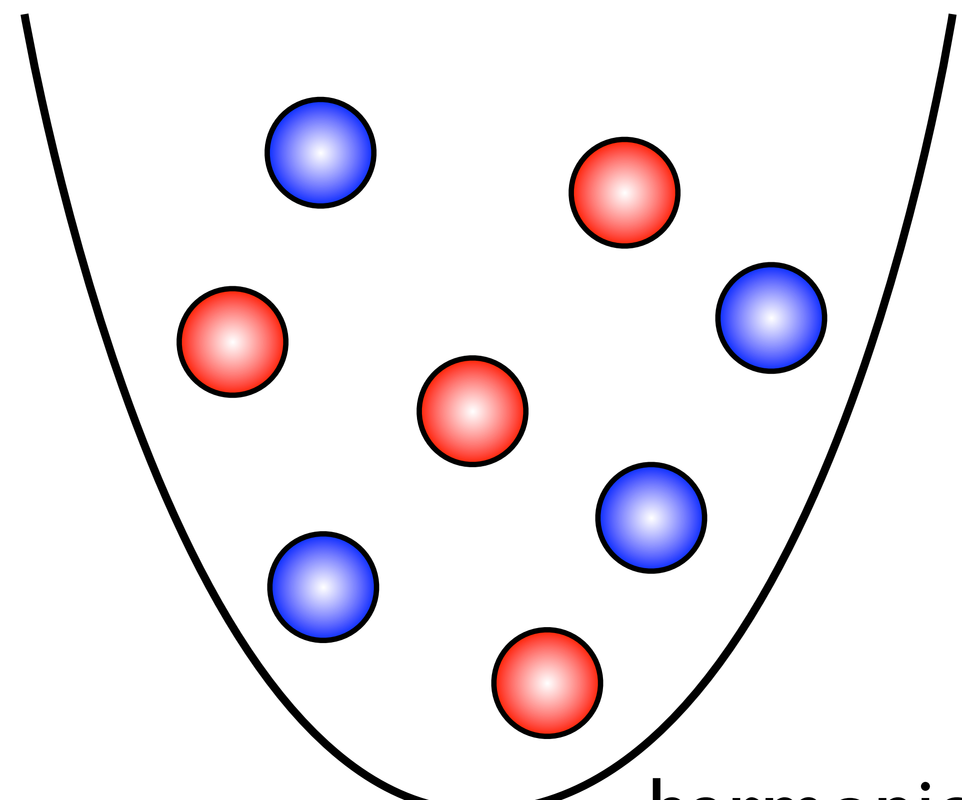
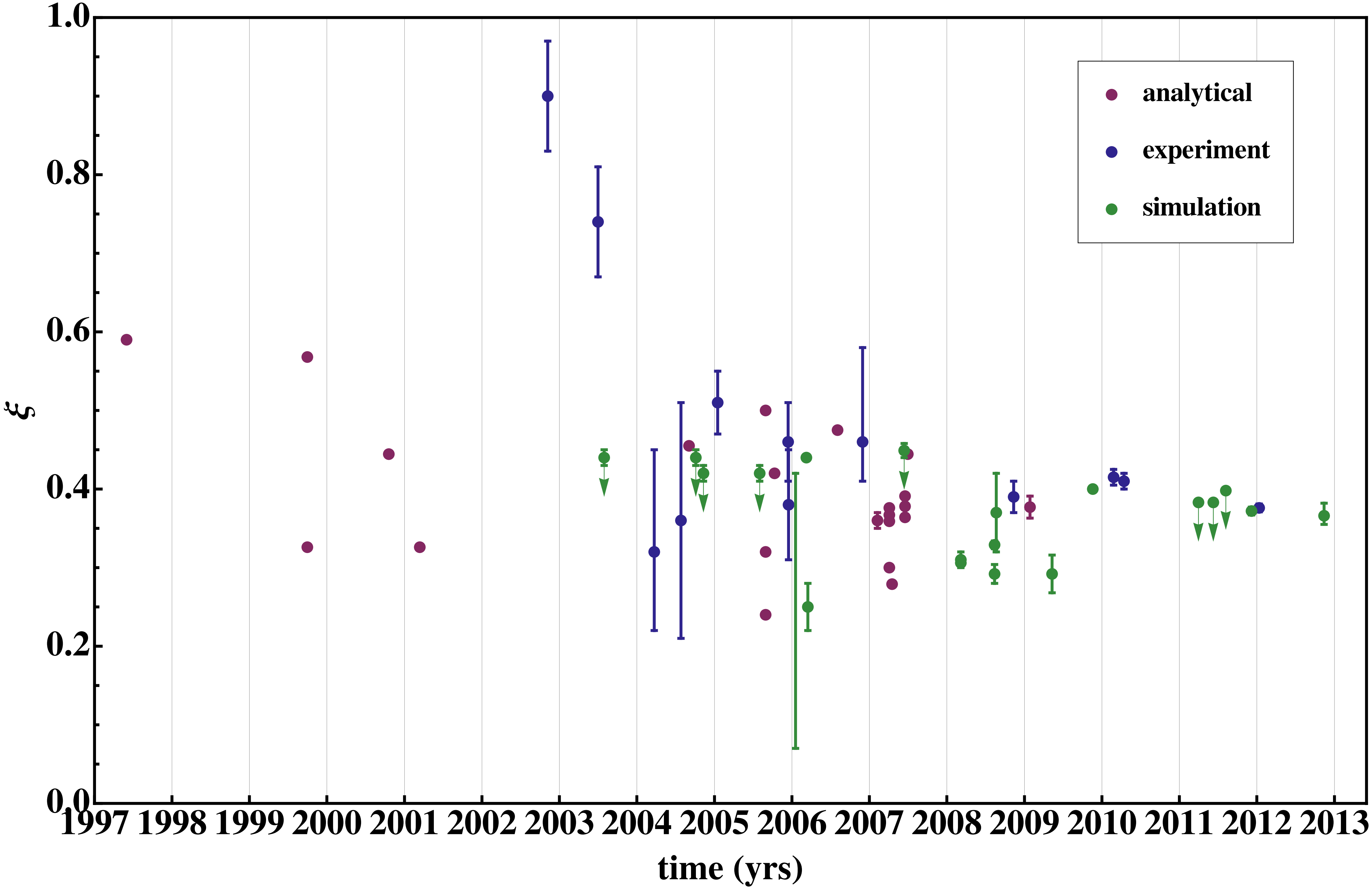


harmonic trap

# Bertsch parameter



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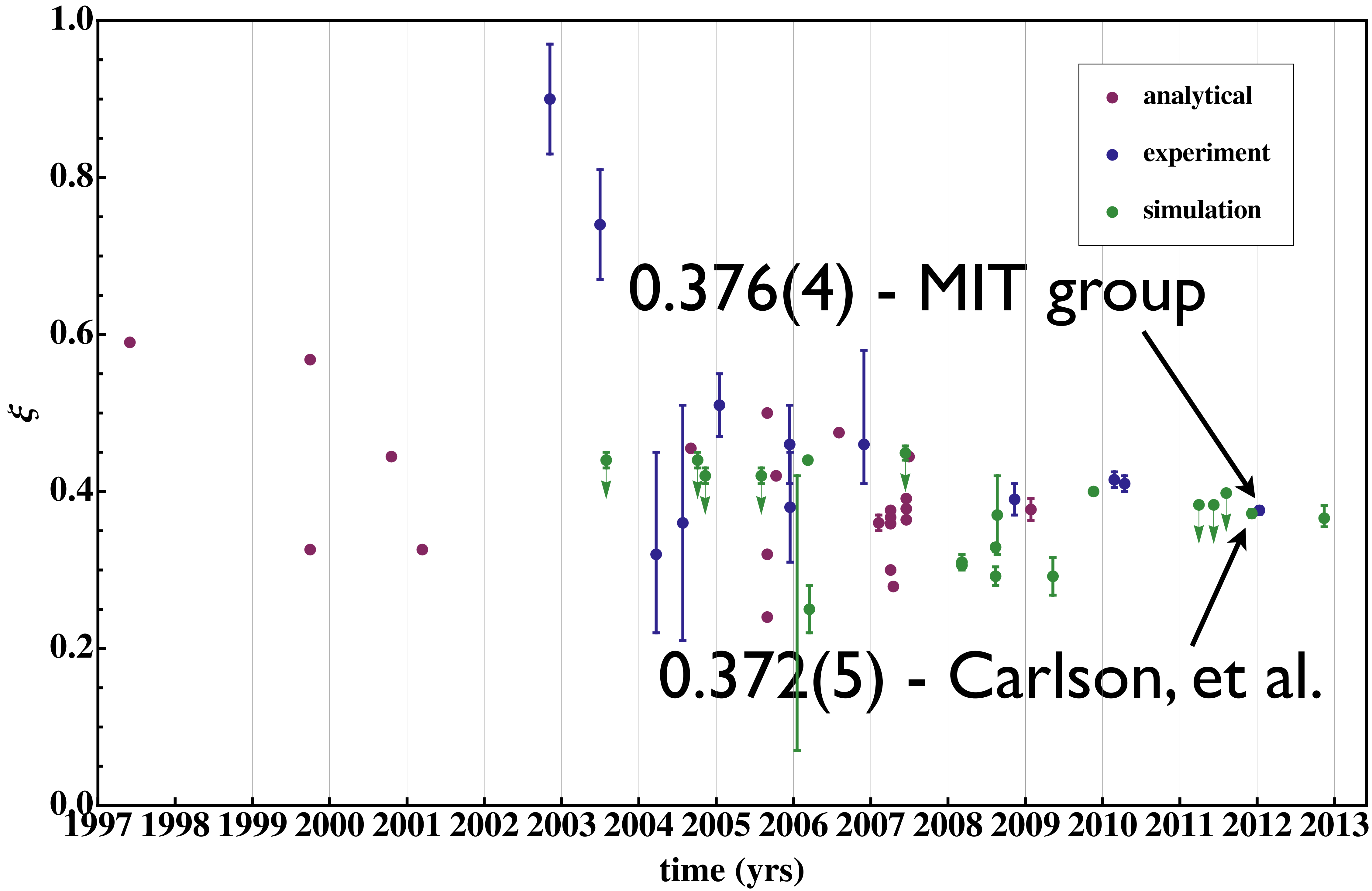

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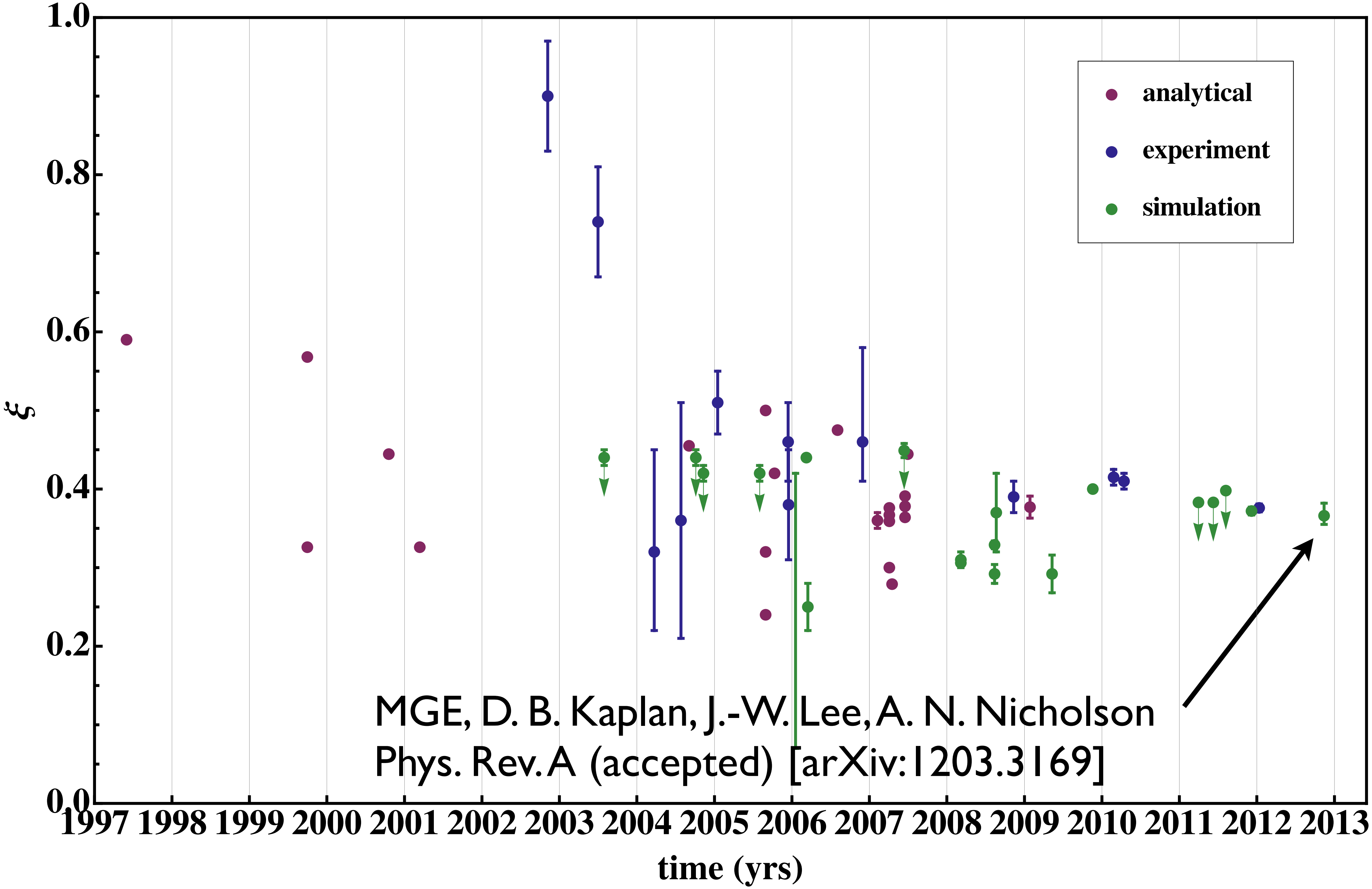

# Universal four-component Fermi gas (one dimension)

# Universal Fermi gases in lower dimensions

- "Universal Fermi gases in mixed dimensions"
  Y. Nishida and S. Tan
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- "Universal four-component Fermi gas in one dimension"
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# Effective field theory

four-body interaction

$$S_{cont}(\mu) = \int d^2x \left[\psi^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\psi - g(\psi^\dagger\psi)^4\right]$$

$$\mu = (\mu_a, \mu_b, \mu_c, \mu_d)$$

1+1 dimensions

$$m = (m_a, m_b, m_c, m_d)$$

$$\psi = (\psi_a, \psi_b, \psi_c, \psi_d)$$

# Effective field theory

$$S_{cont}(\mu) = \int d^2x \left[\psi^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\psi - g(\psi^\dagger\psi)^4\right]$$

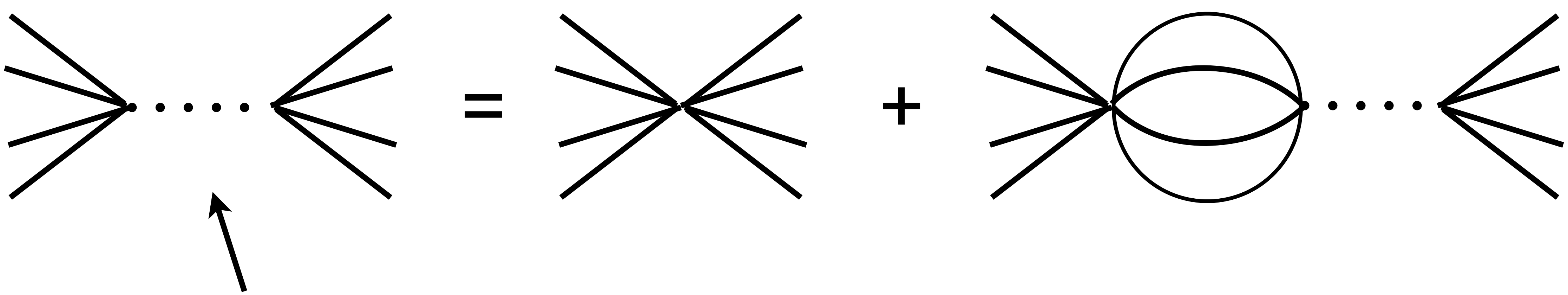
Highly tuned action: lower-dimension ops. absent:

$$\cancel{\left(\psi^\dagger\psi\right)^2} \qquad \cancel{\left(\psi^\dagger\psi\right)^3}$$

# Effective field theory

$$S_{cont}(\mu) = \int d^2x \left[\psi^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\psi - g(\psi^\dagger\psi)^4\right]$$

Relationship between coupling (g) and "scattering length":



four-particle scattering amplitude

$$\mathcal{A}^{-1}(p)\Big|_{p\to 0} \stackrel{\text{def.}}{=} \frac{m}{4\pi a}$$

# Effective field theory

$$S_{cont}(\mu) = \int d^2x \left[\psi^\dagger \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\psi - g(\psi^\dagger\psi)^4\right]$$

Relationship between coupling (g) and "scattering length":

$$a \to \infty \qquad \Leftrightarrow \qquad g \to g_c$$

UV fixed point: "universal", conformal, O(1) coupling

# ...many identical properties with unitary fermions

- Operator state correspondence
- Virial theorems
- Rich and fascinating physics!
  - universal few- and many-body physics
  - universal (Tan) relations
  - Efimov physics

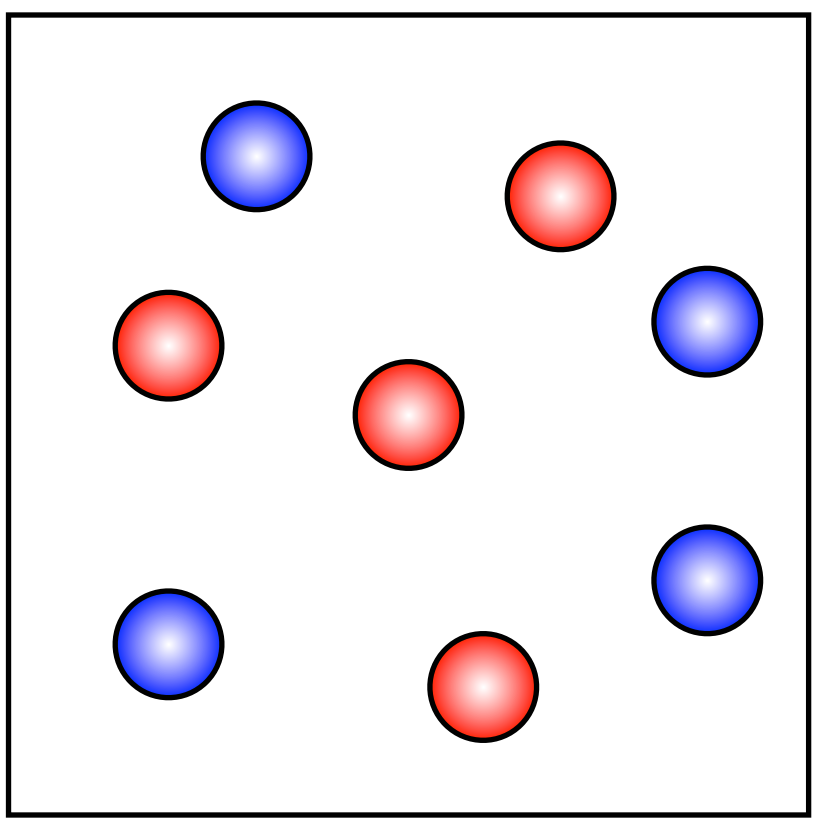
# Example: energy of many-body system

1d Bertsch parameter

$$\frac{E}{E_{FG}} = \xi$$

*same* 1d Bertsch parameter

$$\frac{E}{E_{FG}} = \sqrt{\xi}$$



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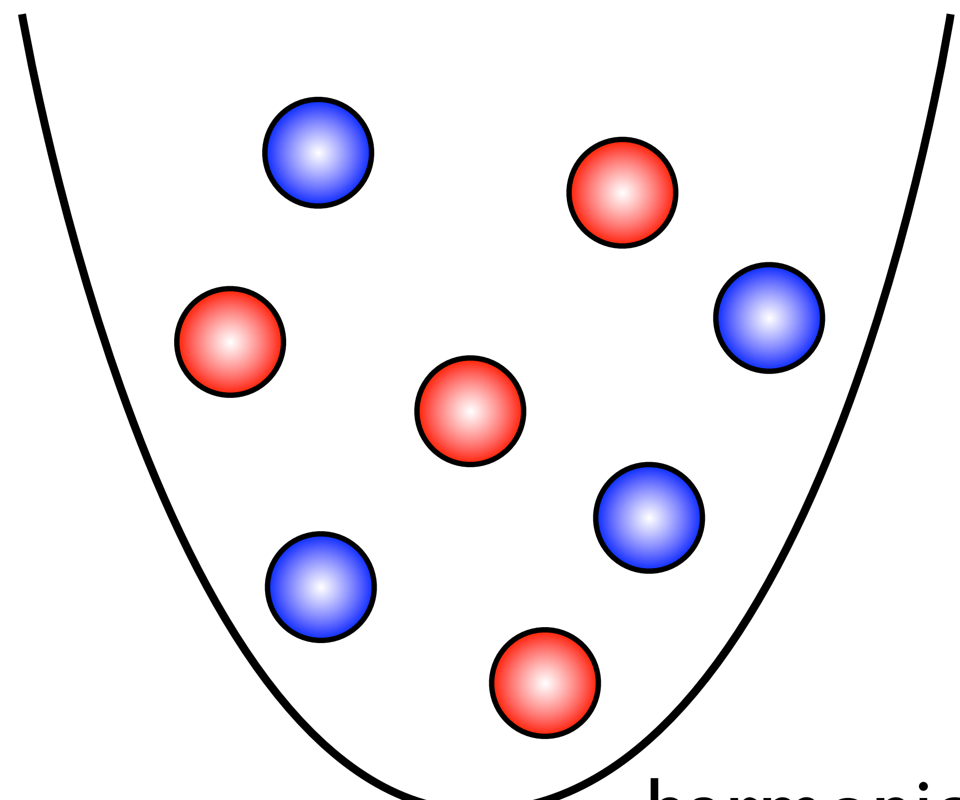

harmonic trap

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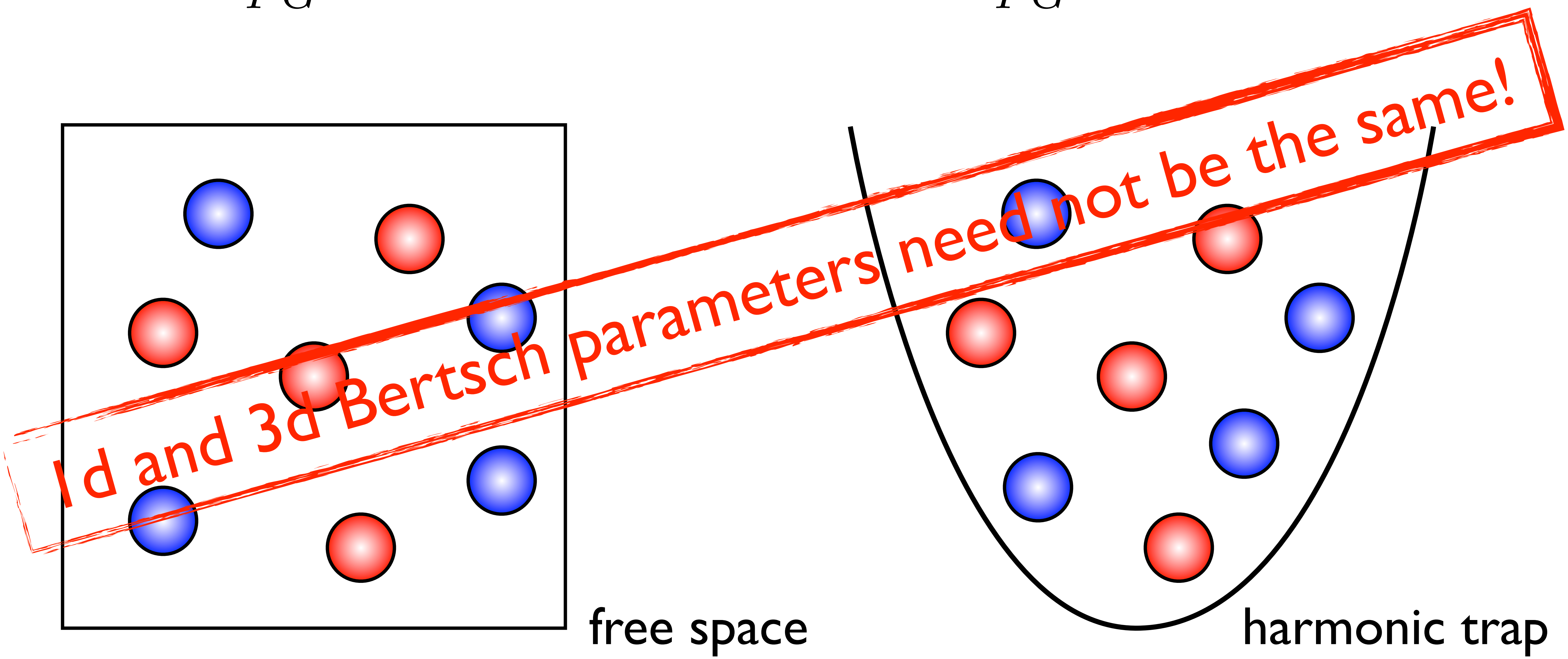


# Objective

- Qualitative similarities of one- and three-dimensional systems make numerical studies of 1D Fermi gas an attractive possibility
- Advantages over the three-dimensional theory:
  - computationally inexpensive
  - no sign problem for imbalanced population, mass and repulsive interactions
- Disadvantages:
  - gain qualitative insights, but how about quantitative ones?

# Lattice discretization

MGE, Phys. Rev. A **85** (2012) 063624 [arXiv:1204.6182]

$$S_{cont}(\mu) = \int d^2x \left[ \psi^\dagger \left( \partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi - g(\psi^\dagger \psi)^4 \right]$$

$$(\partial_\tau \psi - \mu\psi)_{\mathbf{n}} = \frac{1}{b_\tau} \left( \psi_{\mathbf{n}} - e^{b_\tau \mu} \psi_{\mathbf{n} - b_\tau \mathbf{e}_0} \right)$$

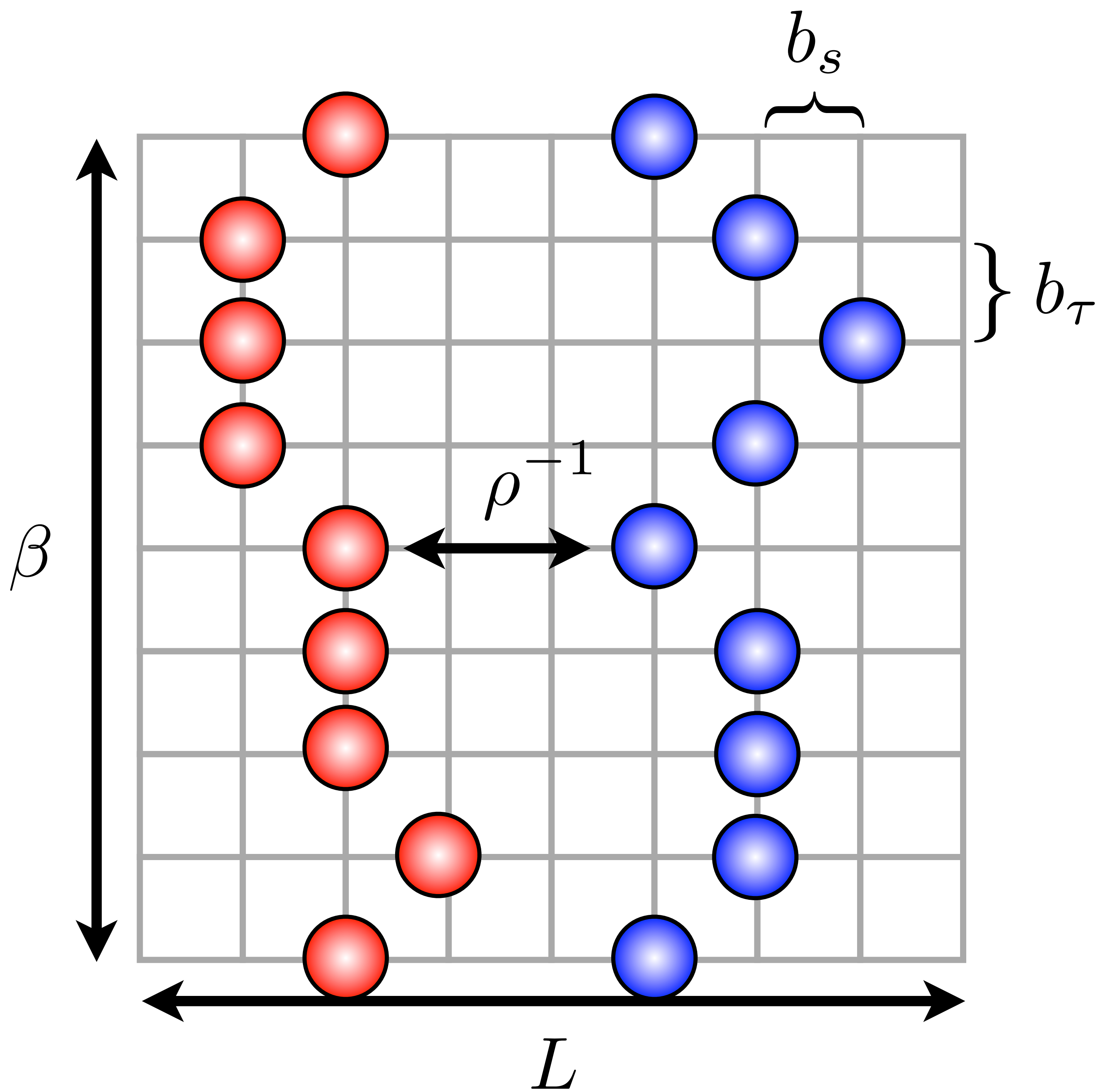
$$(-\nabla^2 \psi)_{\mathbf{n}} = \frac{1}{b_s^2} \left( 2\psi_{\mathbf{n}} - \psi_{\mathbf{n} + b_s \mathbf{e}_1} - \psi_{\mathbf{n} - b_s \mathbf{e}_1} \right)$$

$$(\psi^\dagger \psi)_{\mathbf{n}} = \psi^\dagger_{\mathbf{n}} e^{b_\tau \mu} \psi_{\mathbf{n} - b_\tau \mathbf{e}_0}$$

$$b_\tau = b_s = 1$$

"lattice units"

# Lattice discretization




Continuum & Infinite Volume limits:

$$b_s \ll \rho^{-1} \ll L$$

dilute limit

therm. limit

$$\rho = N/L$$

$$a \to \infty$$

# Path integral formulation

$$-S(\mu) = \sum_{\mathbf{n}\in\Lambda} \left[ -\psi^\dagger_{\mathbf{n}} \left(1 + \frac{1}{m}\right) \psi_{\mathbf{n}} + \psi^\dagger_{\mathbf{n}} e^{\mu} \psi_{\mathbf{n}-\mathbf{e}_0} + \psi^\dagger_{\mathbf{n}} \frac{1}{2m} \left(\psi_{\mathbf{n}+\mathbf{e}_1} + \psi_{\mathbf{n}-\mathbf{e}_1}\right) + g \left(\psi^\dagger_{\mathbf{n}} e^{\mu} \psi_{\mathbf{n}-\mathbf{e}_0}\right)^4 \right]$$

$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

# Path integral formulation

$$-S(\mu) = \sum_{\mathbf{n}\in\Lambda}\left[-\psi^\dagger_{\mathbf{n}}\left(1+\frac{1}{m}\right)\psi_{\mathbf{n}} + \psi^\dagger_{\mathbf{n}} e^{\mu}\psi_{\mathbf{n}-\mathbf{e}_0} + \psi^\dagger_{\mathbf{n}}\frac{1}{2m}\left(\psi_{\mathbf{n}+\mathbf{e}_1}+\psi_{\mathbf{n}-\mathbf{e}_1}\right) + g\left(\psi^\dagger_{\mathbf{n}} e^{\mu}\psi_{\mathbf{n}-\mathbf{e}_0}\right)^4\right]$$

$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

$$g^{1/4}\phi\psi^\dagger e^{\mu}\psi$$

(e.g., φ=$z_4$ field)

Conventional Hubbard-Stratonovich transformation results in a sign problem (after integrating out fermions)

# Path integral formulation

$$-S(\mu) = \sum_{\mathbf{n}\in\Lambda} \left[ -\psi^\dagger_{\mathbf{n}} \left(1 + \frac{1}{m}\right) \psi_{\mathbf{n}} + \psi^\dagger_{\mathbf{n}} e^{\mu} \psi_{\mathbf{n}-\mathbf{e}_0} + \psi^\dagger_{\mathbf{n}} \frac{1}{2m} \left(\psi_{\mathbf{n}+\mathbf{e}_1} + \psi_{\mathbf{n}-\mathbf{e}_1}\right) + g \left(\psi^\dagger_{\mathbf{n}} e^{\mu} \psi_{\mathbf{n}-\mathbf{e}_0}\right)^4 \right]$$

$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

**Solution**: consider a different representation for the partition function based on a hopping parameter expansion

# Path integral formulation

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$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

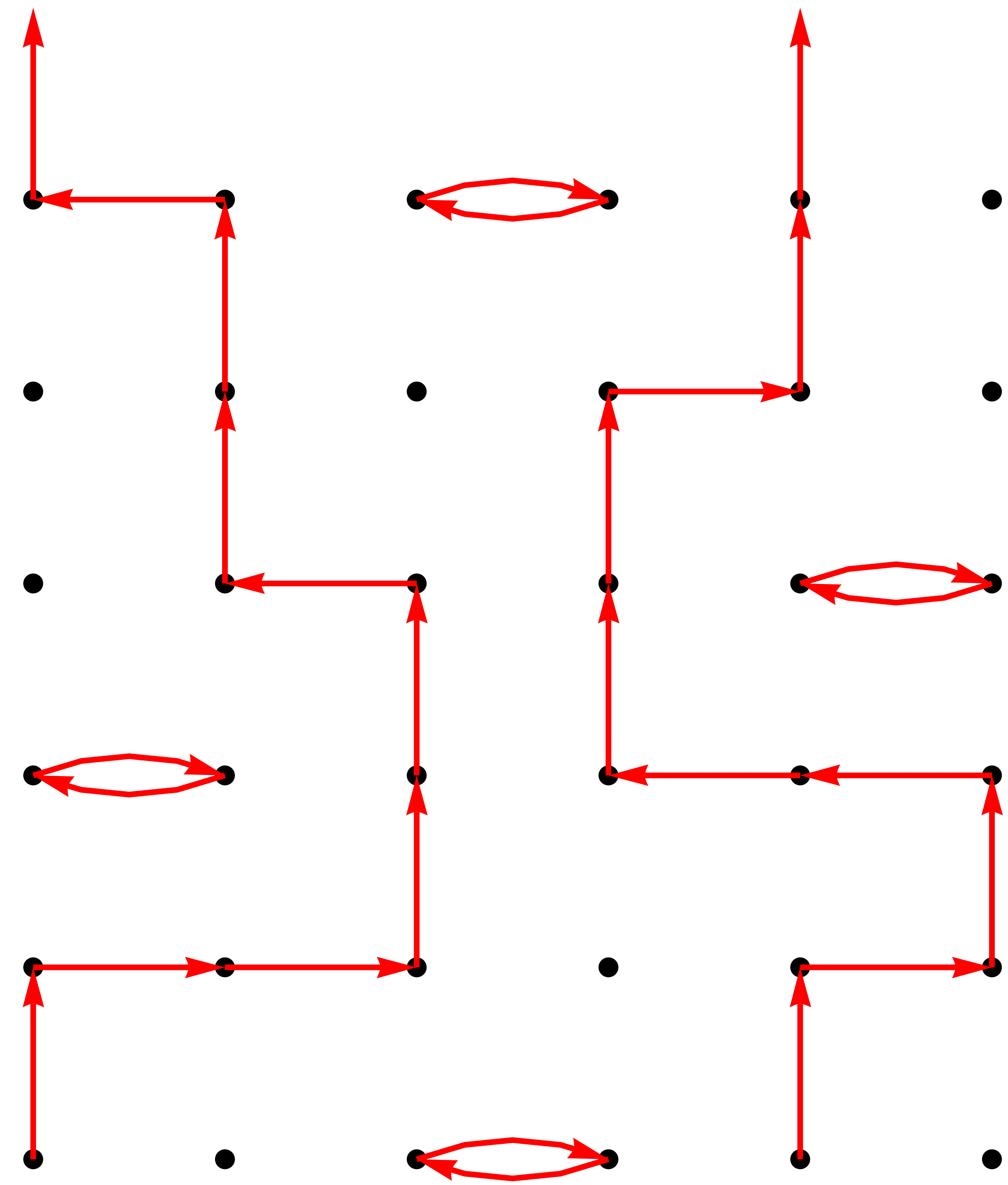
Ignore interaction to begin with...

# Consider a hopping parameter expansion

$$-S(\mu) = \sum_{\mathbf{n}\in\Lambda} \left[ -\psi^\dagger_{\mathbf{n}} \left(1 + \frac{1}{m}\right) \psi_{\mathbf{n}} + \psi^\dagger_{\mathbf{n}} e^{\mu} \psi_{\mathbf{n}-\mathbf{e}_0} + \psi^\dagger_{\mathbf{n}} \frac{1}{2m} \left(\psi_{\mathbf{n}+\mathbf{e}_1} + \psi_{\mathbf{n}-\mathbf{e}_1}\right) \right]$$

$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

Expand in powers of the action, integrate out the fermions term by term



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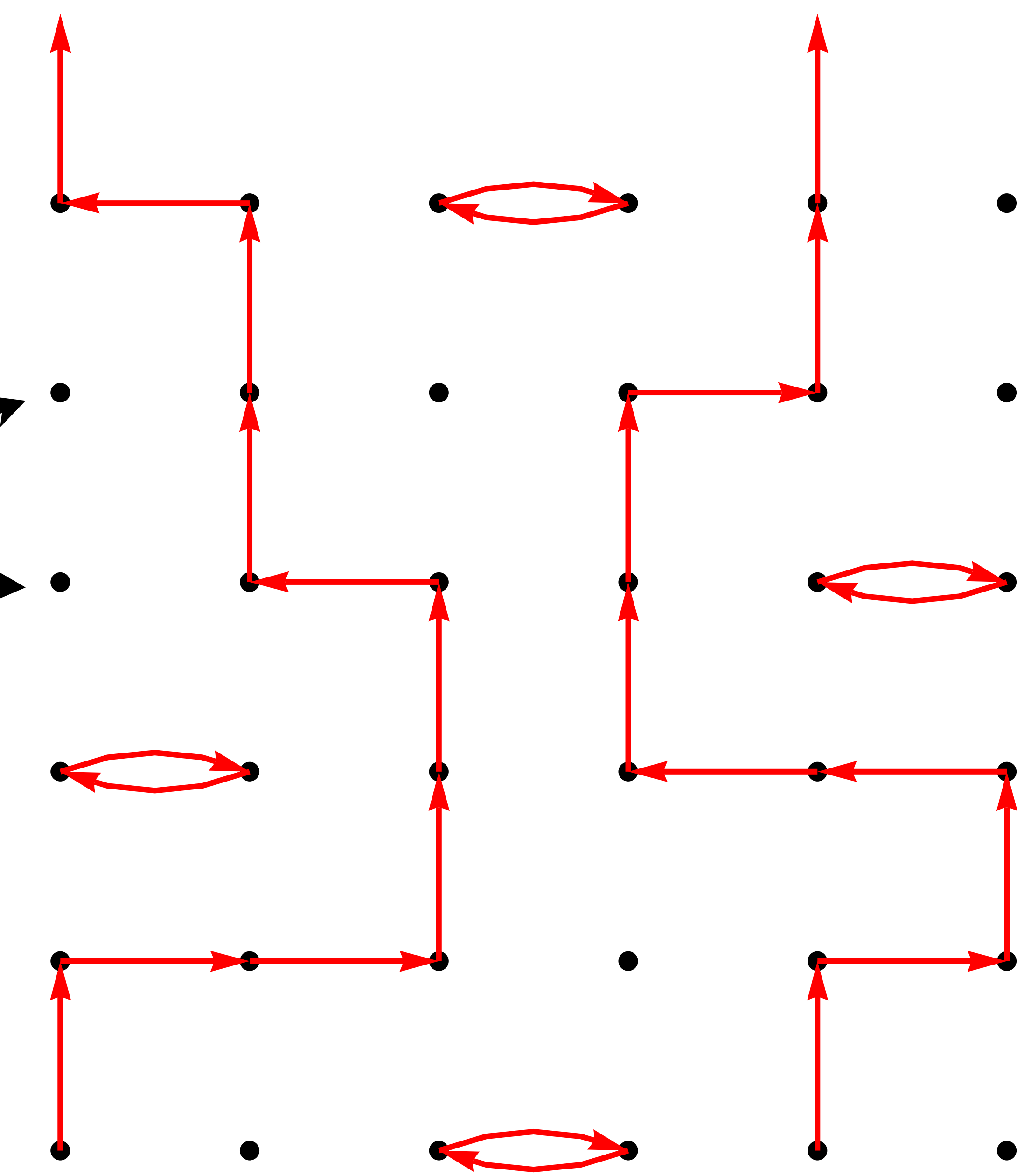
$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

$$-\left(1 + \frac{1}{m}\right)$$



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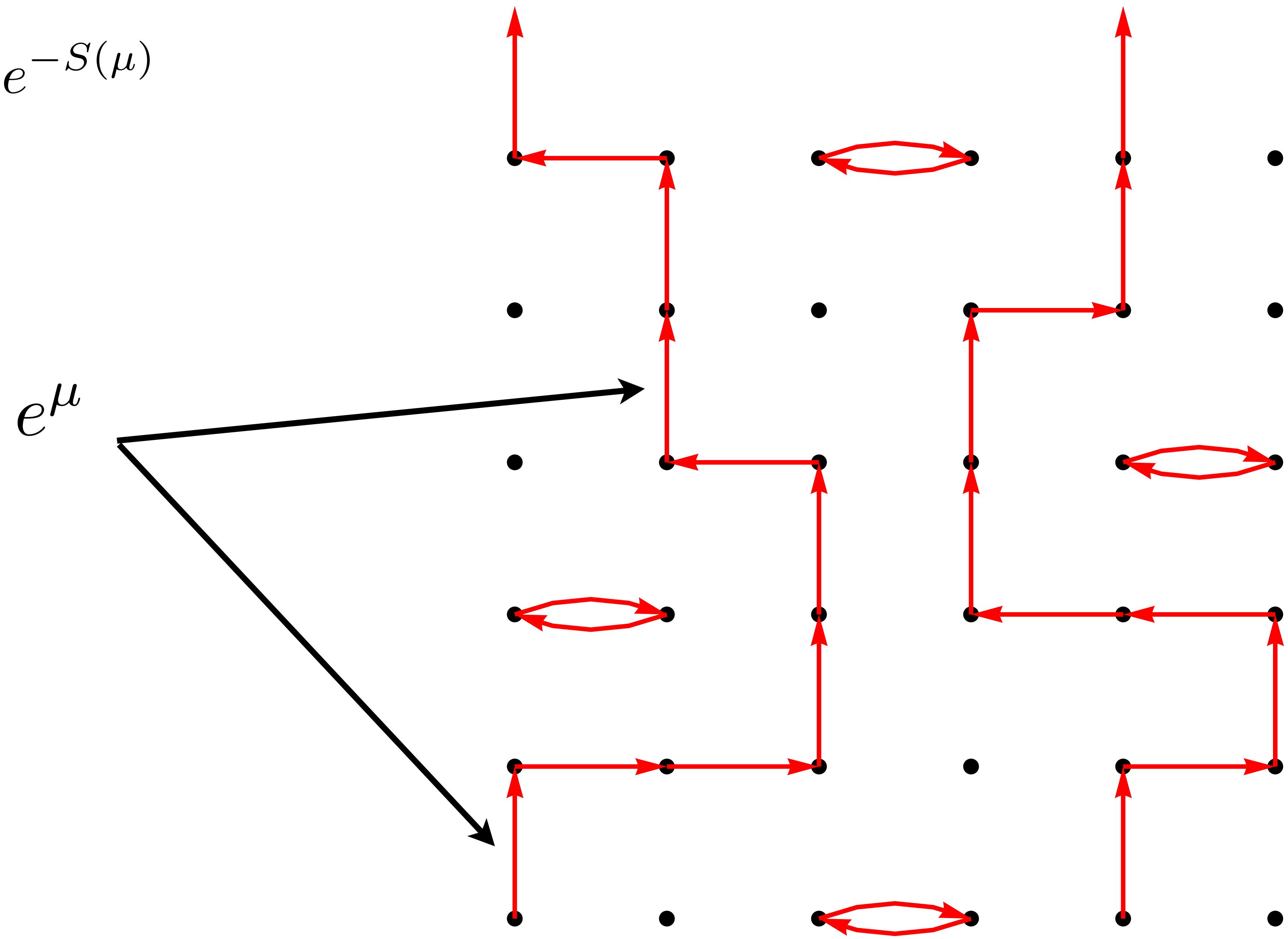

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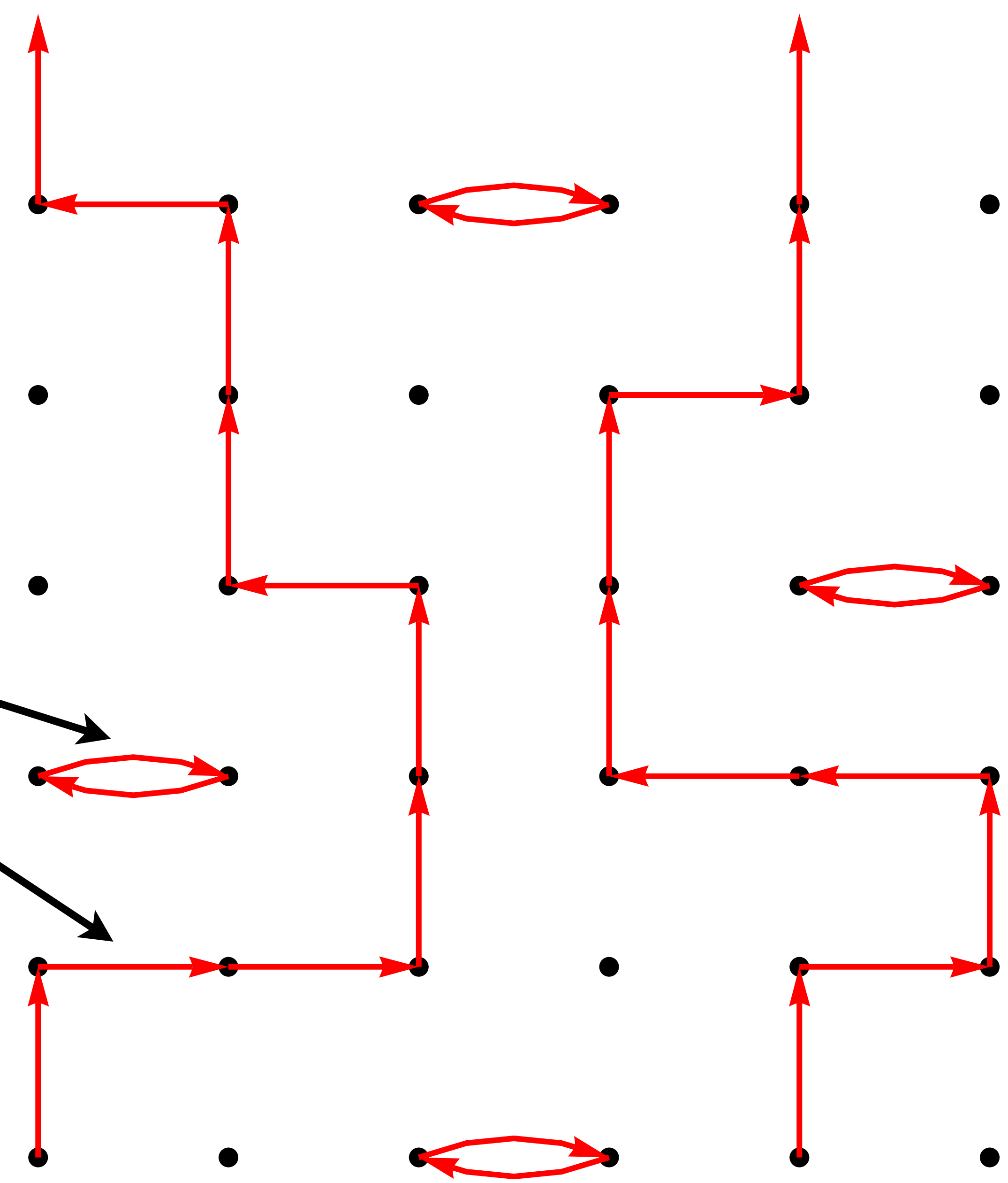
$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

$$\frac{1}{2m}$$



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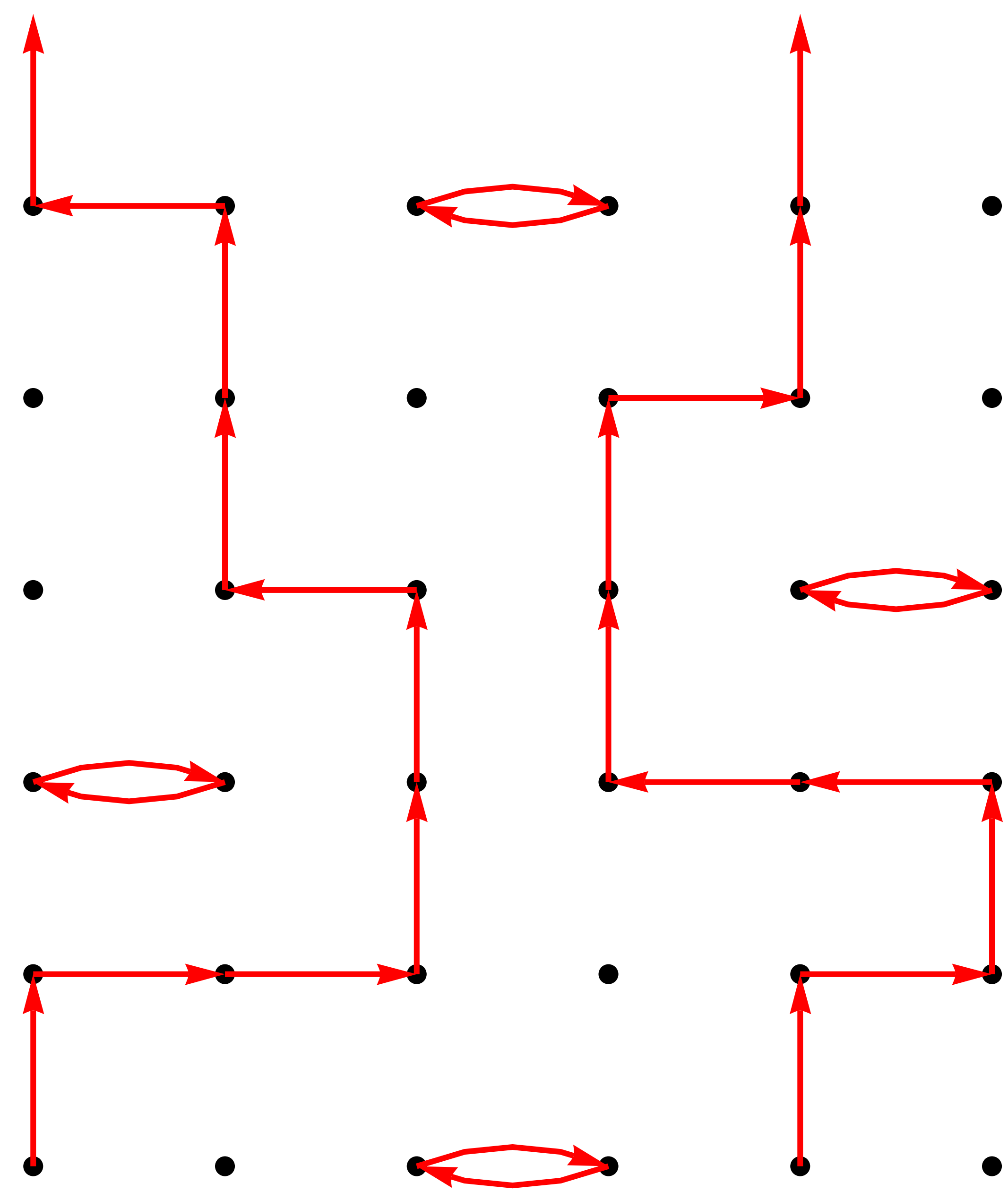
$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

- Fermion paths form closed loops (due to Grassmann integration)
- Fermion loops are self-avoiding (Pauli exclusion)
- Single-hop fermion "bubbles" allowed

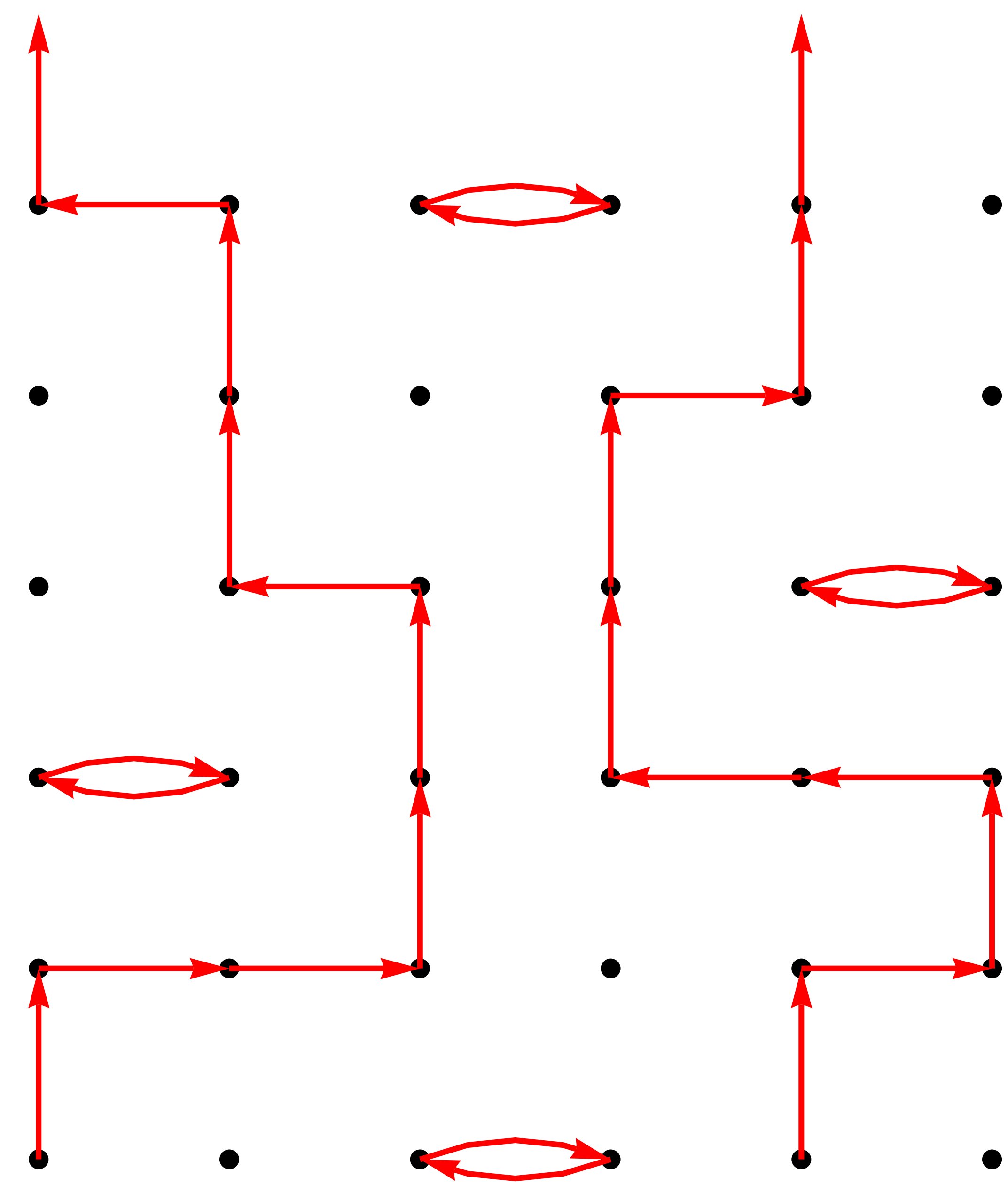


# Consider a hopping parameter expansion

$$-S(\mu) = \sum_{\mathbf{n}\in\Lambda} \left[ -\psi^\dagger_{\mathbf{n}} \left(1 + \frac{1}{m}\right) \psi_{\mathbf{n}} + \psi^\dagger_{\mathbf{n}} e^{\mu} \psi_{\mathbf{n}-\mathbf{e}_0} + \psi^\dagger_{\mathbf{n}} \frac{1}{2m} \left(\psi_{\mathbf{n}+\mathbf{e}_1} + \psi_{\mathbf{n}-\mathbf{e}_1}\right) \right]$$

$$Z(\mu) = \int [d\psi^\dagger][d\psi] e^{-S(\mu)}$$

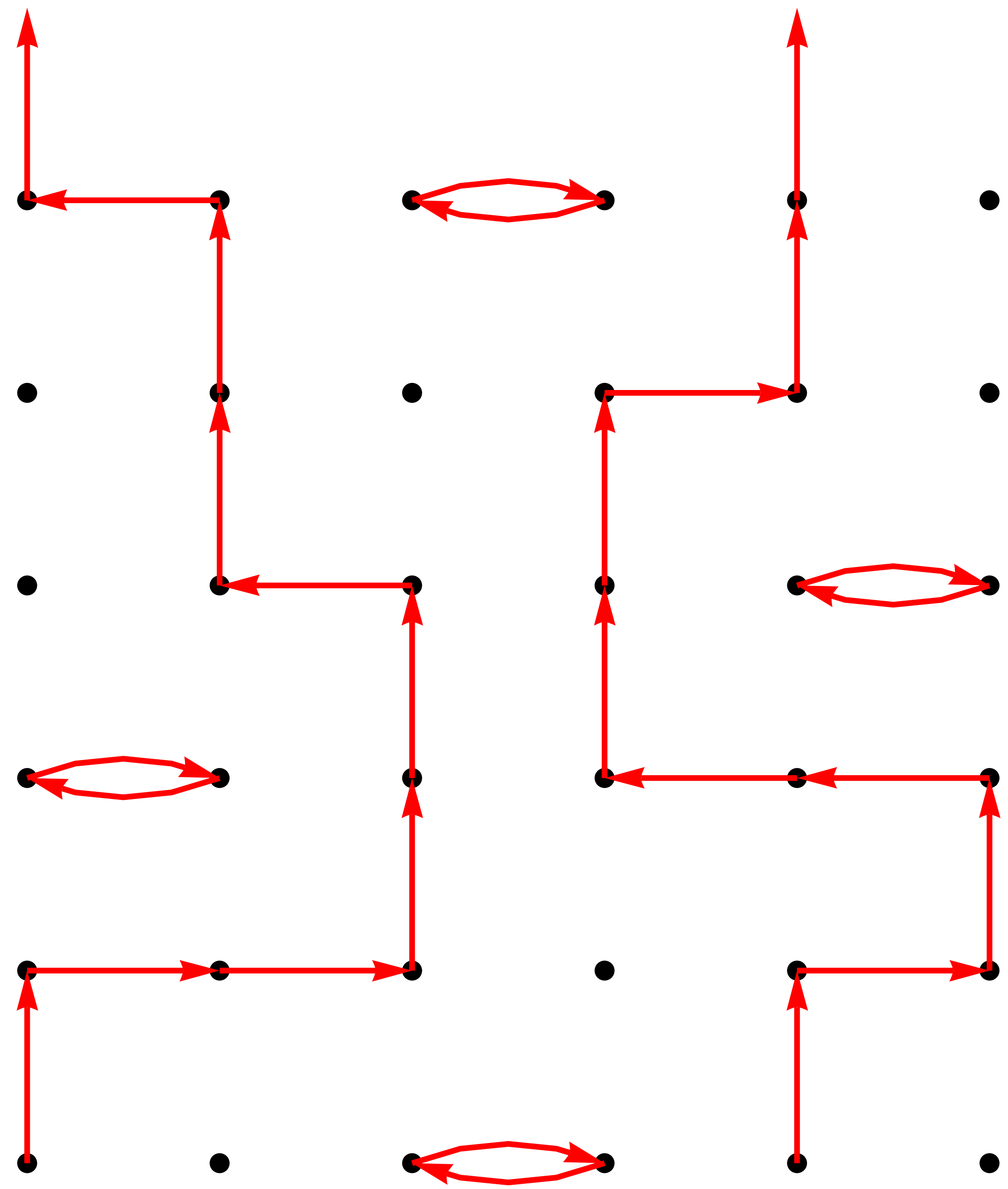
- All fermion loops come with a minus sign
- Every winding in time comes with a minus sign(APBCs)
- Fermion loops in time are disjoint (Pauli exclusion)



# Consider a hopping parameter expansion

$$Z(\mu) = \sum_{\{c_\sigma\}\in C} \left[ \prod_\sigma \left(1 + \frac{1}{m_\sigma}\right)^{\mathcal{S}(c_\sigma)} \left(\frac{1}{2m_\sigma}\right)^{\mathcal{B}_s(c_\sigma)} (-1)^{\mathcal{F}(c_\sigma)} e^{\mu_\sigma \mathcal{B}_\tau(c_\sigma)} \right]$$

- S = # unvisited sites
- $B_s$ = # space-like links
- $B_t$ = # time-like links
- F = # space-like fermion bubble loops



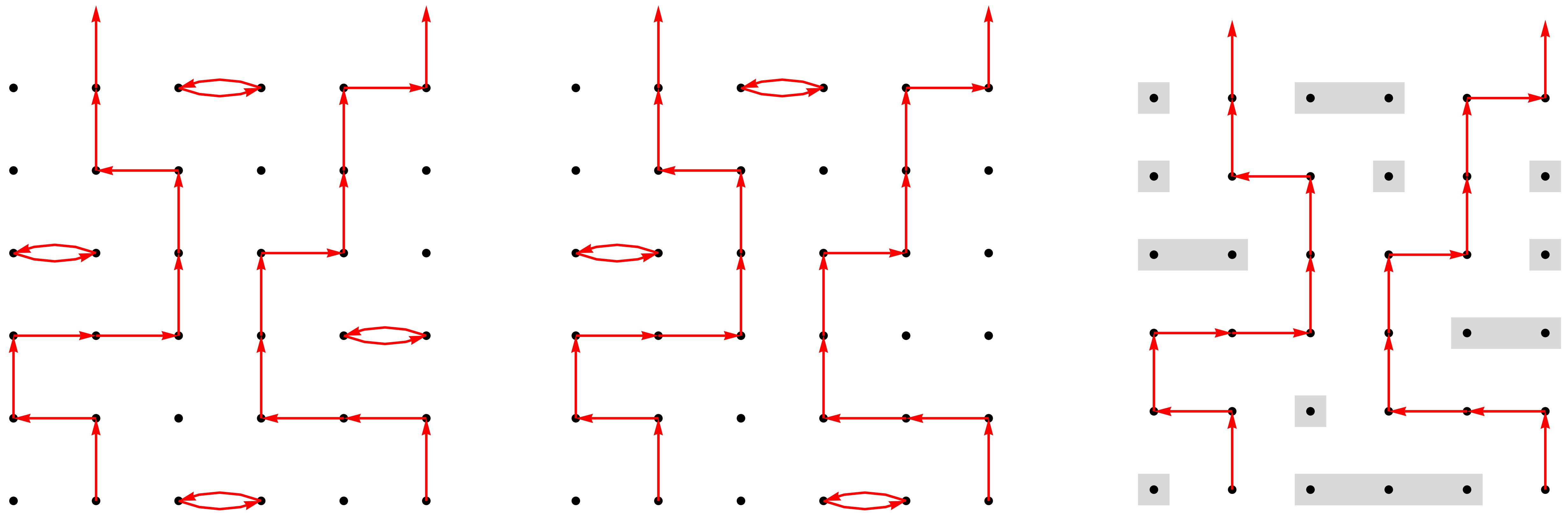
# Consider a hopping parameter expansion

$$Z(\mu) = \sum_{\{c_\sigma\}\in C} \left[ \prod_\sigma \left(1 + \frac{1}{m_\sigma}\right)^{\mathcal{S}(c_\sigma)} \left(\frac{1}{2m_\sigma}\right)^{\mathcal{B}_s(c_\sigma)} (-1)^{\mathcal{F}(c_\sigma)} e^{\mu_\sigma \mathcal{B}_\tau(c_\sigma)} \right]$$

...but we still have a sign problem.

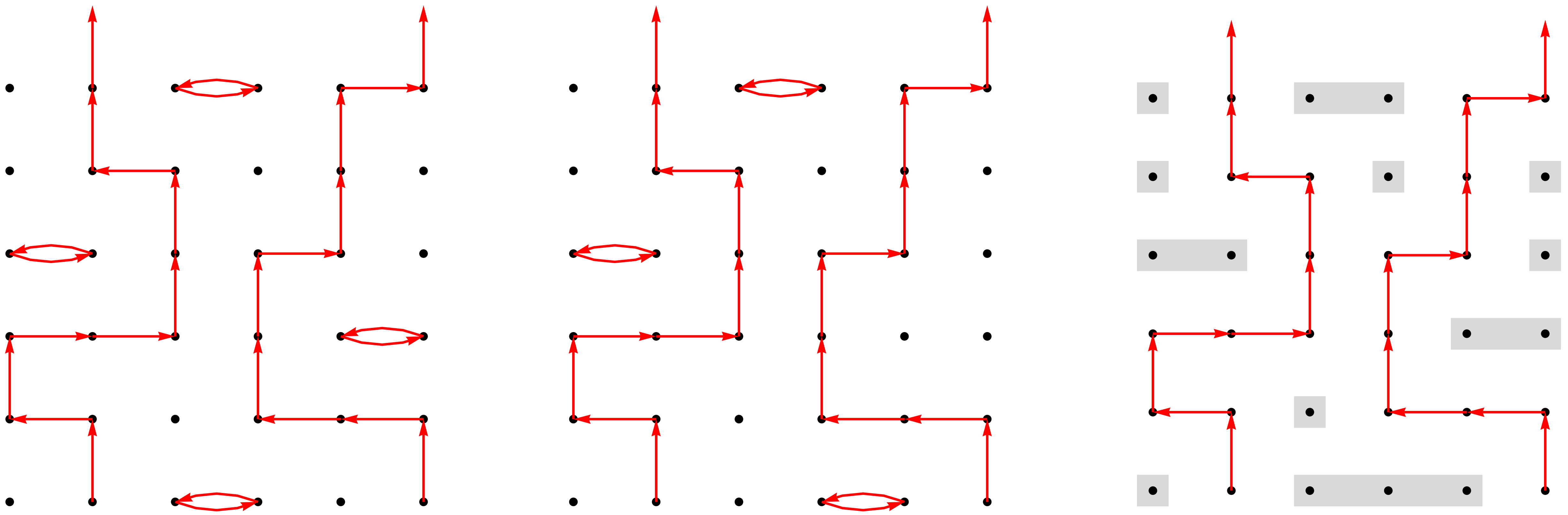
# Solving the sign problem

**Observation**: configurations fall into classes designated by the time-like loops



# Solving the sign problem

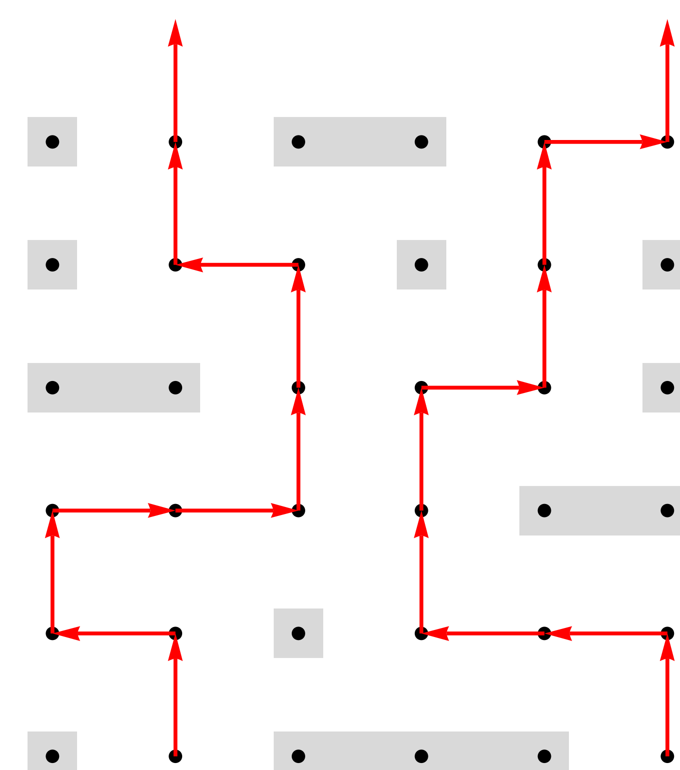
**Idea**: sum all up the fermion bubbles within each class



# Evaluation of the fermion bubble sum


$$z_n(m) = z_{n-1}(m)\left(1+\frac{1}{m}\right) - \frac{1}{(2m)^2} z_{n-2}(m)$$

$$z_0(m) = 1 \qquad z_1(m) = 1 + \frac{1}{m}$$



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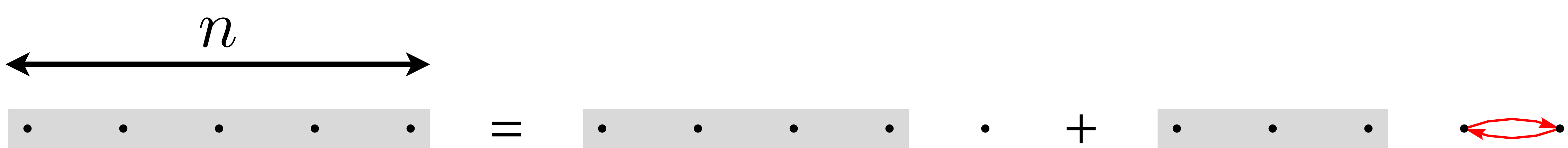
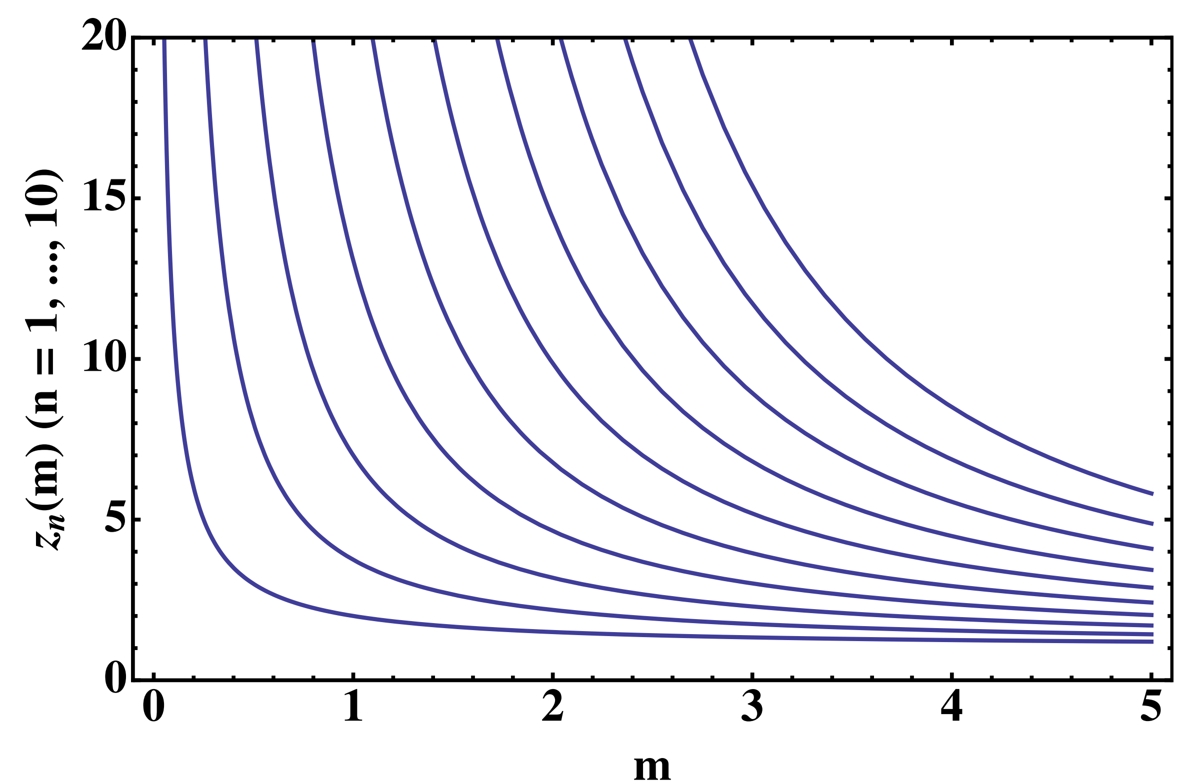



$$z_n(m) = \frac{1}{2^{n+1}\sqrt{1+2/m}}\left[\left(1+\frac{1}{m}+\sqrt{1+\frac{2}{m}}\right)^{n+1} - \left(1+\frac{1}{m}-\sqrt{1+\frac{2}{m}}\right)^{n+1}\right]$$



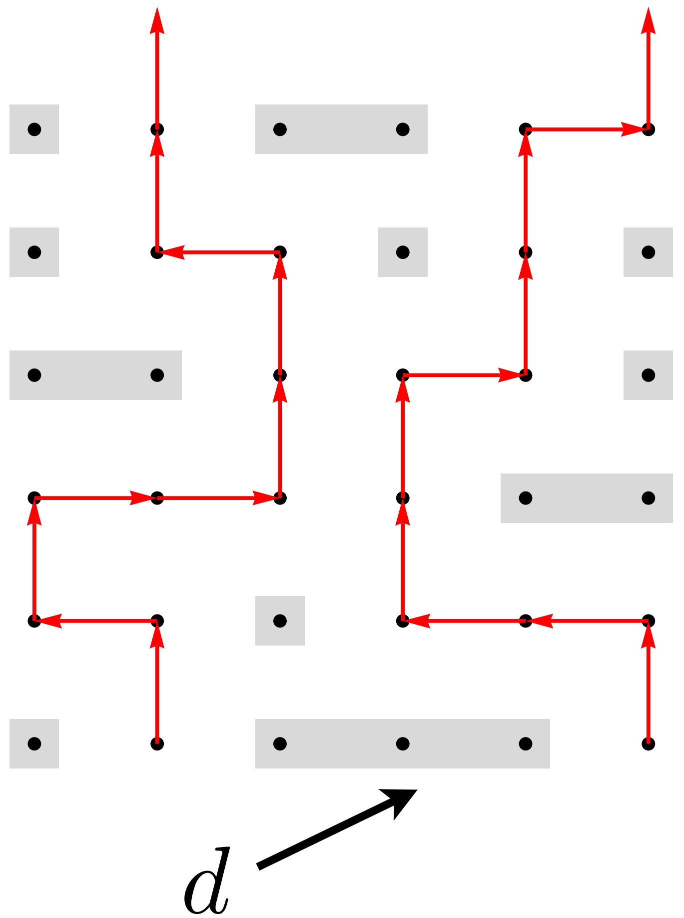
# Final result for free fermions

$$Z(\mu) = \sum_{\{c_\sigma\}\in C^*} \left[ \prod_\sigma \left( \prod_{d\in\mathcal{D}(c_\sigma)} z_{\mathcal{L}(d)}(m_\sigma) \right) \left( \frac{1}{2m_\sigma} \right)^{\mathcal{B}_s(c_\sigma)} e^{\mu_\sigma \mathcal{B}_\tau(c_\sigma)} \right]$$

$\mathcal{D}(c) = \text{set of domains } d \text{ associated with } c$

$\mathcal{L}(d) = \text{length of } d$

C* = set of all possible "bubble free" configurations



# Final result for free fermions

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Adding back the interaction...

# Final result for interacting fermions

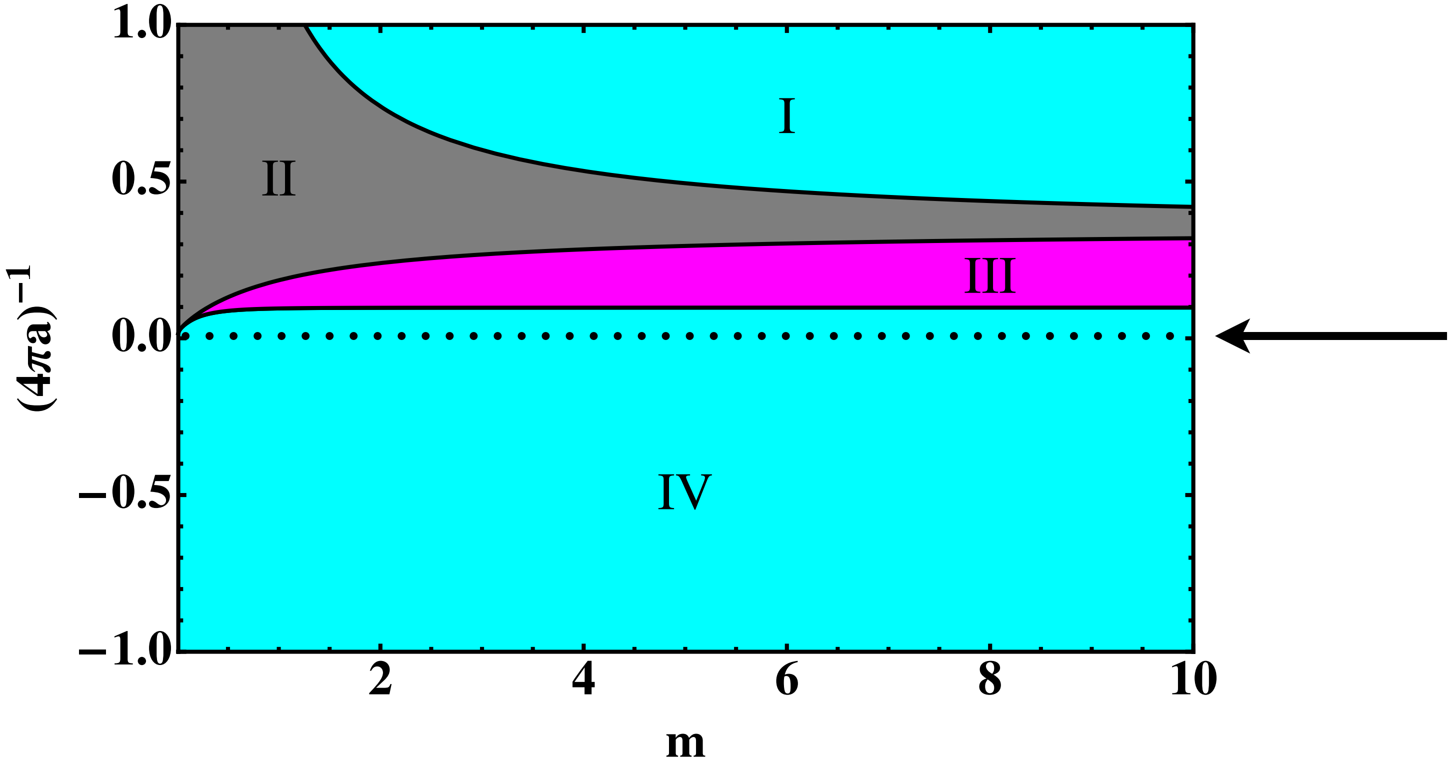
$$Z(\mu) = \sum_{\{c_\sigma\}\in C^*} \left[ \prod_\sigma \left( \prod_{d\in\mathcal{D}(c_\sigma)} z_{\mathcal{L}(d)}(m_\sigma) \right) \left( \frac{1}{2m_\sigma} \right)^{\mathcal{B}_s(c_\sigma)} e^{\mu_\sigma \mathcal{B}_\tau(c_\sigma)} \right] (1+g)^{\mathcal{B}_\tau(\cap_\sigma c_\sigma)}$$

$$c_a \cap c_b \cap c_c \cap c_d$$

- Resulting partition function free of sign problems even with:
  - mass imbalance
  - polarization imbalance
  - repulsive interactions (provided g > -1)

# Mean field results

# Mean-field results: m-$a^{-1}$ phase diagram

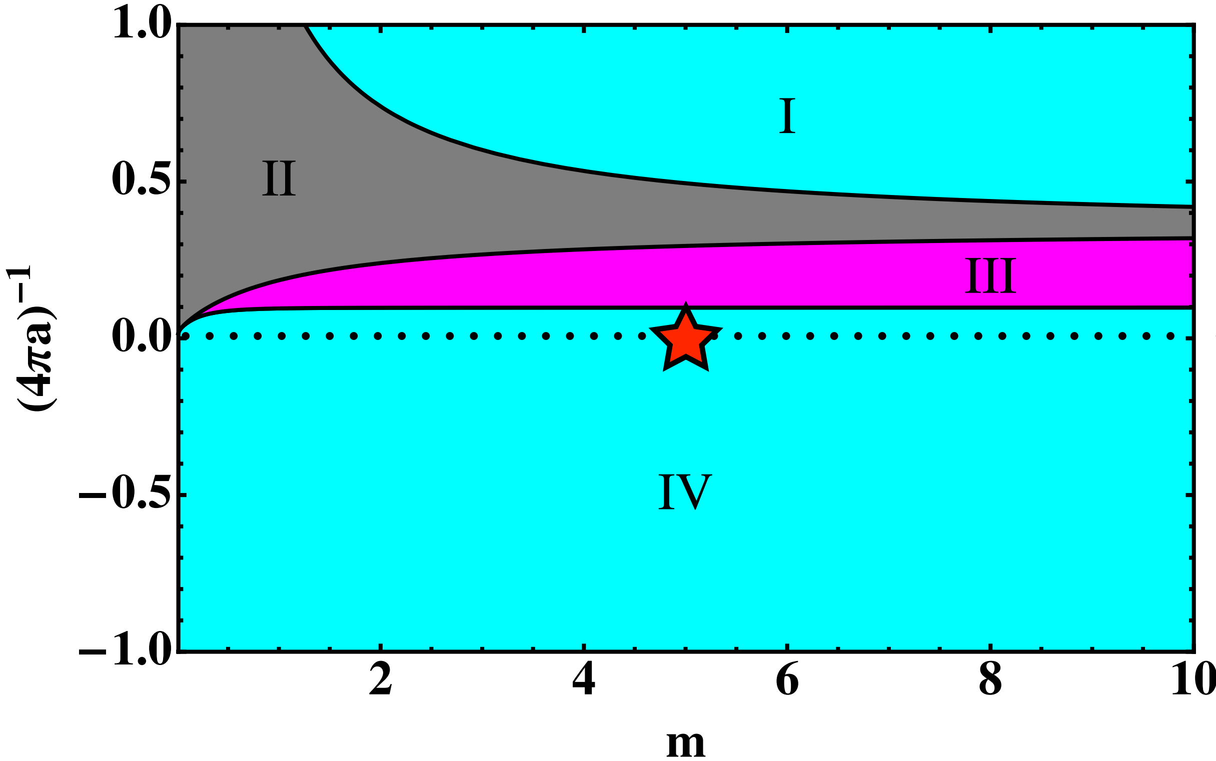



g = $g_c$

$$-\frac{m}{4\pi a} = \frac{1}{g} - \frac{1}{g_c}$$

- I & IV: zero density regime
- II: inaccessible within variational approach (complex action)
- III: saturated lattice, density equals four

# Mean-field results: m-a$^{-1}$ phase diagram




g = g$_c$

$$-\frac{m}{4\pi a} = \frac{1}{g} - \frac{1}{g_c}$$

- I & IV: zero density regime
- II: inaccessible within variational approach (complex action)
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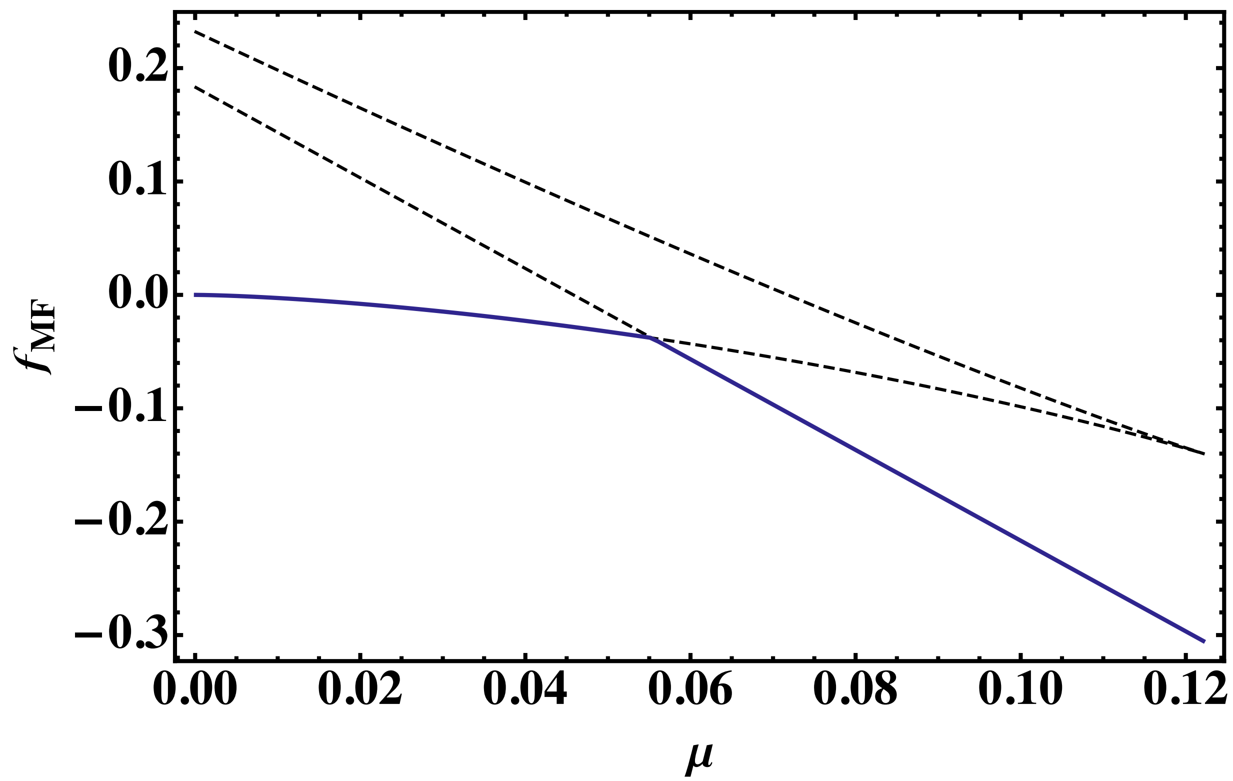
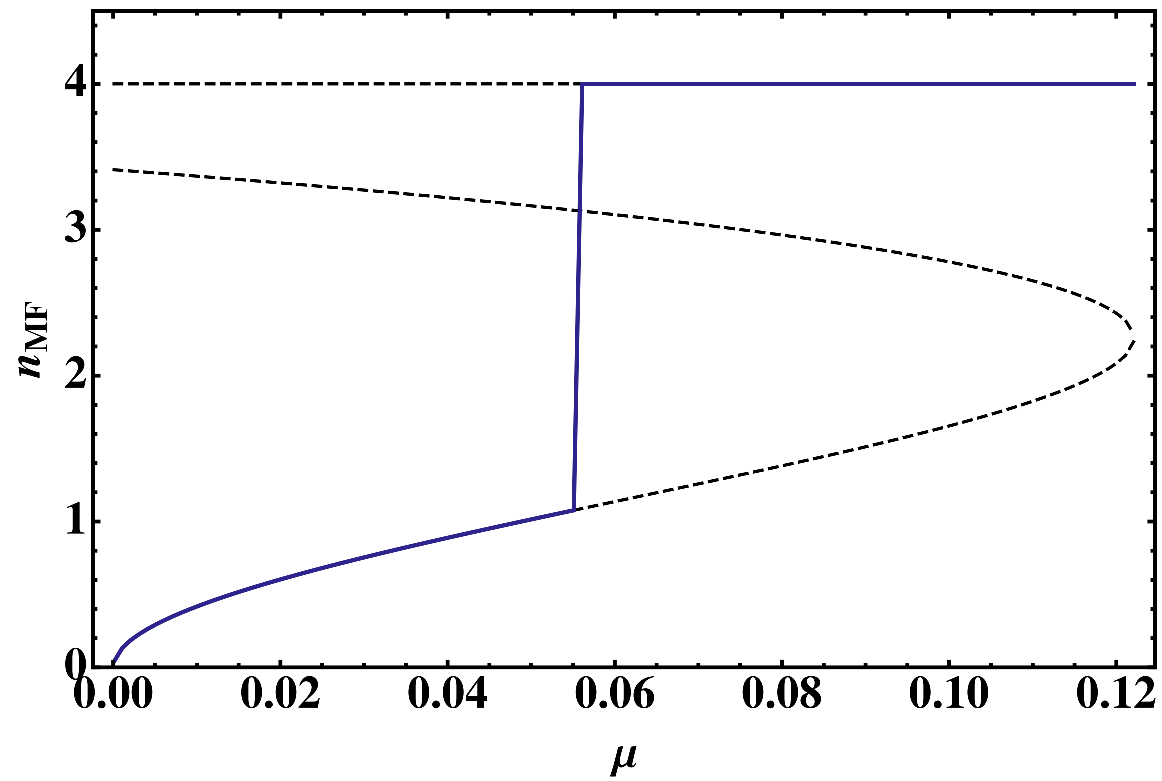
# Mean-field results: free energy & number density




- Number density at critical coupling jumps discontinuously from region of low(-ish) density to region in which lattice is saturated with fermions as a function of μ

- Continuum: ρ << 1 with aρ=fixed
  - exists within mean-field theory at low density

# Numerical results

# Numerical simulations

MGE, Phys. Rev. Lett. **109** (2012) 250403 [arXiv:1210.3104]

- Implemented Monte Carlo simulation of the canonical partition function for one-dimensional Fermi gas:
  - in a finite box
  - in a harmonic trap
- Studies include:
  - few-body energies
  - virial theorem
  - one-dimensional Bertsch parameter

# Energy observable

$$E = \lim_{\beta\to\infty} \frac{1}{\beta} \frac{d \log \hat{Z}(q)}{d \log \omega} \qquad \omega = \frac{1}{m L_0^2}$$

$$= \lim_{\beta\to\infty} \frac{1}{\beta} \left[ \frac{\partial \log \hat{Z}(q)}{\partial \log m} + \frac{\partial \log \hat{Z}(q)}{\partial \log \kappa} + \left( - \frac{\partial \log g_c}{\partial \log m} \right) \frac{\partial \log \hat{Z}(q)}{\partial \log g_c} \right]$$

kinetic (T) potential (V) interaction (I)

# Energy observable

$$E = \lim_{\beta\to\infty} \frac{1}{\beta} \frac{d \log \hat{Z}(q)}{d \log \omega} \qquad \omega = \frac{1}{mL_0^2}$$

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kinetic (T) potential (V) interaction (I)

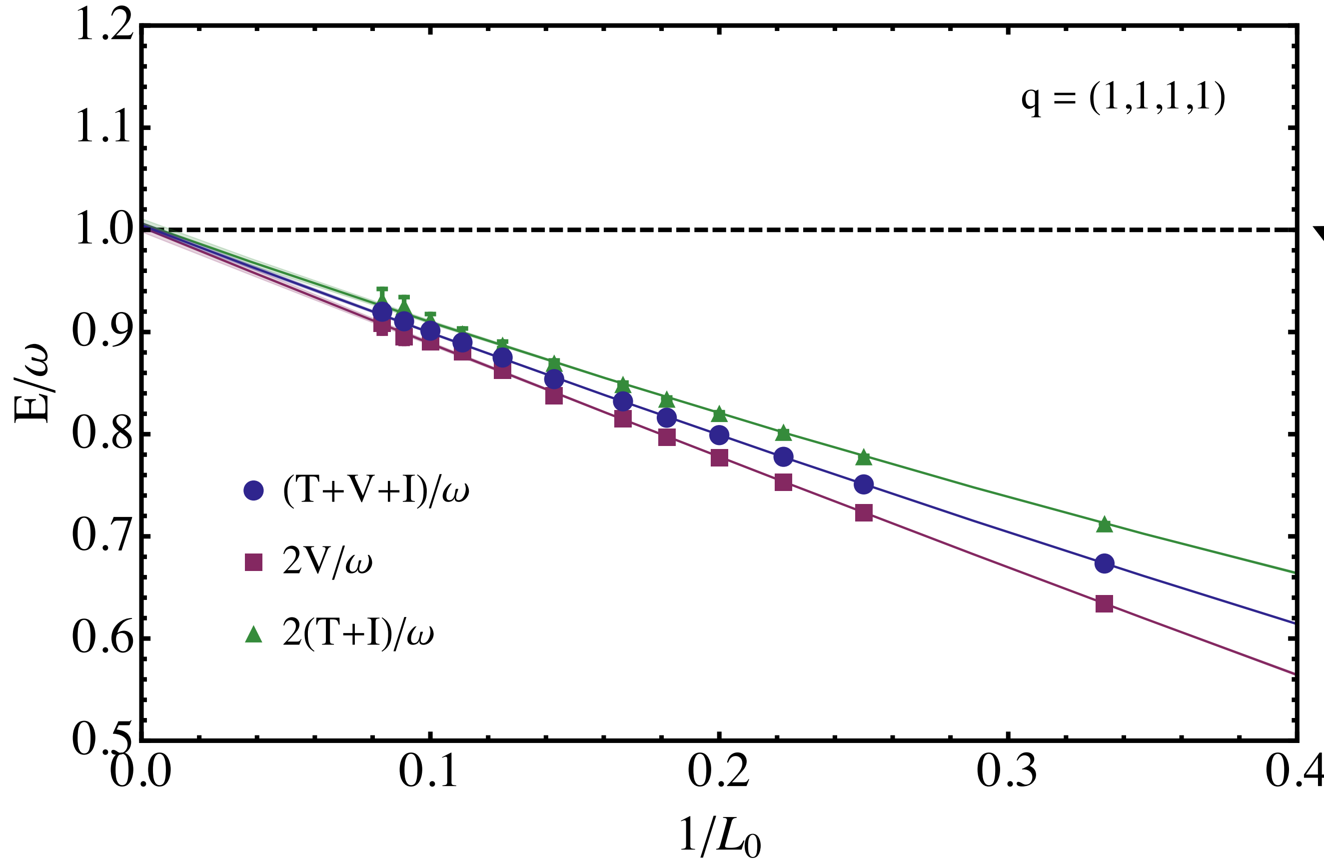
E = T+V+I E = 2V (Virial) E = 2(T+I) (Virial)

# Continuum limit

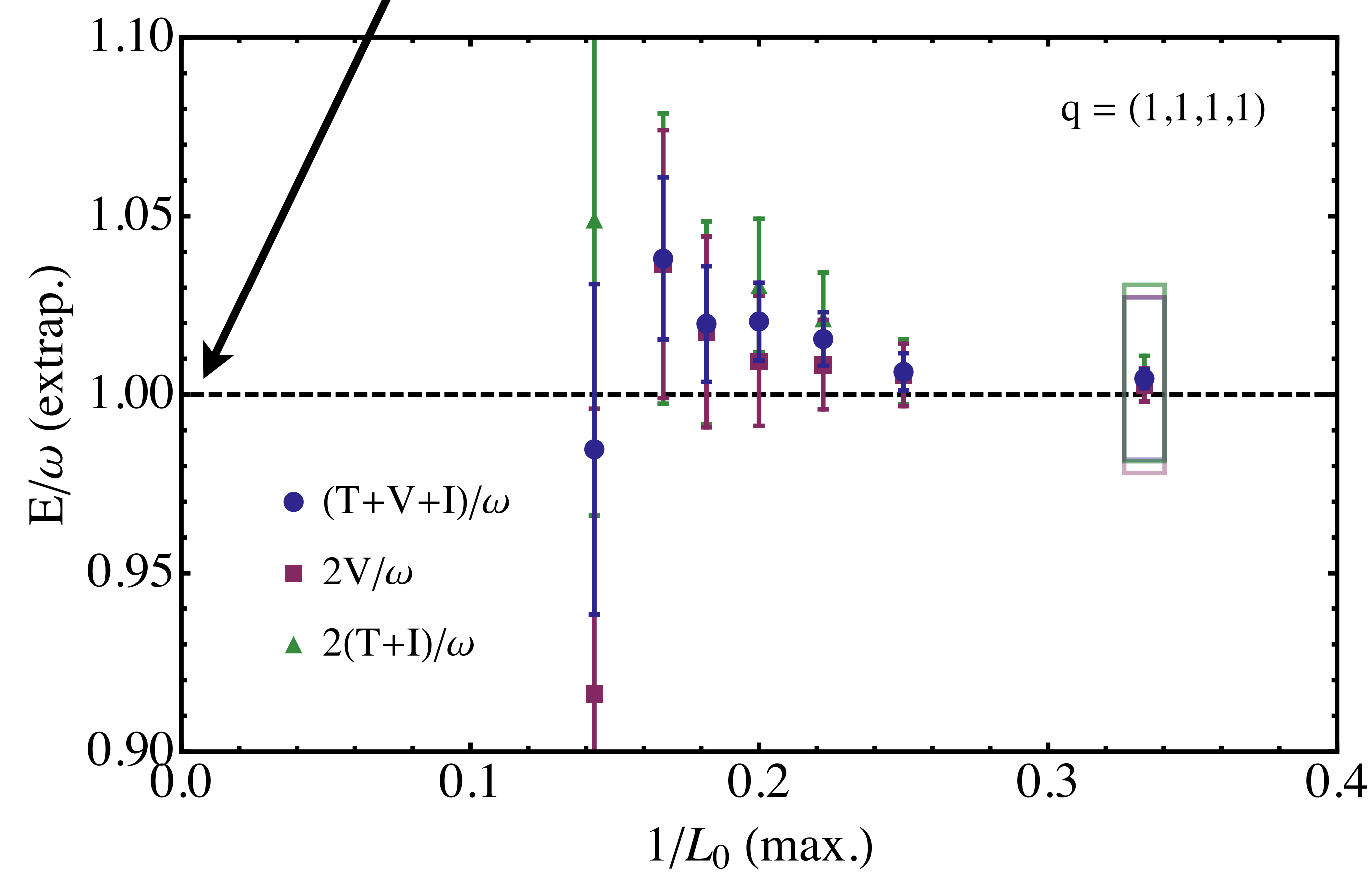
- Symanzik action: lattice artifacts associated with higher-dimension operators in a *continuum* effective theory
  - operator-state correspondence allows us to identify scaling dimensions of few-body operators
  - lack of scales allows us to identify volume scaling via dimensional analysis in a perturbative expansion in couplings
- Non-trivial volume scaling for dimensionless observables:

$$\mathcal{O}\left(\frac{b_s}{L_0}\right) = \mathcal{O}_{cont} + \mathcal{O}_1\left(\frac{b_s}{L_0}\right) + \mathcal{O}_{1.666}\left(\frac{b_s}{L_0}\right)^{1.6666} + \ldots$$

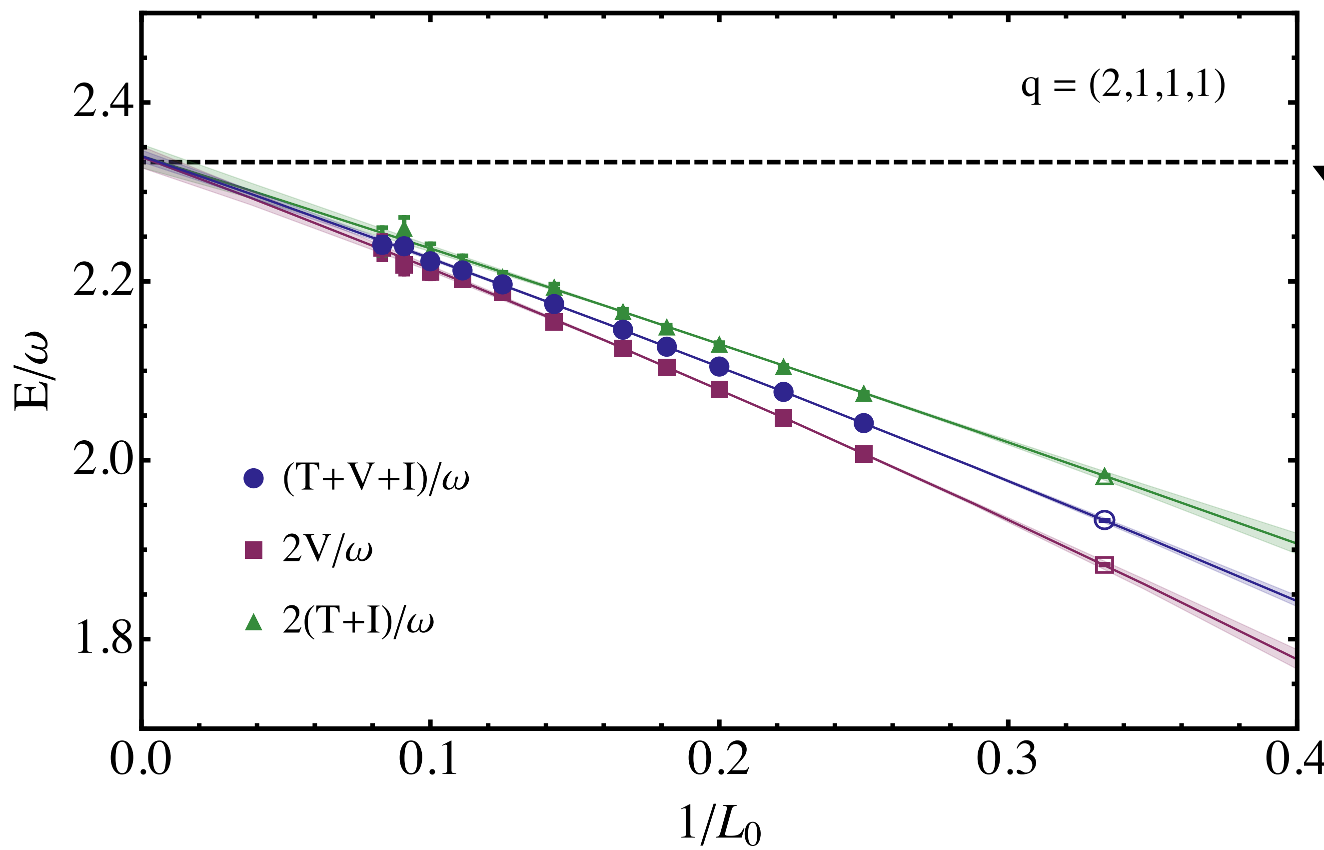
# Four-body system (trapped)



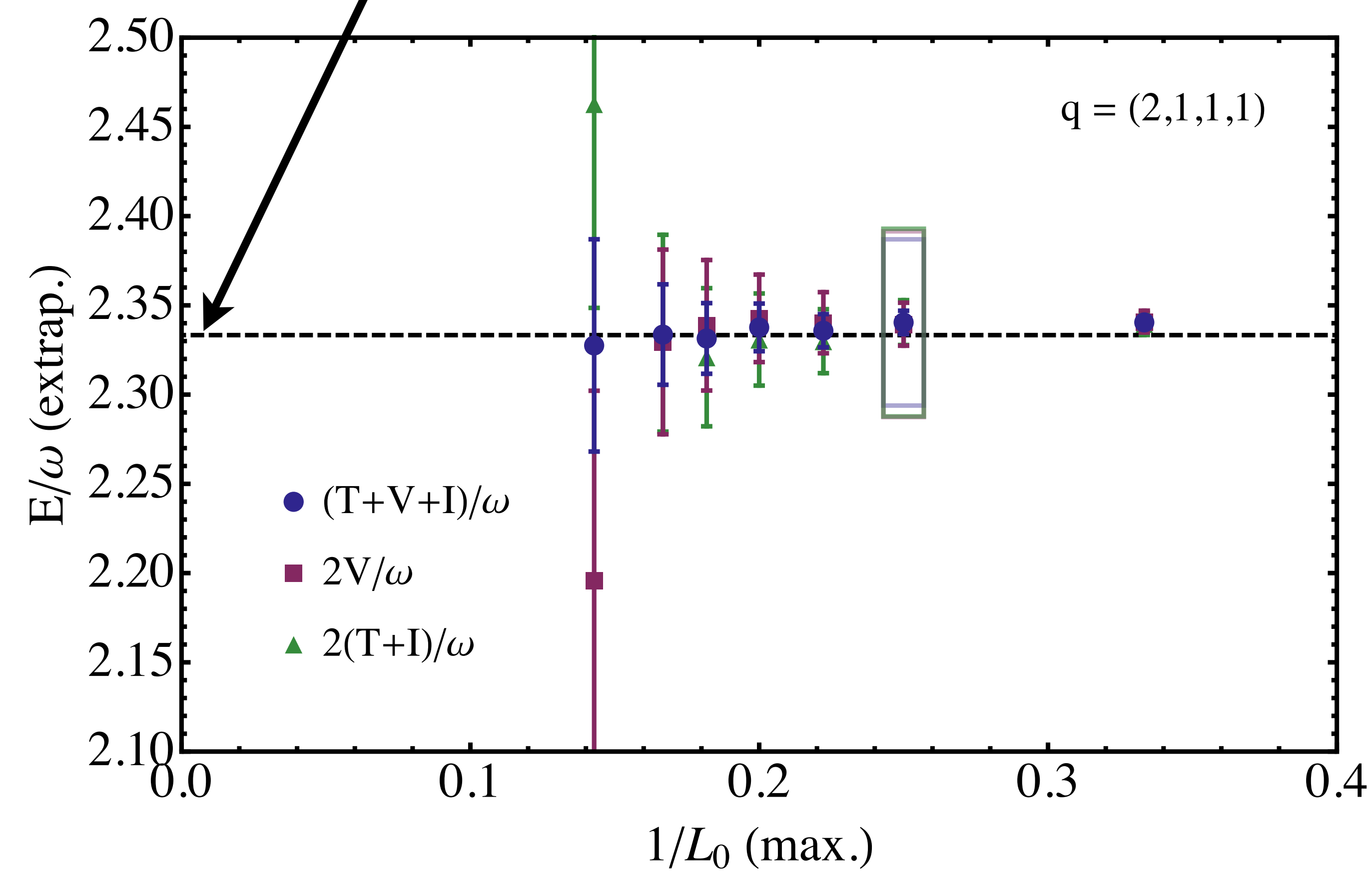

(exact value = unity)



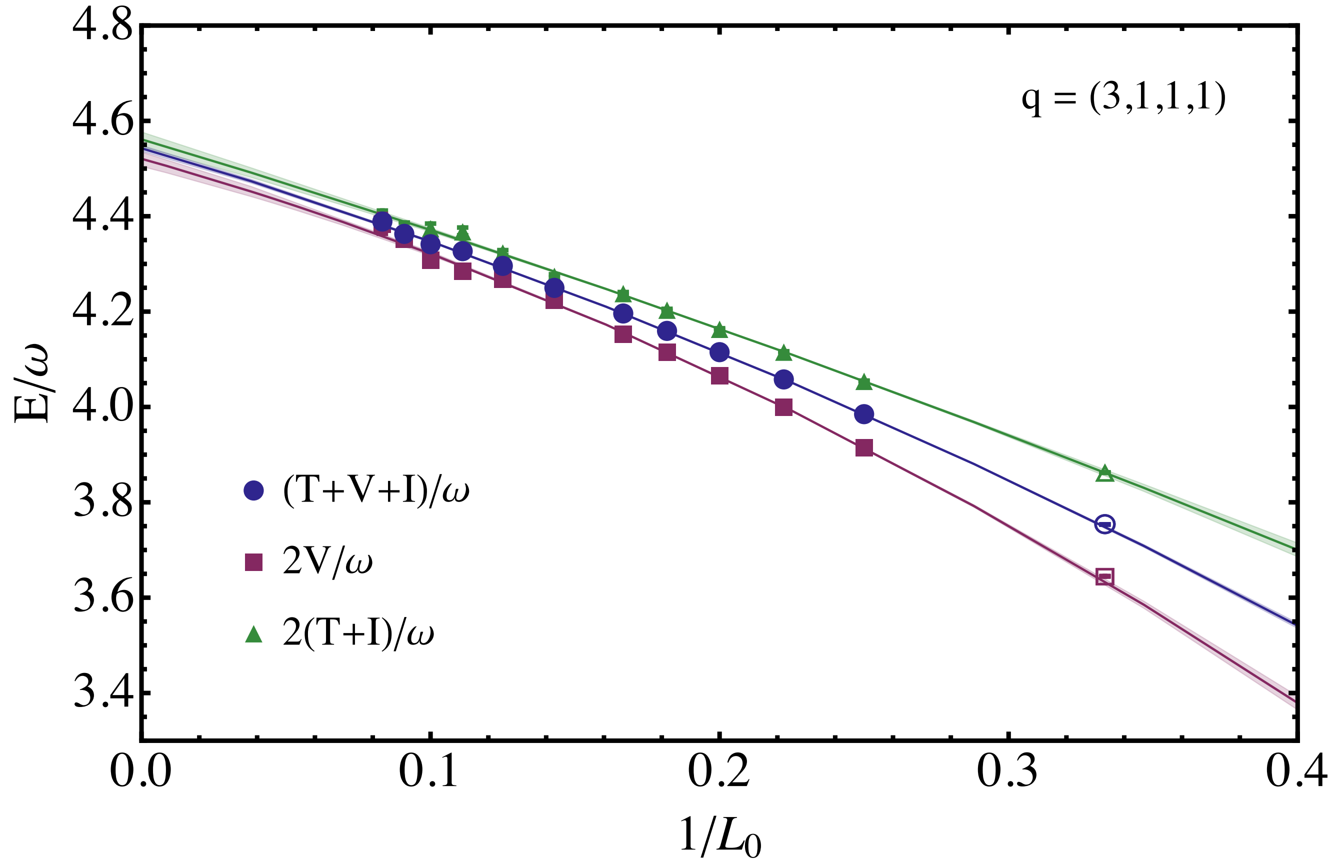
# Five-body system (trapped)

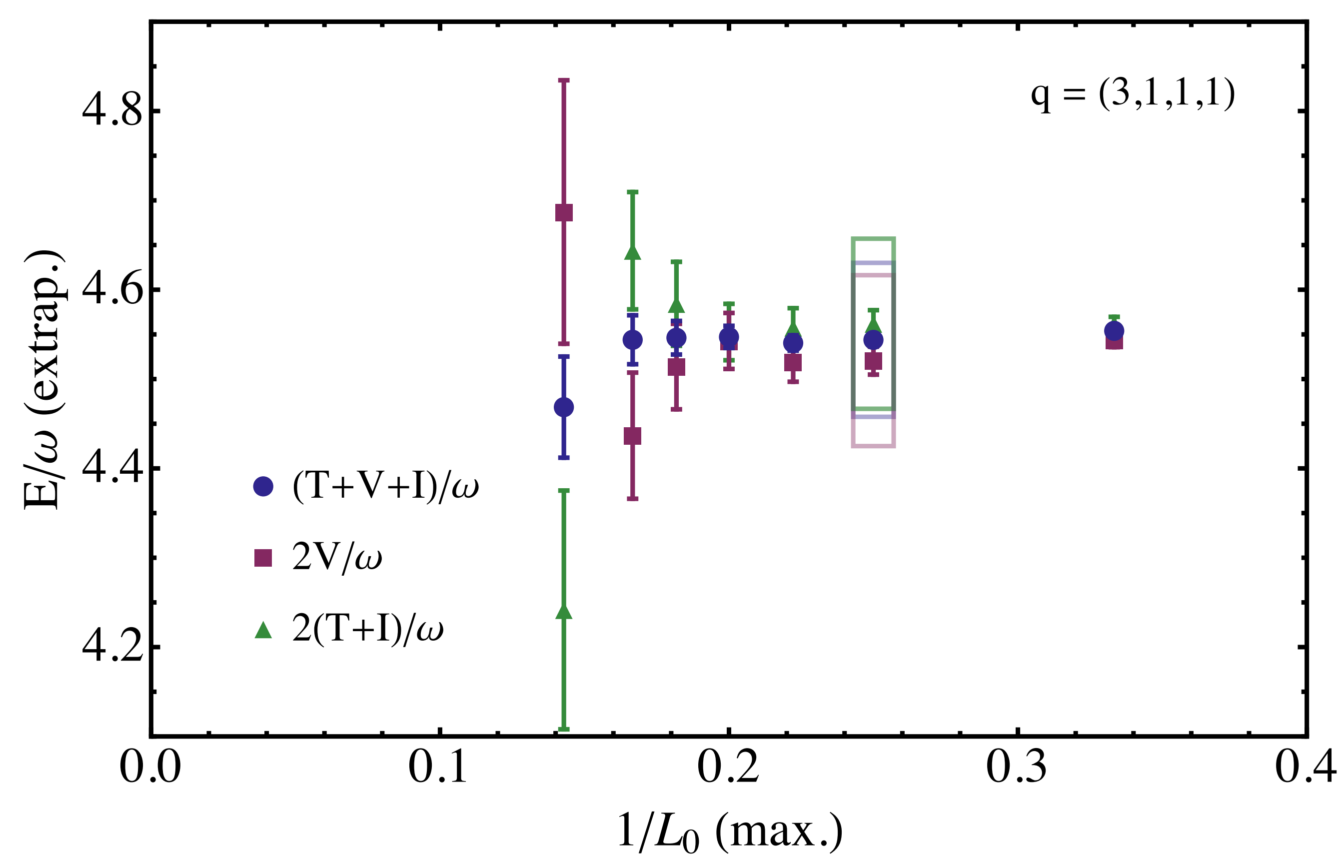



(exact value = 2.333)

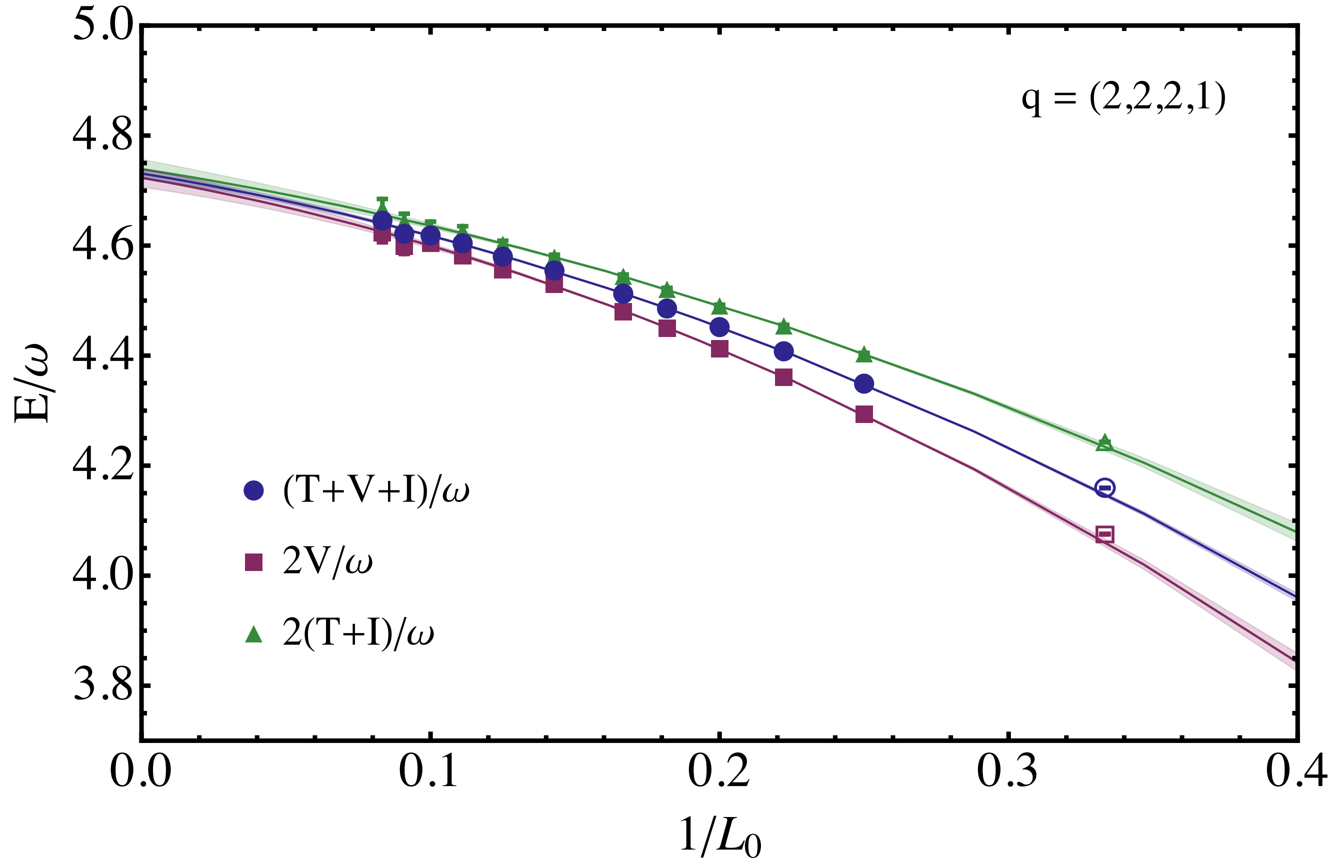


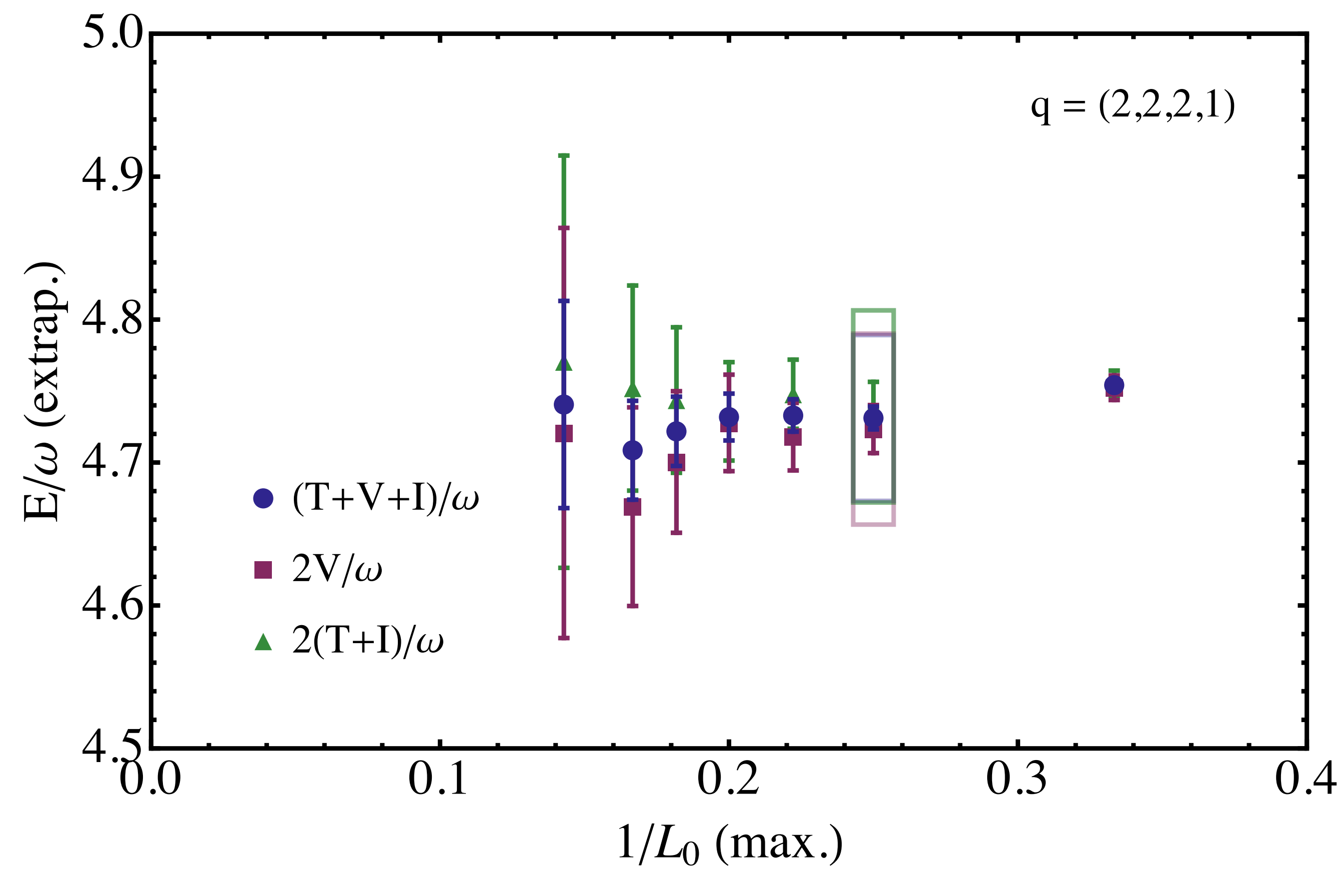
# Six-body system(s) (trapped)



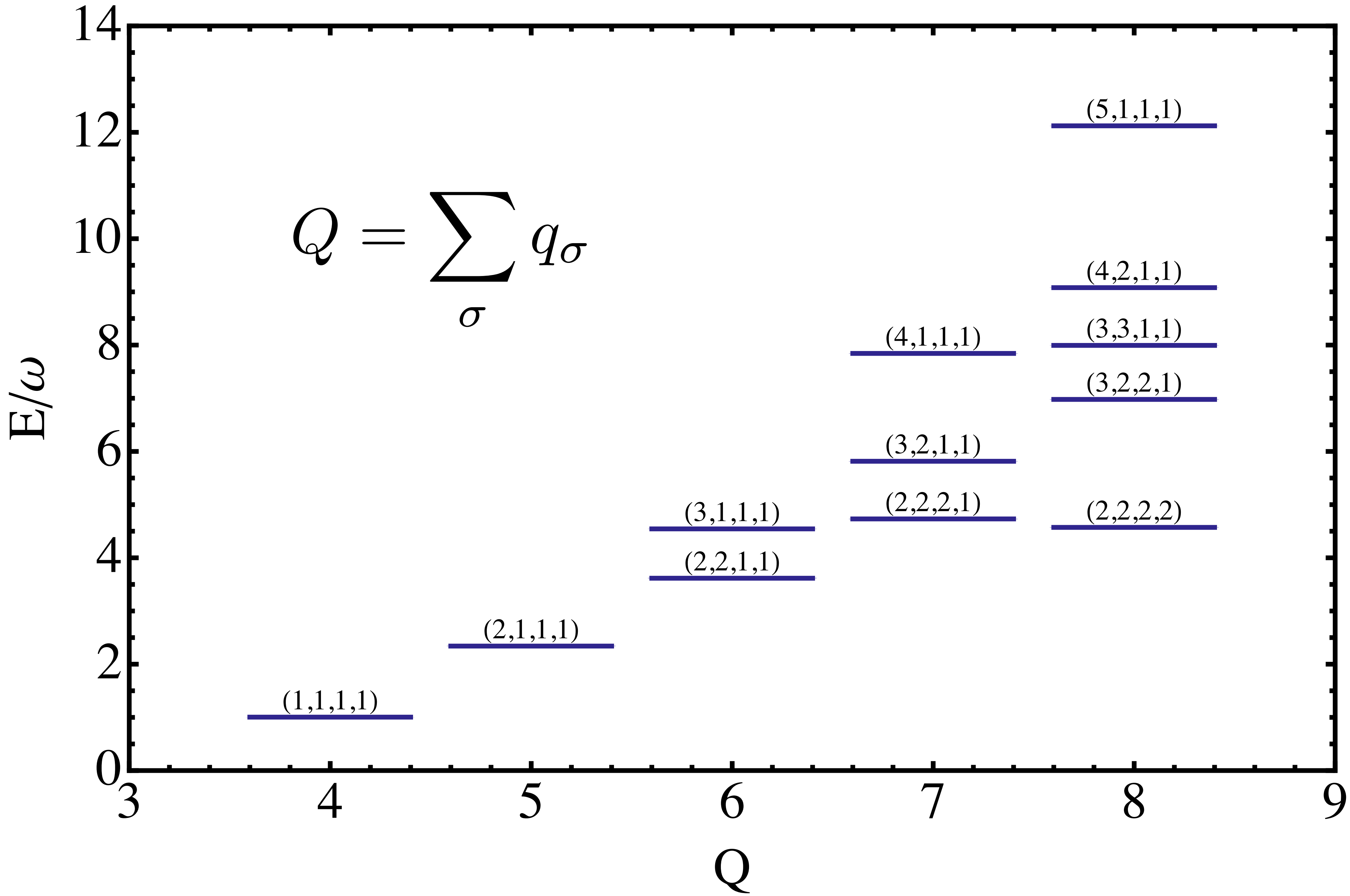



# Seven-body system(s) (trapped)

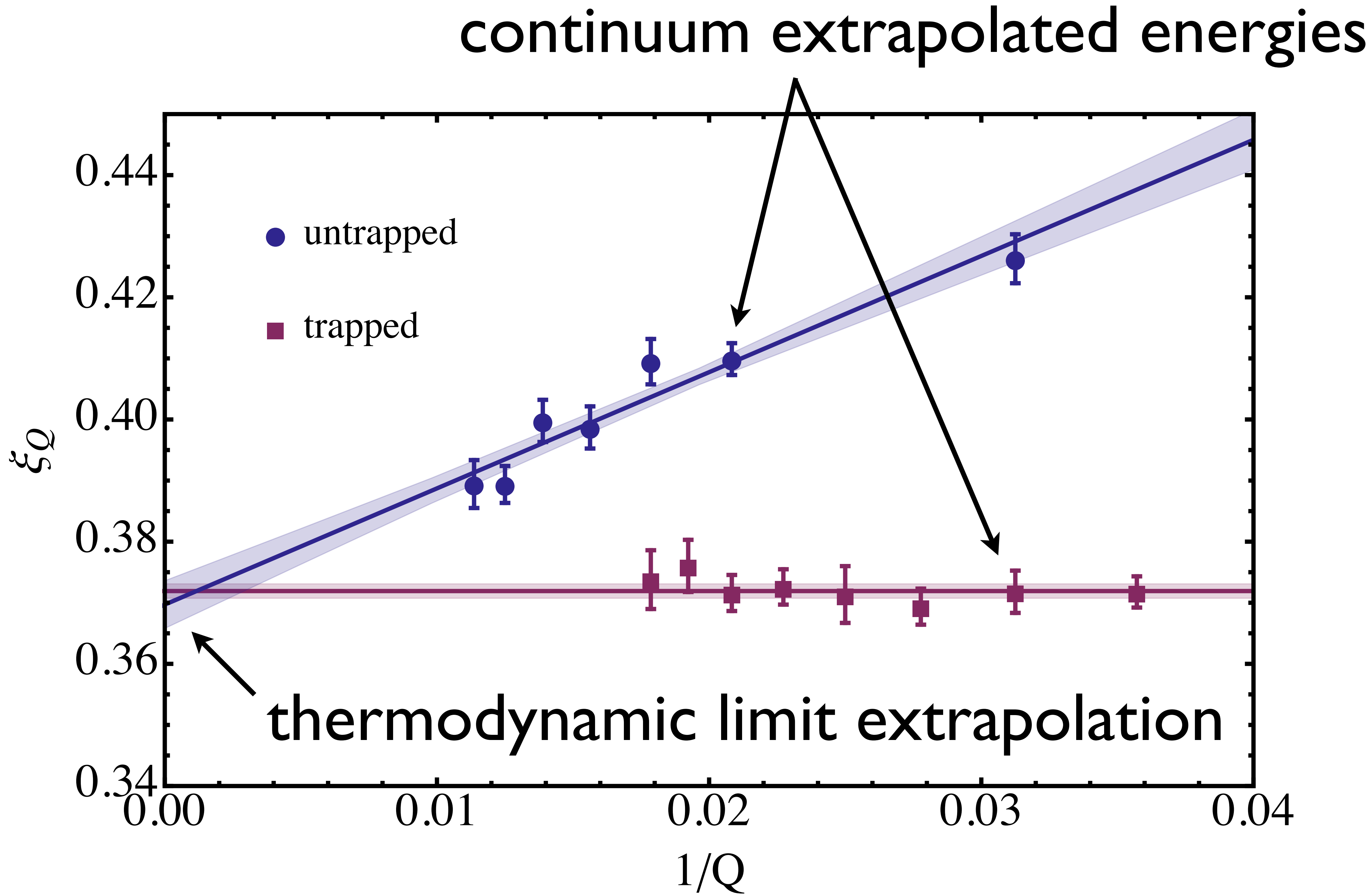


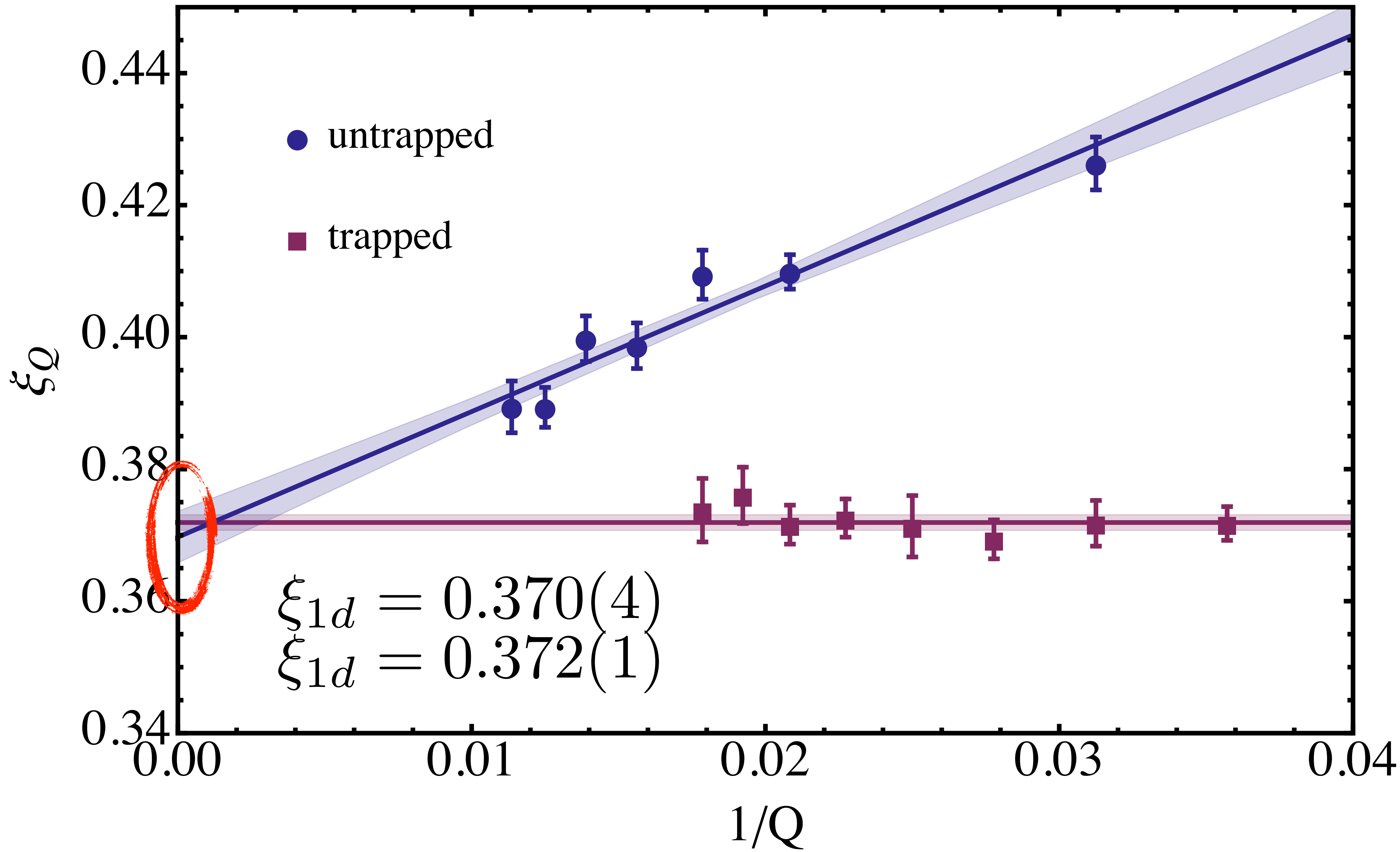
# Few-body summary (≤8 trapped fermions)



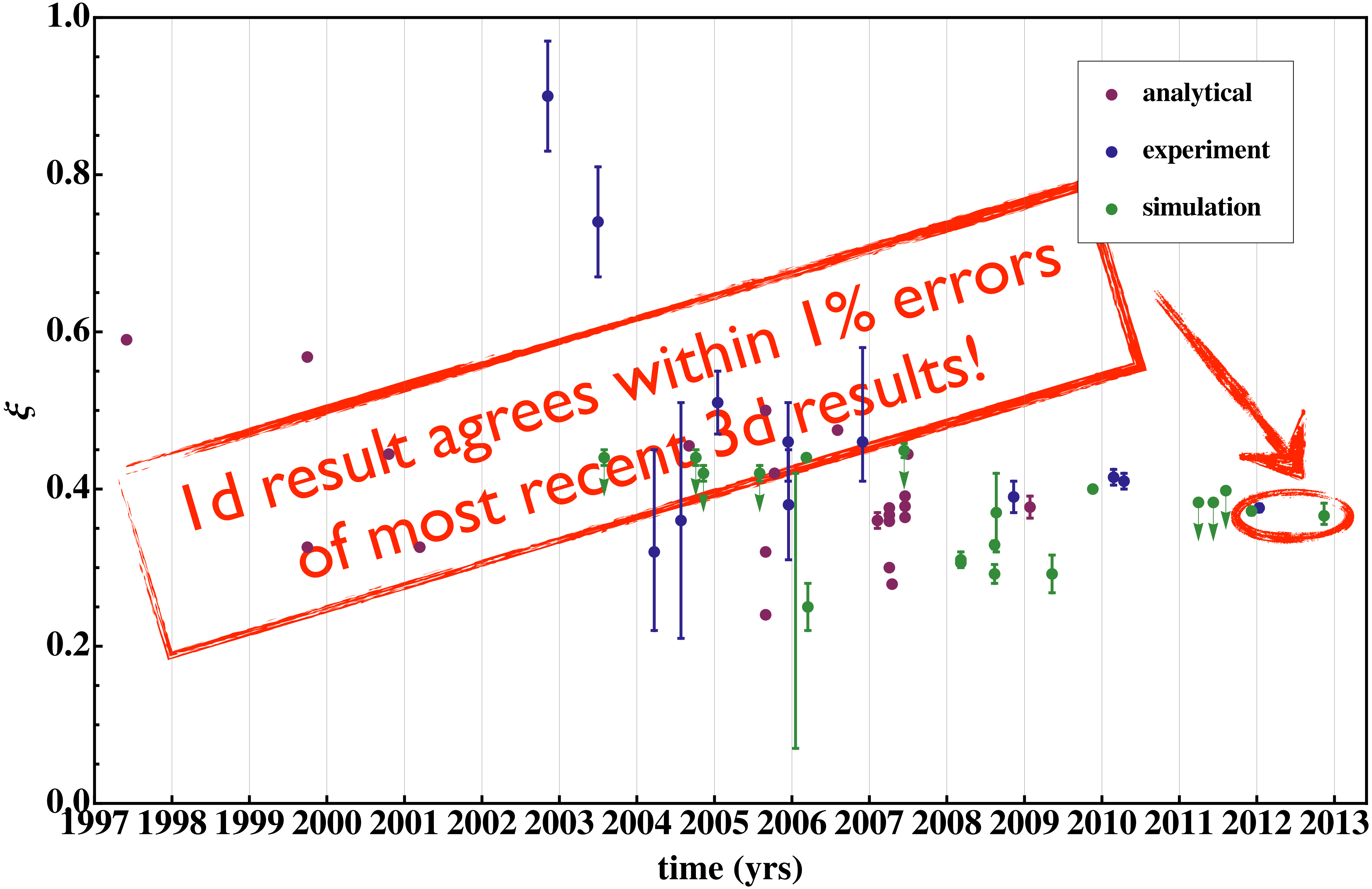
# Many-body systems (untrapped & trapped)



# Many-body systems (untrapped & trapped)



# 3d Bertsch parameter



# Summary/Outlook

# Summary

- Despite their simplicity, universal Fermi gases exhibit rich and fascinating physics!
- Found a solution to the "sign problem" for 1d system
- Simulated a universal four-component Fermi gas in one spatial dimension
  - few-body energies in a trap agree with exact results
  - demonstrated restoration of virial theorem
  - 1d & 3d Bertsch parameters are equal to within 1% errors

# Outlook/Future plans

- Theoretical understanding of Bertsch equality
  - dynamical in origin?
  - due to symmetries (conformal, scale invariance)?
- Continue few/many body simulations:
  - “integrated contact density”
  - imbalanced few- and many-body systems

Thank you!