# Harmonically trapped unitary few-body systems at finite temperature

Yangqian Yan and D. Blume

See:

Y. Yan and D. Blume, PRA **88**, 023616 (2013)
Y. Yan and D. Blume, arXiv: 1312.4470 (2013)
Y. Yan and D. Blume, in preparation (2014)

# Outline

- Introduction
  - Motivation
  - Systems considered
- Finite-temperature method:
  - Path integral Monte Carlo
- Results:
  - Two-component Fermi gas
  - Single-component Bose gas

# Motivation
## Finite systems at finite temperature

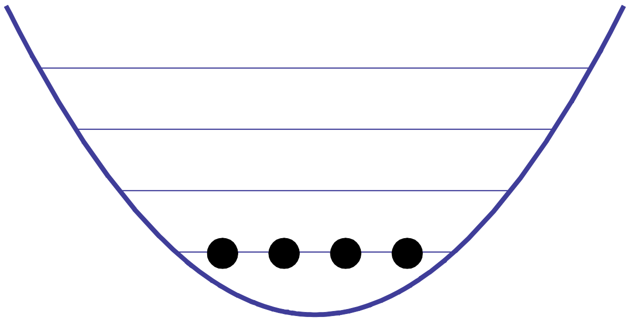
- Quantum dots
- Nuclei

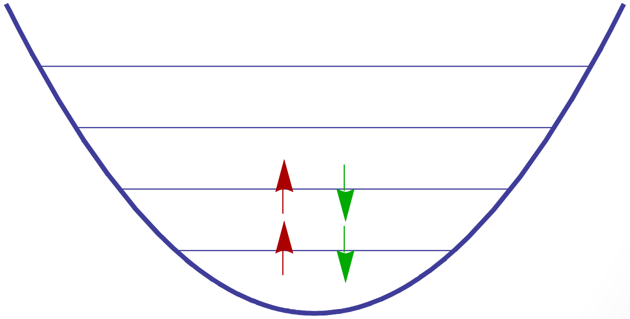
- Cold atom experiments:
  - Selim Jochim’s group: Effectively one-dimensional Fermi gas consisting of 2, 3, 4,… fermions at low T.
  - Deterministic number of particles per optical lattice site.
  - Large Bose/Fermi gases: Loss measurements.

- Treatment of few-body systems is “exact” and “easier” than that of many-body system.

# Systems considered

- N particles with equal mass in a spherically symmetric trap.
  - N small; N fixed.

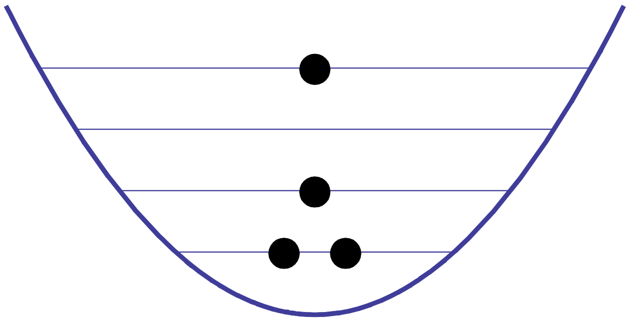


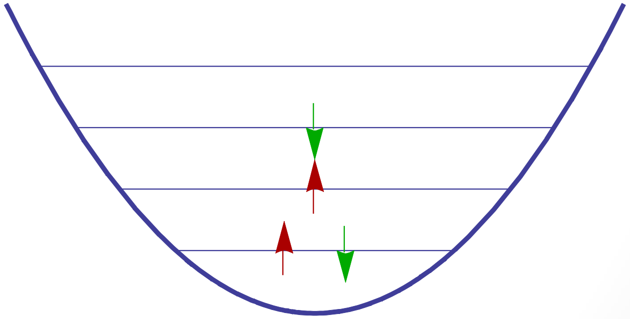


- Finite temperature?
- Effect of interactions?
- Particle statistics?

# Systems considered

- N particles with equal mass in a spherically symmetric trap.
    - N small; N fixed.

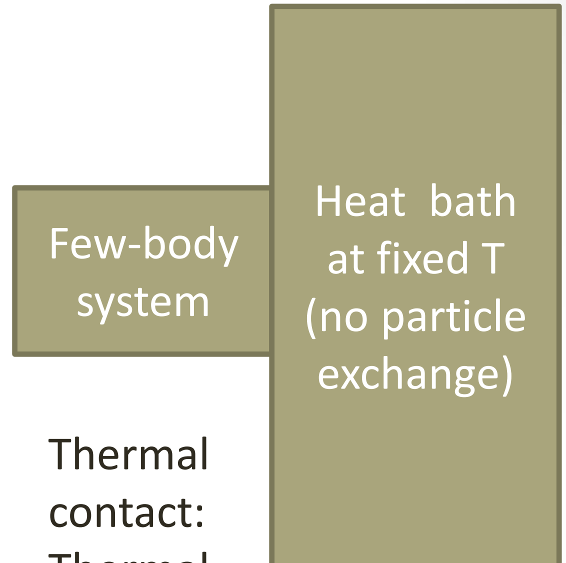




- Finite temperature?
- Effect of interactions?
- Particle statistics?

# Temperature of finite-sized system

- Canonical ensemble:
  - Fixed number of particles N
  - Fixed temperature T
  - Fixed harmonic trapping frequency $\omega$




Thermal contact: Thermal equilibrium

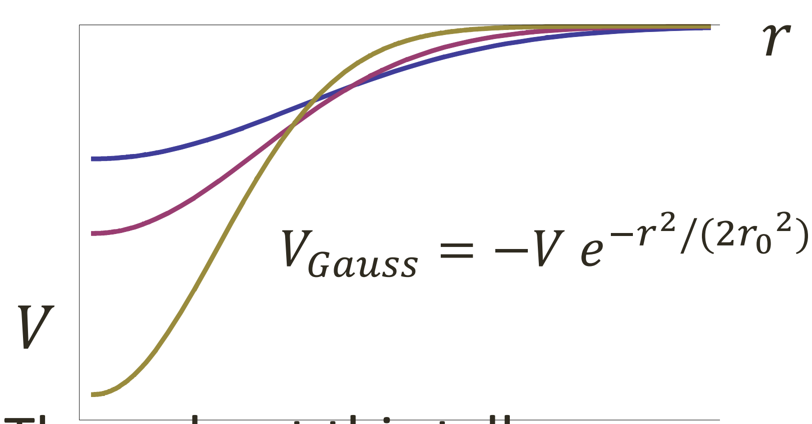
- Partition function: $$Z = \sum_j e^{-\beta E_j}$$

- Temperature region of interest:

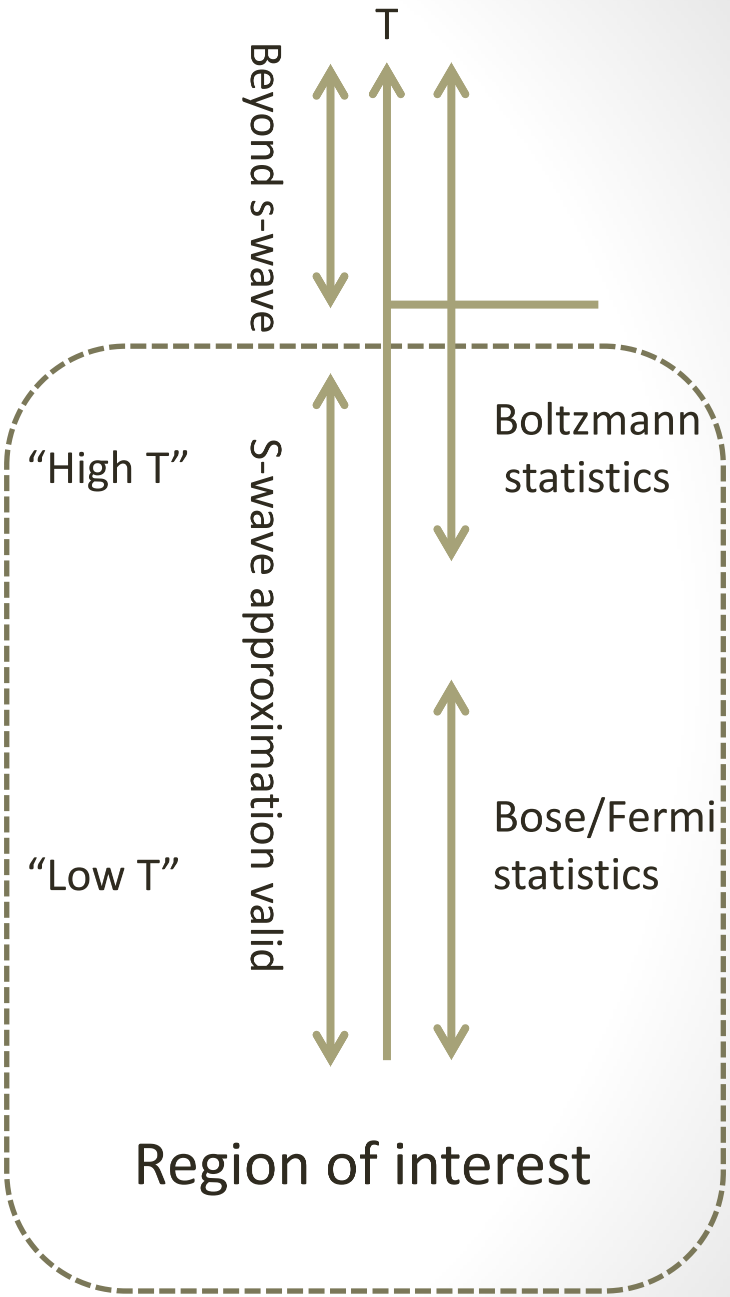
  $T < T_F$ and $T > T_F$

# Model interaction

- Short-range potential with tunable scattering length:
  - Gaussian potential (smeared out delta-function)
  - Range of interaction $r_0 \approx 0.06 a_{ho}$

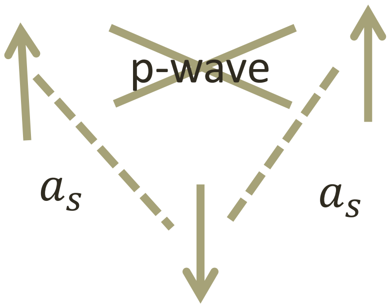



- Throughout this talk: $|a_s| = \infty$ (at unitarity)



# Statistics

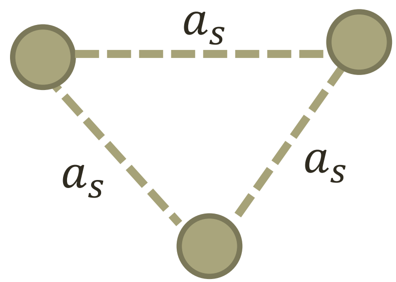
Fermions




Fully determined by $a_s$. $a_{ho}$ is the only length scale.

Here: We do not consider spin flips. Denoted as (2, 1) system.

Bosons




Determined by $a_s$ and three-body parameter $\kappa_*$.
Length scales: $a_{ho}, 1/\kappa_*$.

Here: finite-range of two-body potential serves as a regulator and determines $\kappa_*$.

# How to treat finite N system at finite T?

- Use numerical technique: Path integral Monte Carlo (can treat bosons and fermions (?); for bosons, any N).
- All thermodynamic properties can be calculated from

the density matrix: $\hat{\rho} = e^{-\beta \hat{H}}$

Inverse temperature: $\beta = \frac{1}{k_B T}$

Project to position basis: $\rho(\mathbf{R}, \mathbf{R}', \beta) = \langle \mathbf{R} \,|\, \hat{\rho} \,|\, \mathbf{R}' \rangle$

Partition function: $Z = \int \mathrm{d}\mathbf{R} \rho(\mathbf{R}, \mathbf{R}, \beta)$

Observables: $\langle \hat{\mathcal{O}} \rangle = Z^{-1} \int \mathrm{d}\mathbf{R}\mathrm{d}\mathbf{R}' \rho(\mathbf{R}, \mathbf{R}', \beta) \langle \mathbf{R}' | \hat{\mathcal{O}} | \mathbf{R} \rangle$

# How to get the density matrix?

"Hard": Low T $\beta = \frac{1}{k_B T}$

"Trick": $\langle x_0 | e^{-\beta H} | x_0 \rangle \rightarrow$

$$\left\langle x_0 \middle| e^{-\frac{\beta}{M}H} \middle| x_1 \right\rangle \dots \left\langle x_{M-1} \middle| e^{-\frac{\beta}{M}H} \middle| x_0 \right\rangle$$

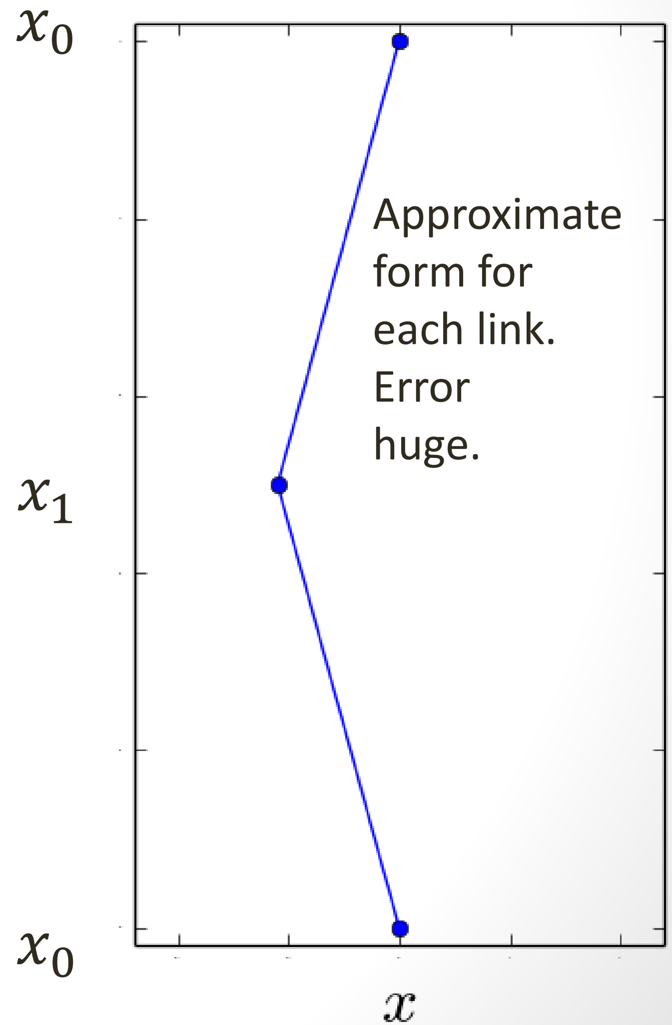
"Easy": High T

"Easy": High T

$$\frac{\beta}{M} = \frac{1}{M\, k_B T}$$

"Hard": Needs to be done M times

M=2



# How to get the density matrix?

"Hard": Low T $\qquad \beta = \frac{1}{k_B T}$

"Trick": $\langle x_0 | e^{-\beta H} | x_0 \rangle \rightarrow$

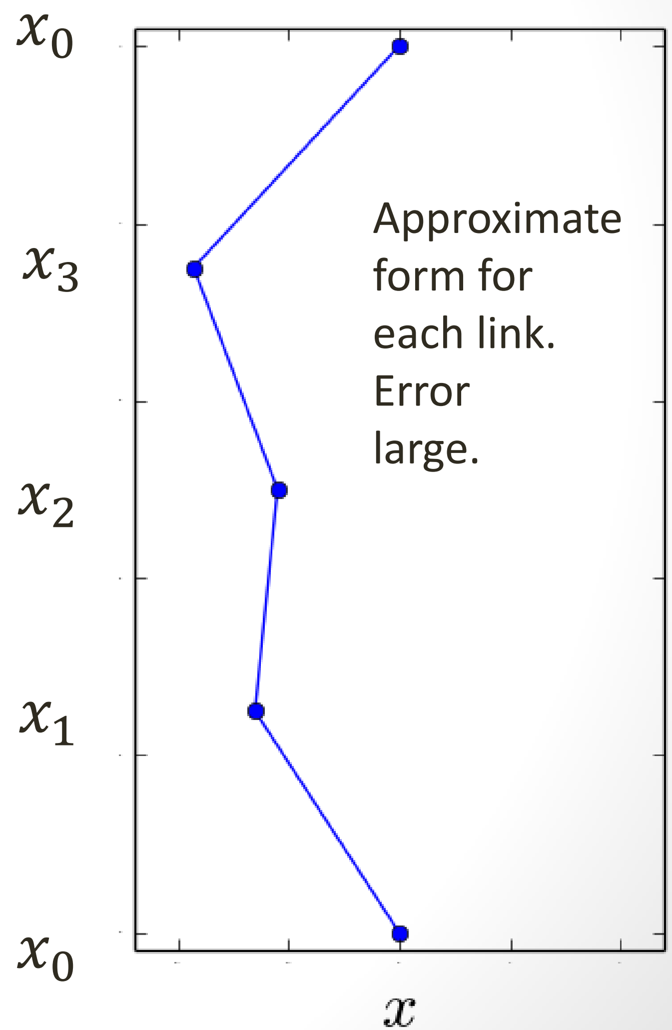
$$\left\langle x_0 \middle| e^{-\frac{\beta}{M} H} \middle| x_1 \right\rangle \ldots \left\langle x_{M-1} \middle| e^{-\frac{\beta}{M} H} \middle| x_0 \right\rangle$$

"Easy": High T $\qquad$ "Easy": High T

$$\frac{\beta}{M} = \frac{1}{M\, k_B T}$$

"Hard": Needs to be done M times

M=4



# How to get the density matrix?

"Hard": Low T $\quad \beta = \frac{1}{k_B T}$

"Trick": $\langle x_0 | e^{-\beta H} | x_0 \rangle \rightarrow$

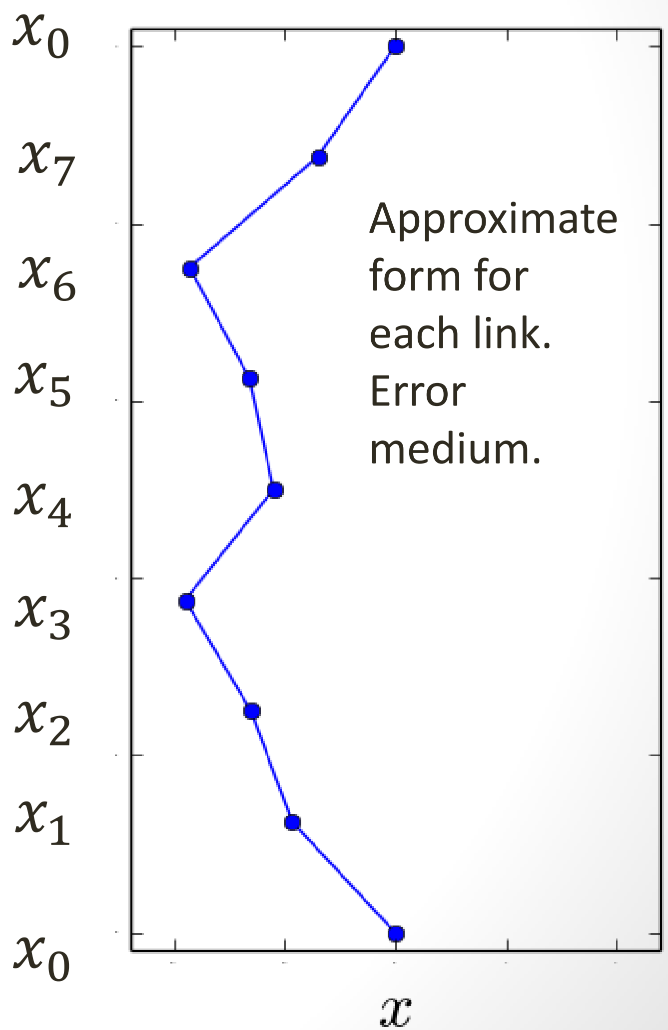
$$\left\langle x_0 \middle| e^{-\frac{\beta}{M}H} \middle| x_1 \right\rangle \ldots \left\langle x_{M-1} \middle| e^{-\frac{\beta}{M}H} \middle| x_0 \right\rangle$$

"Easy": High T $\qquad$ "Easy": High T

$$\frac{\beta}{M} = \frac{1}{M\, k_B T}$$

"Hard": Needs to be done M times

M=8



# How to get the density matrix?

“Hard”: Low T $\beta = \frac{1}{k_B T}$

“Trick”: $\langle x_0 | e^{-\beta H} | x_0 \rangle \rightarrow$

$$\left\langle x_0 \middle| e^{-\frac{\beta}{M}H} \middle| x_1 \right\rangle \ldots \left\langle x_{M-1} \middle| e^{-\frac{\beta}{M}H} \middle| x_0 \right\rangle$$

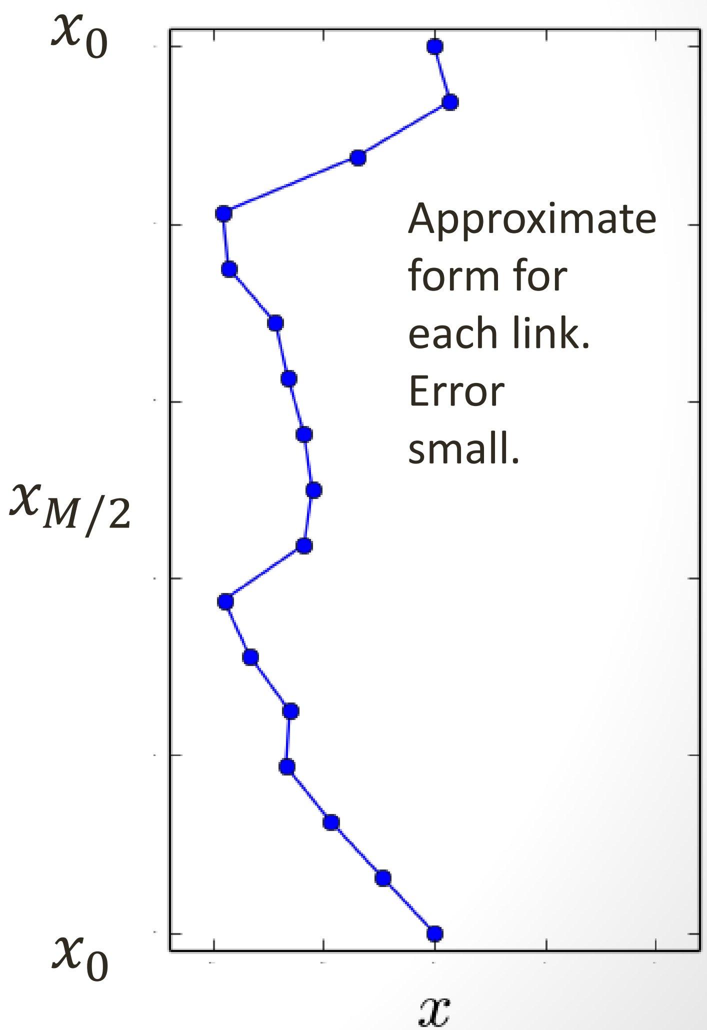
“Easy”: High T

“Easy”: High T

$$\frac{\beta}{M} = \frac{1}{M\, k_B T}$$

“Hard”: Needs to be done M times

M=16



# How to get the density matrix?

"Hard": Low T $\beta = \frac{1}{k_B T}$

"Trick": $\langle x_0 | e^{-\beta H} | x_0 \rangle \rightarrow$

$$\left\langle x_0 \middle| e^{-\frac{\beta}{M}H} \middle| x_1 \right\rangle \ldots \left\langle x_{M-1} \middle| e^{-\frac{\beta}{M}H} \middle| x_0 \right\rangle$$

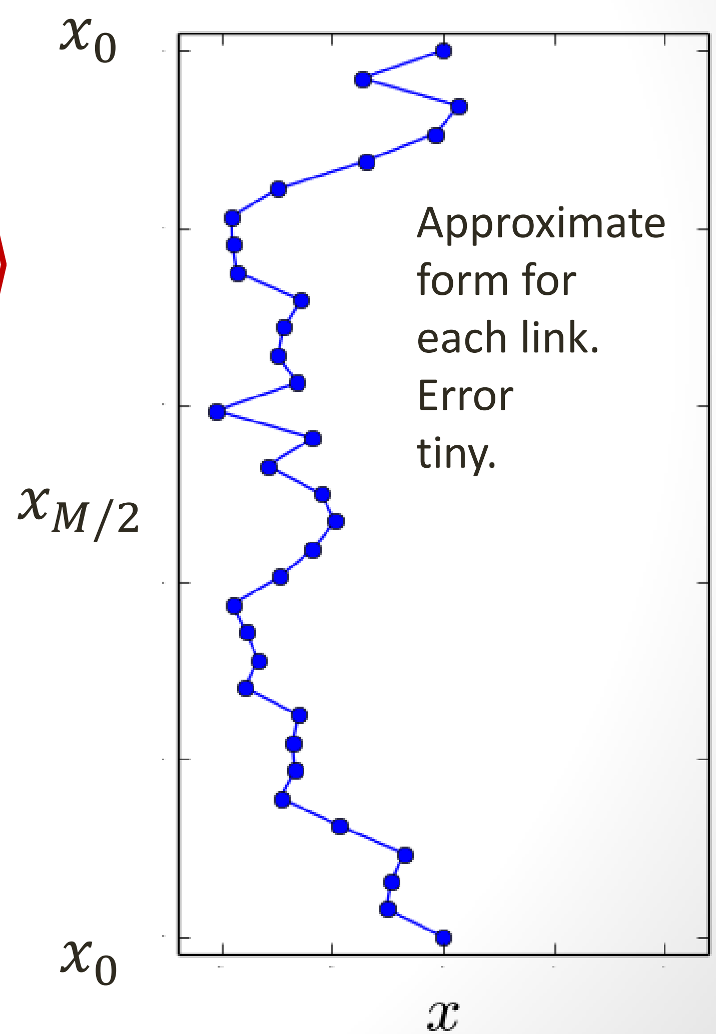
"Easy": High T

"Easy": High T

$$\frac{\beta}{M} = \frac{1}{M\,k_B T}$$

"Hard": Needs to be done M times

M=32




Approximate form for each link. Error tiny.

# How to get the density matrix?

M=32

"Hard": Low T $\beta = \frac{1}{k_B T}$

"Trick": $\langle x_0 | e^{-\beta H} | x_0 \rangle \rightarrow$

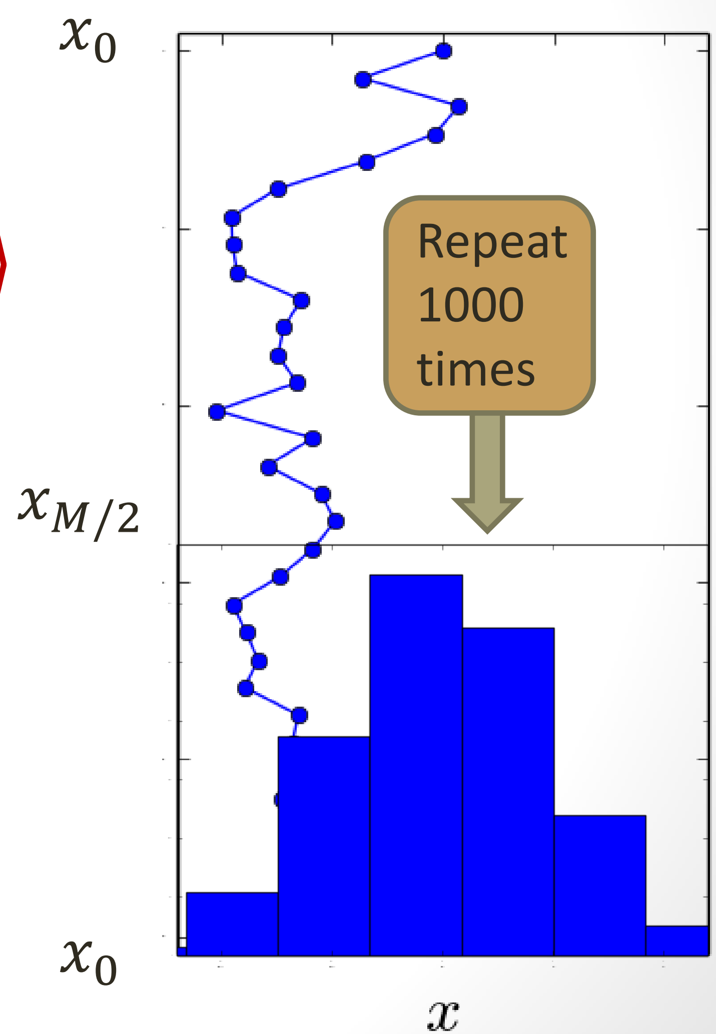
$$\left\langle x_0 \middle| e^{-\frac{\beta}{M}H} \middle| x_1 \right\rangle \ldots \left\langle x_{M-1} \middle| e^{-\frac{\beta}{M}H} \middle| x_0 \right\rangle$$

"Easy": High T

"Easy": High T

$$\frac{\beta}{M} = \frac{1}{M\, k_B T}$$

"Hard": Needs to be done M times



# Particle symmetry

$\hat{\rho}$ -> $\hat{\rho}\mathcal{P}$

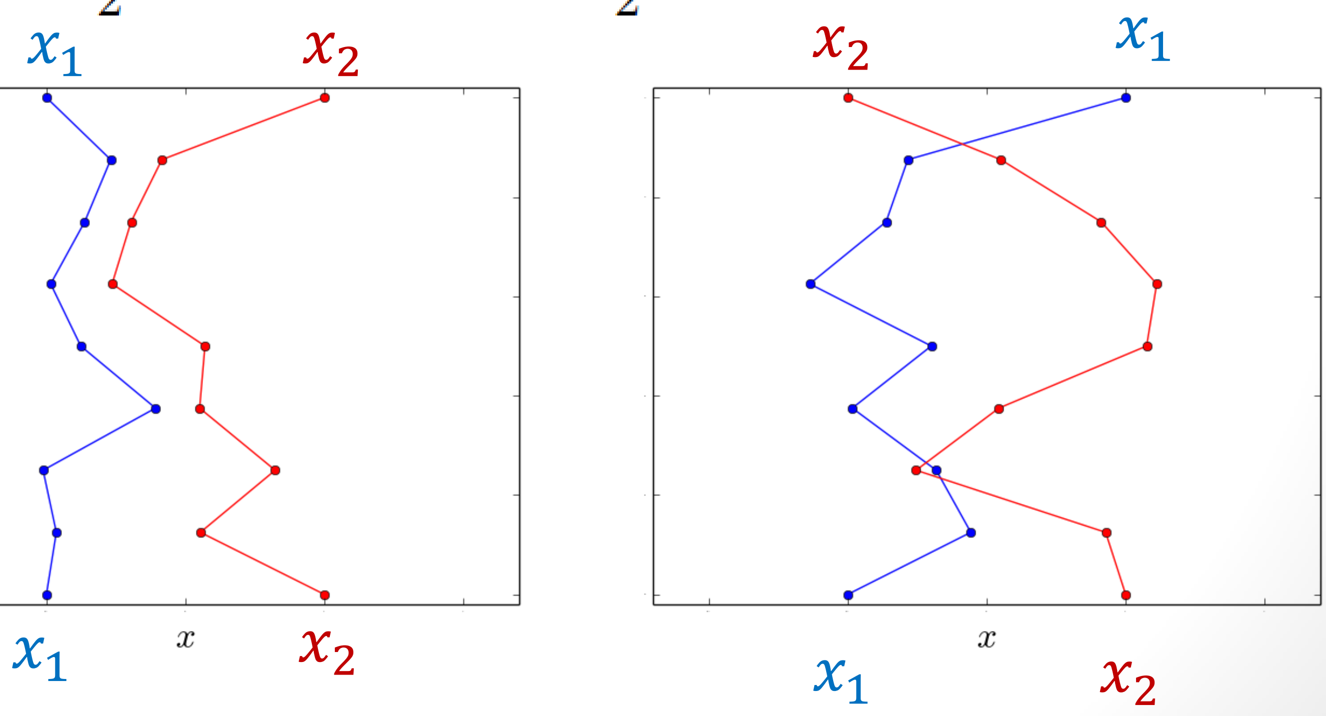
$$Z = \int \mathrm{d}\mathbf{R}\rho(\mathcal{P}\mathbf{R}, \mathbf{R}, \beta)$$

+: bosons

−: fermions

Example: For two particles $\mathcal{P} = \frac{1}{2}\hat{1} \pm \frac{1}{2}\hat{P_{21}}$

$$\frac{1}{2}\rho(x_1, x_2; x_1, x_2; \beta) \pm \frac{1}{2}\rho(x_2, x_1; x_1, x_2; \beta)$$

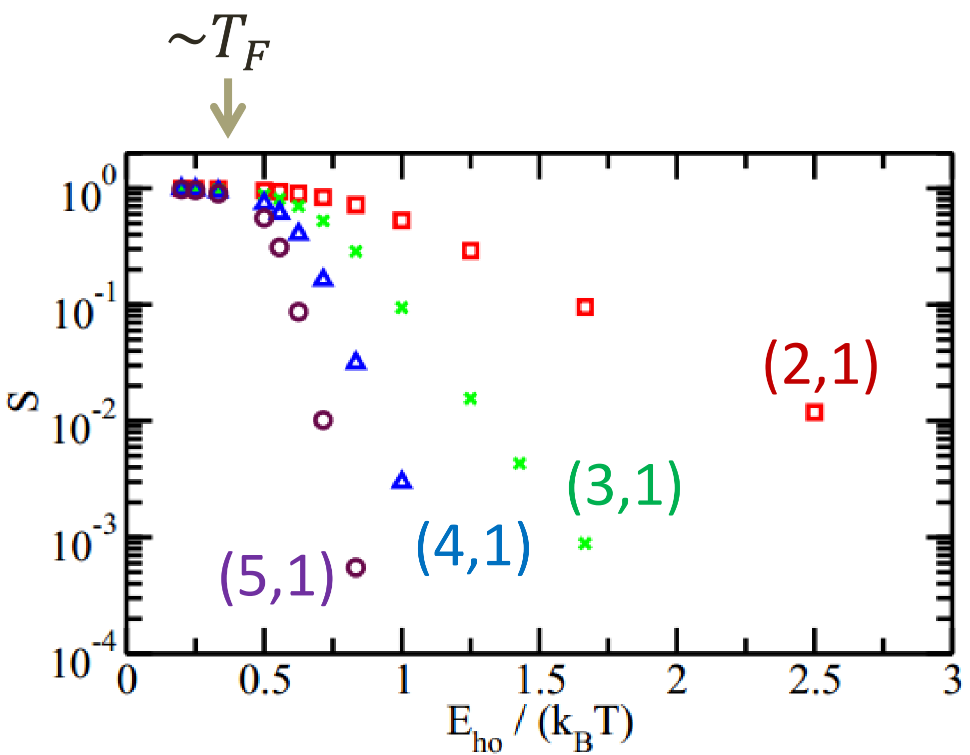


# Monte Carlo and the Fermi sign problem

- No exchanges at high T.
- Exchanges give positive and negative contributions and add up to a small number. Signal to noise ratio decreases.

$$S \sim \frac{\text{Signal}}{\text{Noise}}$$

Small S:
Poor signal for fermions.
Bose/Fermi statistics important.



# Contact of two-component Fermi gas

Why contact? S. Tan, Ann. Phys. (2008)

- Proven to be fundamental (valid at zero and finite T).
- T dependence unknown for trapped few-body system (N>2).
- Relates physically distinct observables:
  - Short-range behavior of pair distribution function:

$$C_{N_1,N_2} = 4\pi \lim_{s\to 0} \frac{\langle N_{\text{pair}}^{r<s} \rangle_{\text{th}}}{s}$$

  - Slope of eigen energy/free energy: $C_{N_1,N_2} = \frac{4\pi m}{\hbar^2} \left\langle \frac{\partial E(a_s)}{\partial\left(-a_s^{-1}\right)} \right\rangle_{\text{th}}$
  - Tail of momentum distribution, tail of radio-frequency spectrum, etc…

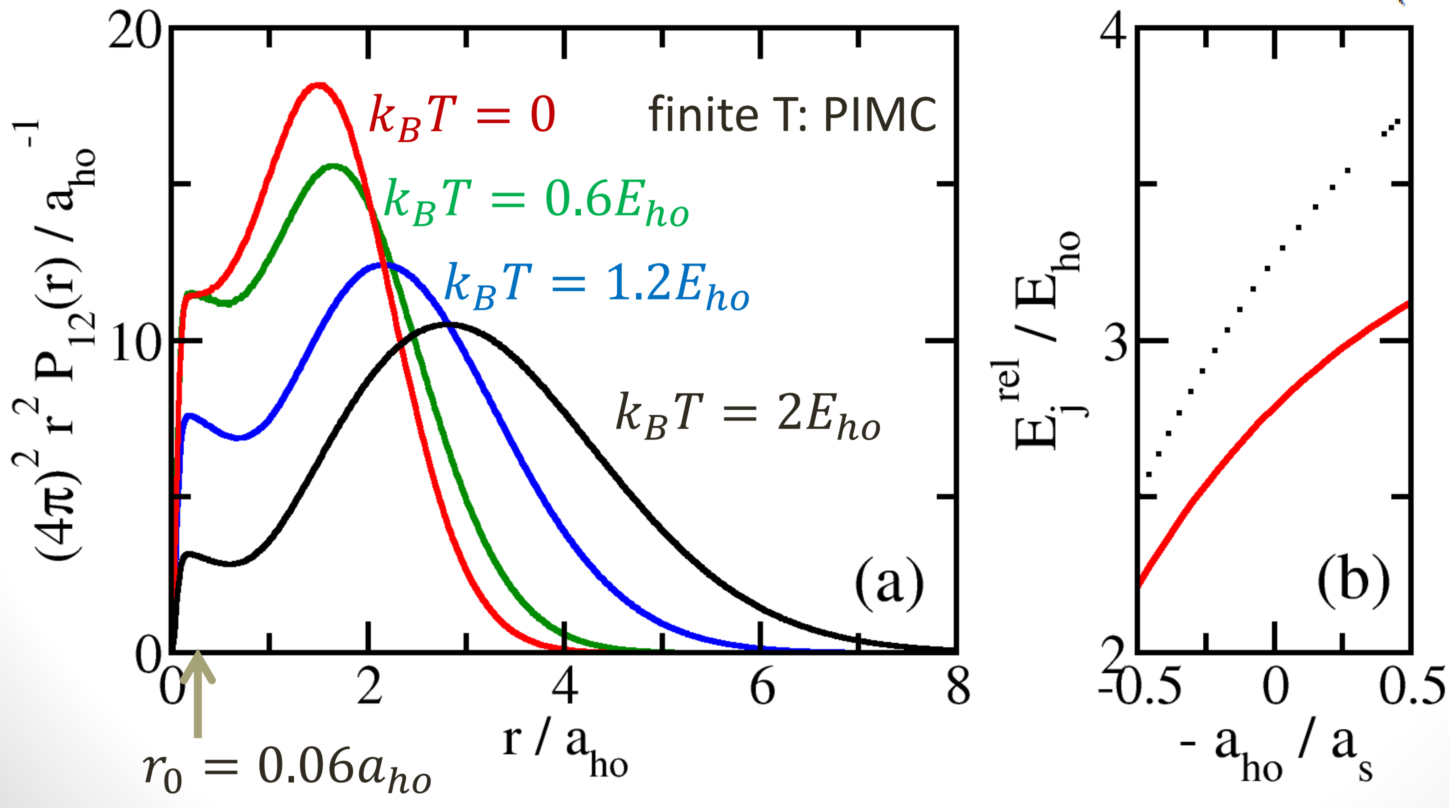
# Contact of (3,1) & (2,1) Fermi gases: $r_0 = 0.06\, a_{ho}$

Pair relation

$$C_{N_1,N_2} = 4\pi \lim_{s\to 0} \frac{\langle N_{\text{pair}}^{r<s}\rangle_{\text{th}}}{s}$$

Adiabatic relation

$$C_{N_1,N_2} = \frac{4\pi m}{\hbar^2}\left\langle \frac{\partial E(a_s)}{\partial(-a_s^{-1})}\right\rangle_{\text{th}}$$

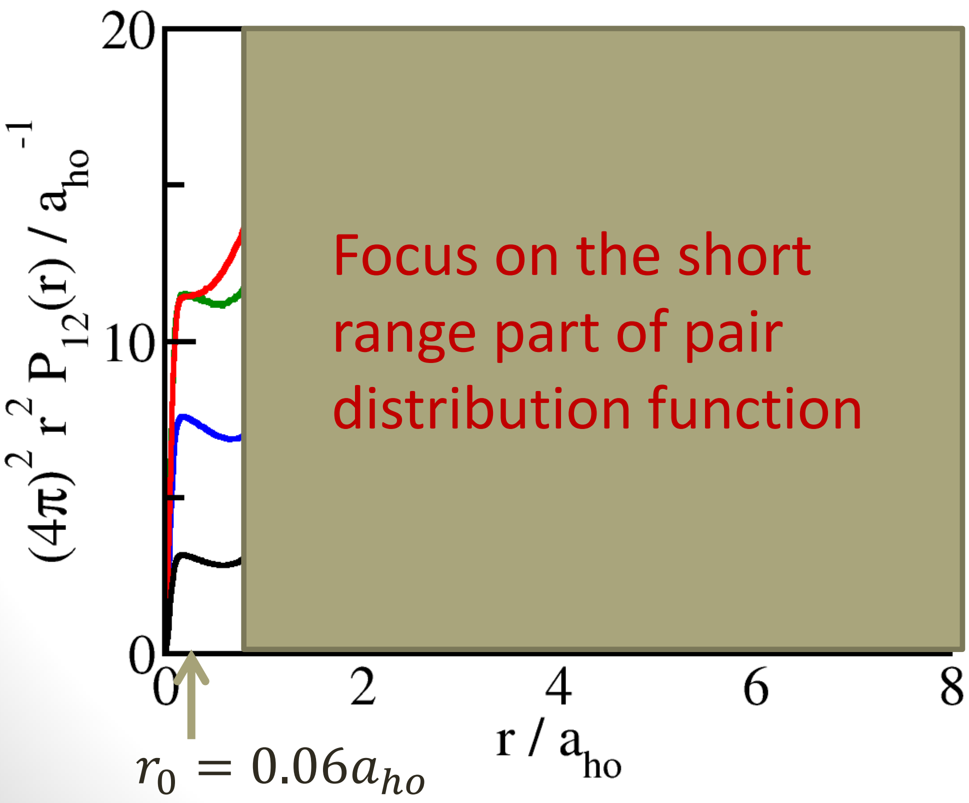



Correlated Gaussian for zero T.

# Contact of (3,1) & (2,1) Fermi gases: $r_0 = 0.06\, a_{ho}$

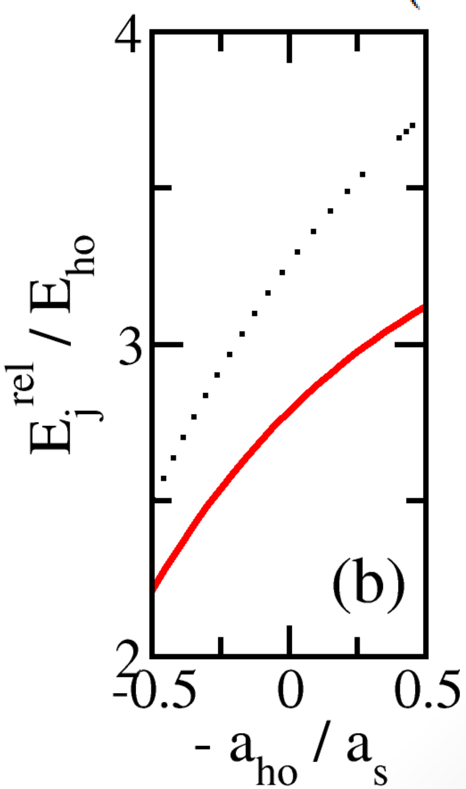
Pair relation

$$C_{N_1,N_2} = 4\pi \lim_{s\to 0} \frac{\langle N_{\text{pair}}^{r<s}\rangle_{\text{th}}}{s}$$




Adiabatic relation

$$C_{N_1,N_2} = \frac{4\pi m}{\hbar^2}\left\langle \frac{\partial E(a_s)}{\partial(-a_s^{-1})}\right\rangle_{\text{th}}$$




Correlated Gaussian for zero T.

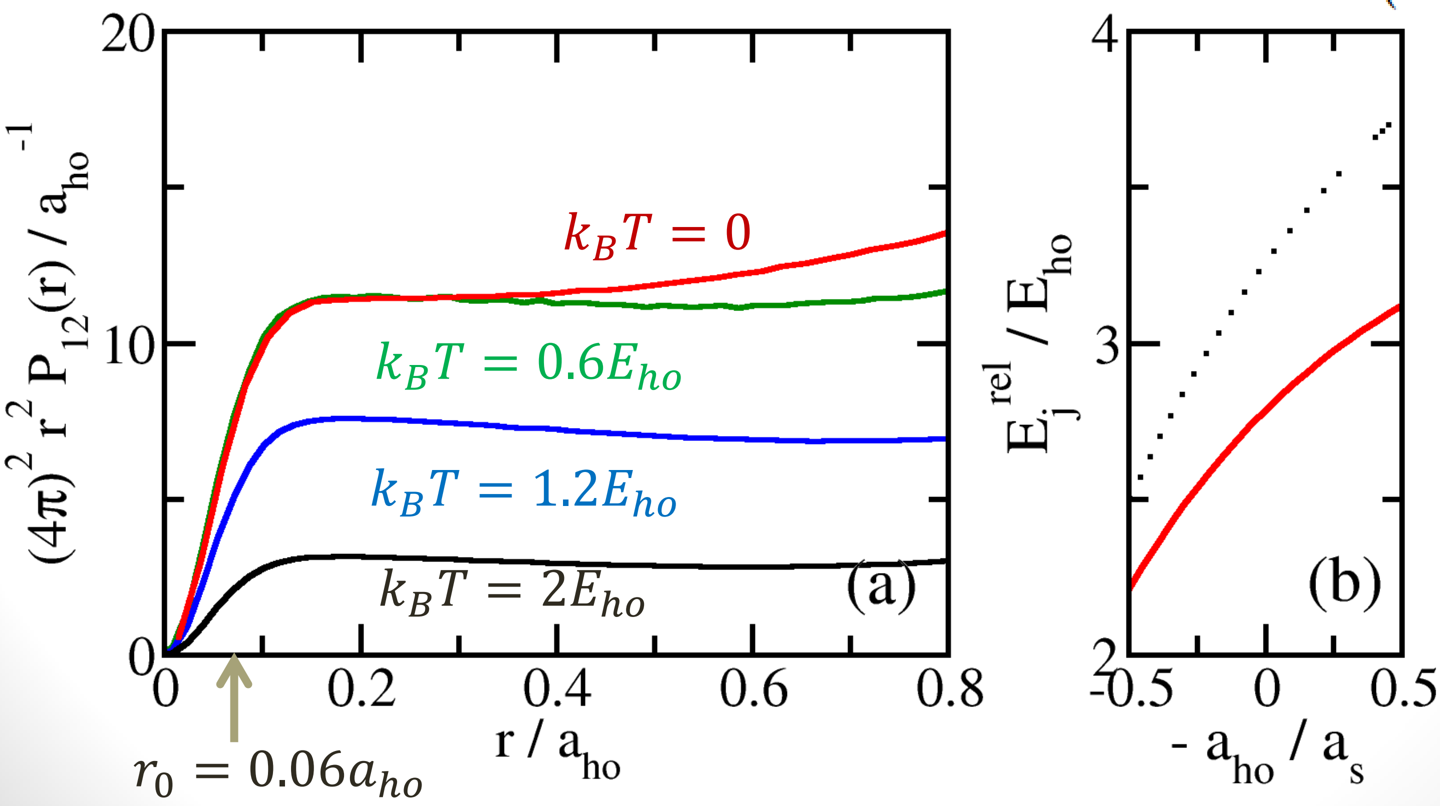
# Contact of (3,1) & (2,1) Fermi gases: $r_0 = 0.06\, a_{ho}$

Pair relation

$$C_{N_1,N_2} = 4\pi \lim_{s\to 0} \frac{\langle N_{\text{pair}}^{r<s}\rangle_{\text{th}}}{s}$$

Adiabatic relation

$$C_{N_1,N_2} = \frac{4\pi m}{\hbar^2}\left\langle \frac{\partial E(a_s)}{\partial(-a_s^{-1})}\right\rangle_{\text{th}}$$



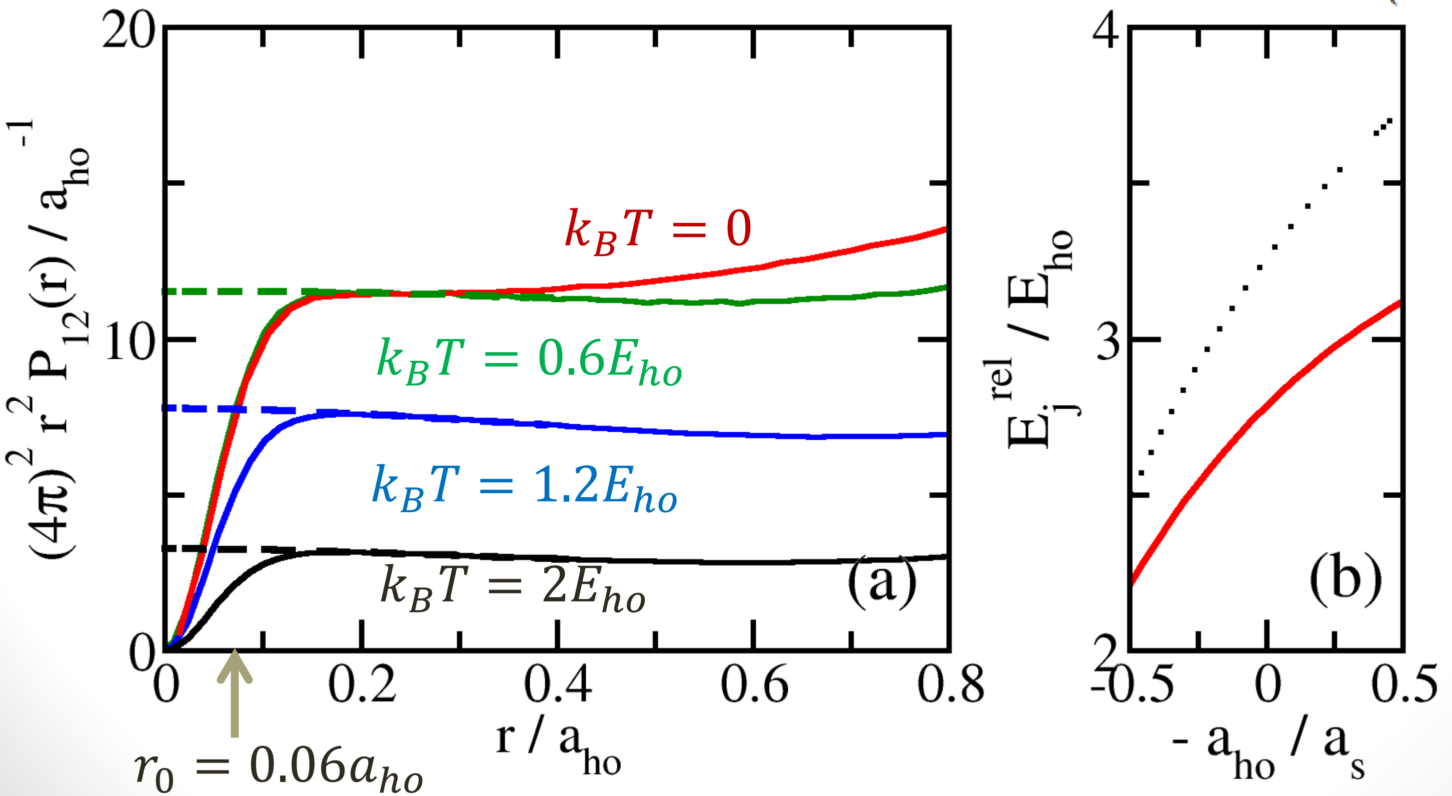
# Contact of (3,1) & (2,1) Fermi gases: $r_0 = 0.06\, a_{ho}$

Pair relation

$$C_{N_1,N_2} = 4\pi \lim_{s\to 0} \frac{\langle N_{\text{pair}}^{r<s} \rangle_{\text{th}}}{s}$$

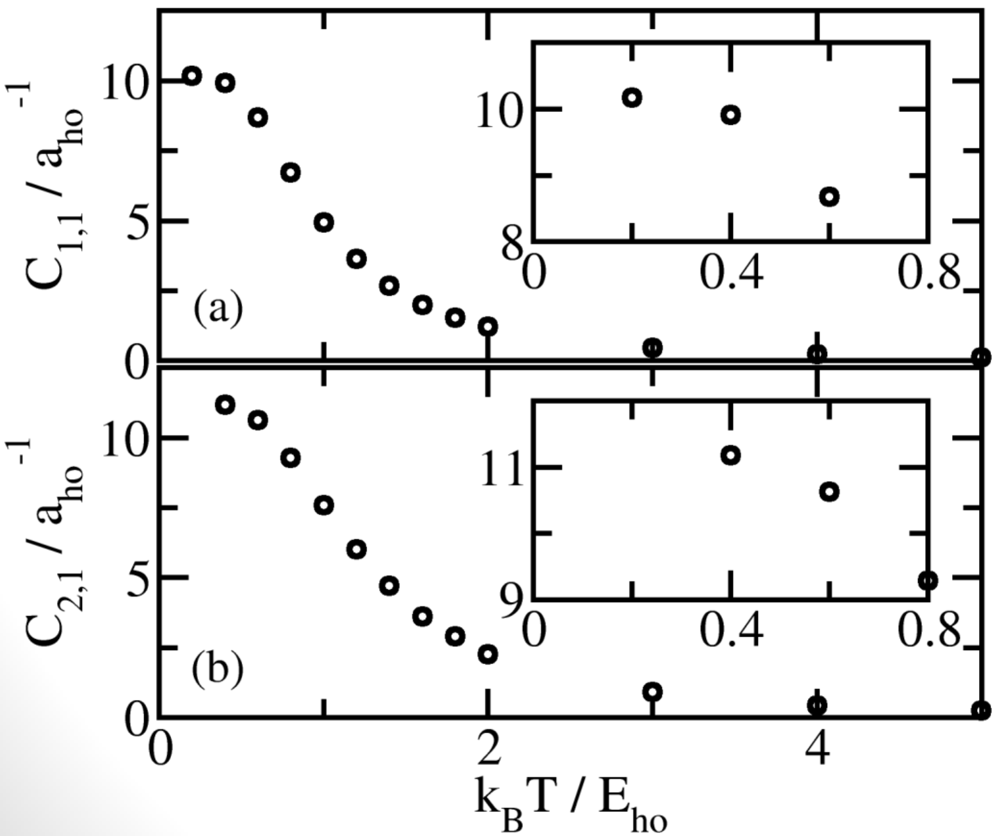
Adiabatic relation

$$C_{N_1,N_2} = \frac{4\pi m}{\hbar^2} \left\langle \frac{\partial E(a_s)}{\partial(-a_s^{-1})} \right\rangle_{\text{th}}$$



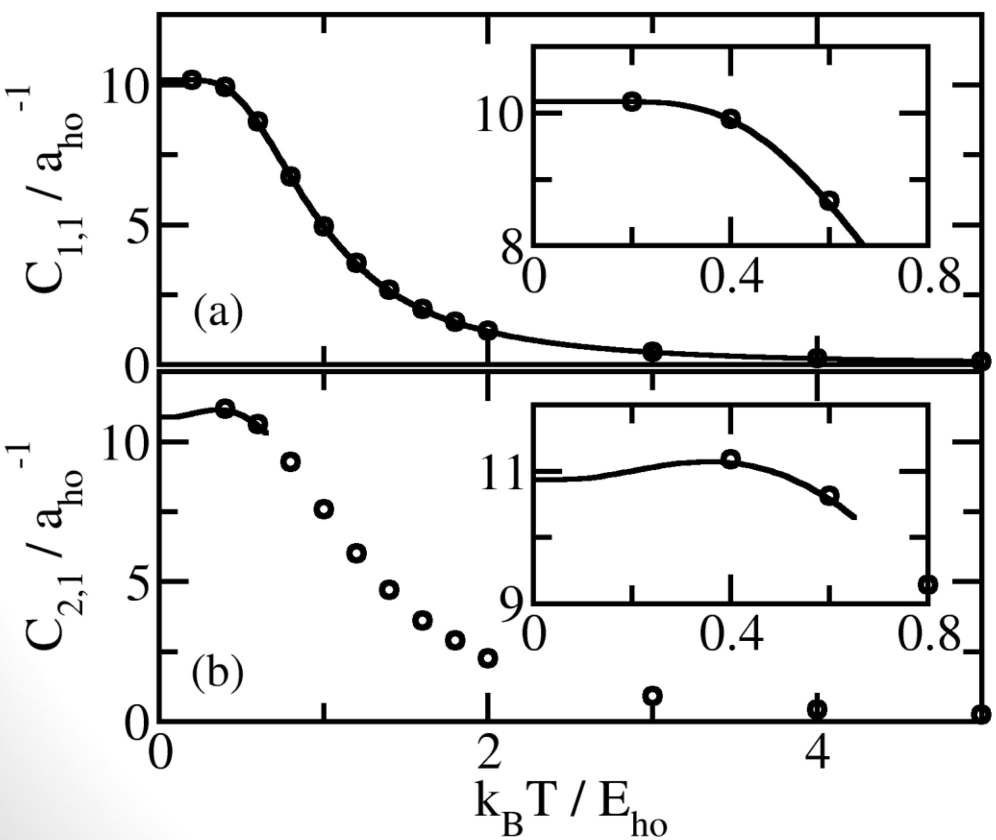
# Contact of (1,1) & (2,1) systems

- Symbols: PIMC data for $r_0 = 0.06a_{ho}$



# Contact of (1,1) & (2,1) systems

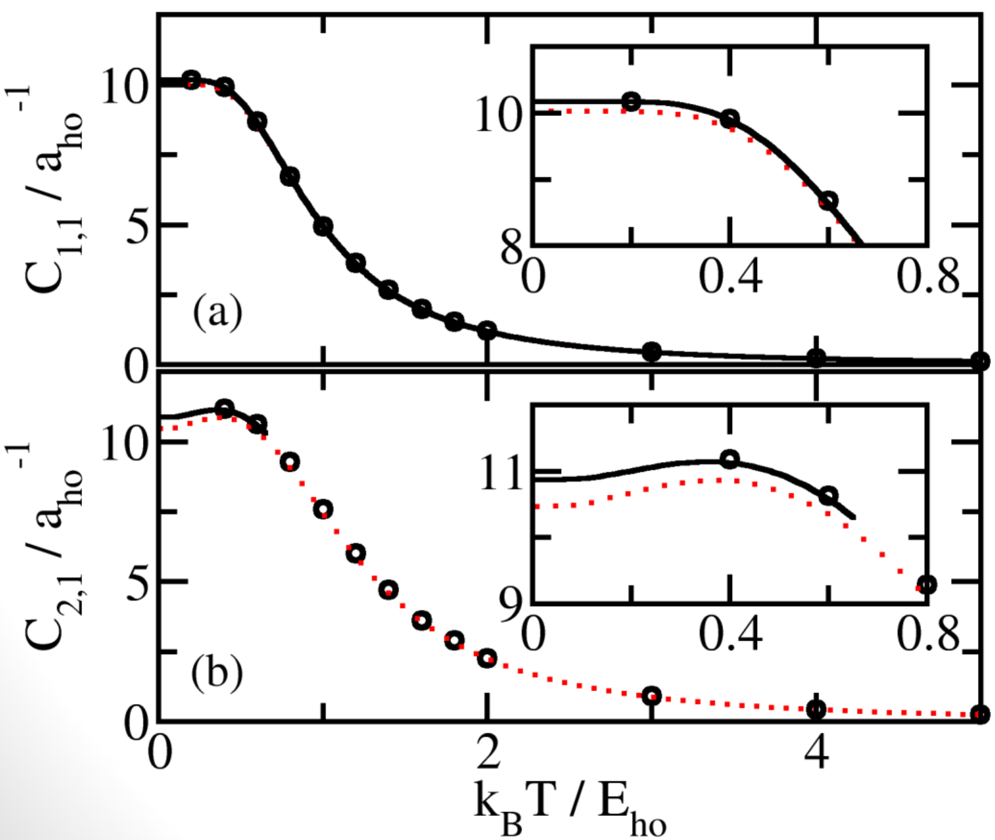
Non monotonic at low T for (2,1) system.




- Symbols: PIMC data for $r_0 = 0.06a_{ho}$
- Solid lines: B-spline & CG for the same range

# Contact of (1,1) & (2,1) systems

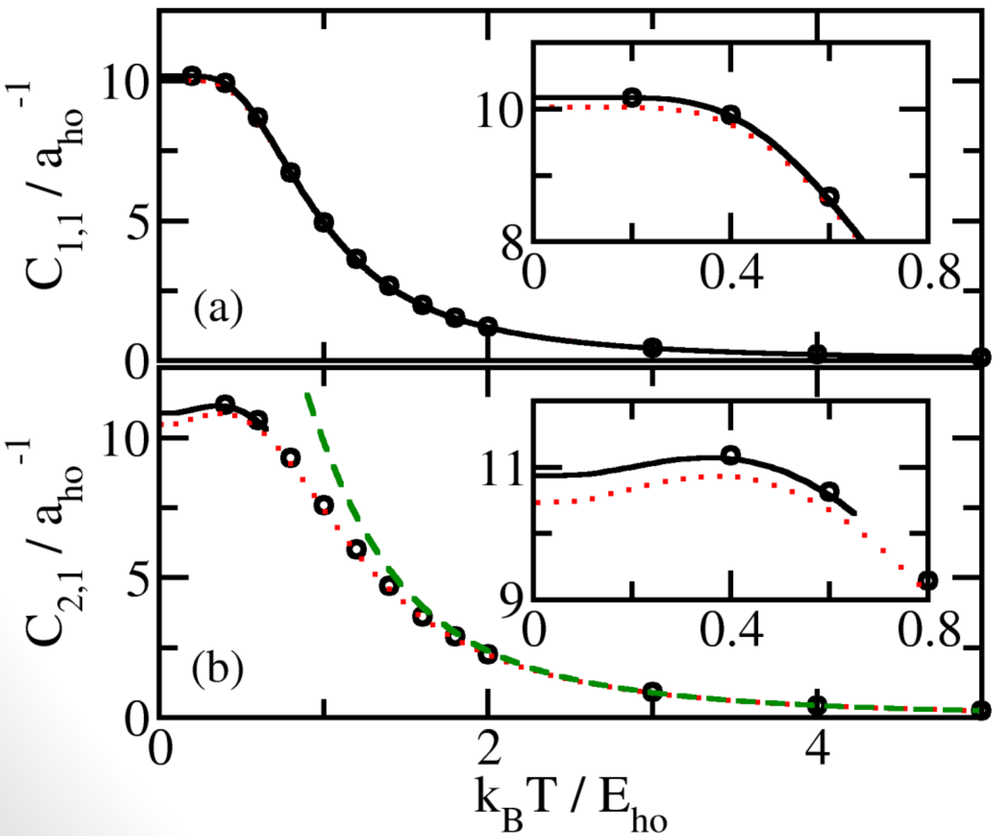
Non monotonic at low T for (2,1) system.
Range of interaction effect is small.




- Symbols: PIMC data for $r_0 = 0.06a_{ho}$
- Solid lines: B-spline & CG for the same range
- Dotted lines: zero-range model

# Contact of (1,1) & (2,1) systems

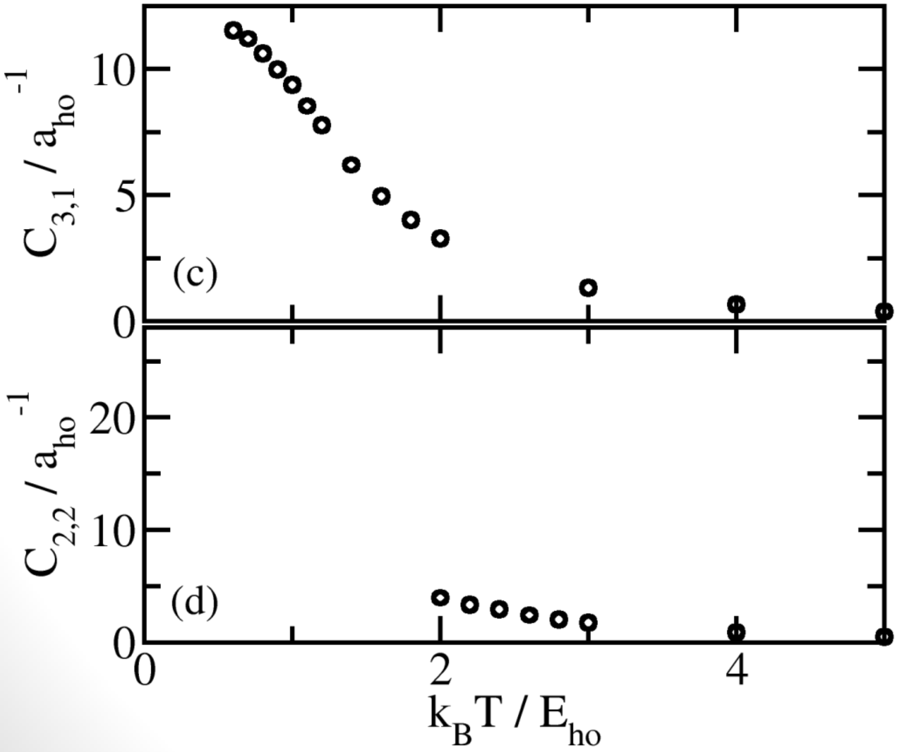
Non monotonic at low T for (2,1) system.
Range of interaction effect is small.




- Symbols: PIMC data for $r_0 = 0.06a_{ho}$
- Solid lines: B-spline & CG for the same range
- Dotted lines: zero-range model
- High T cluster expansion $C_{2,1} \approx 2C_{1,1}$ (canonical ensemble analog of virial expansion)

# Contact of (3,1) & (2,2) systems

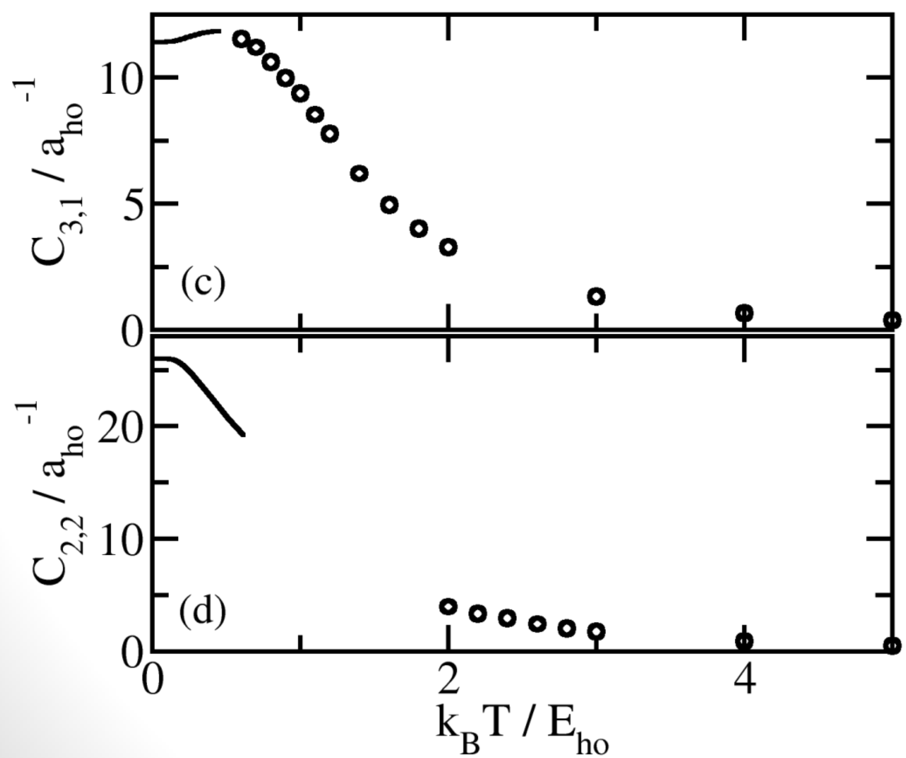
- Symbols: PIMC data for $r_0/a_{ho} = 0.06$



# Contact of (3,1) & (2,2) systems

Spin-imbalanced gas has non-monotonic behavior. Balanced gas has monotonic behavior.

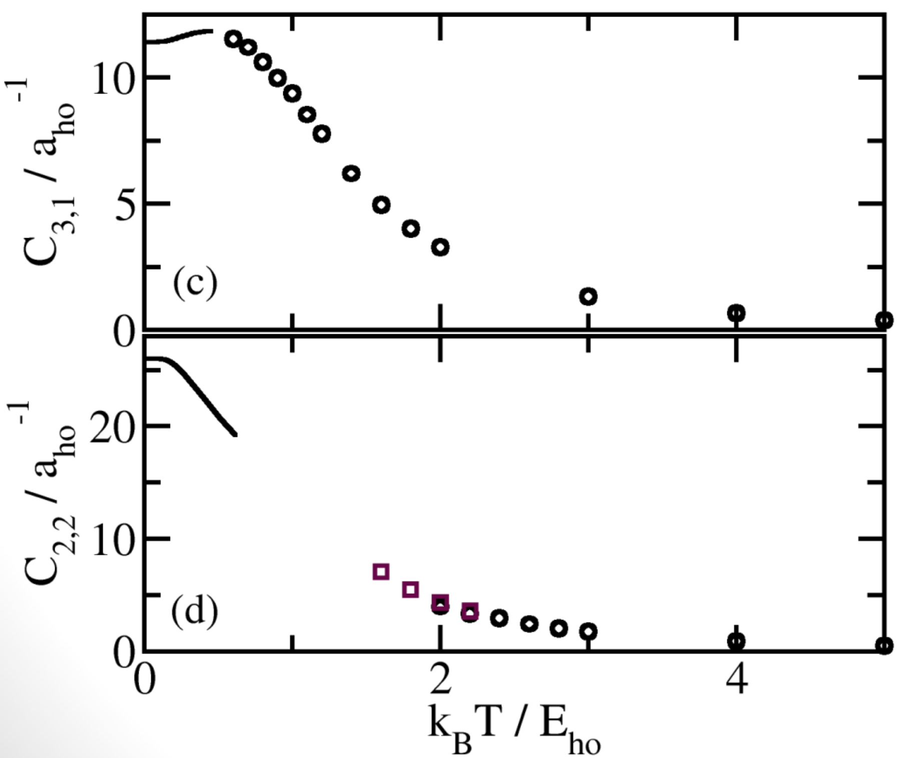
- Symbols: PIMC data for $r_0/a_{ho} = 0.06$
- Solid lines: CG using Gaussian potential



# Contact of (3,1) & (2,2) systems

Spin-imbalanced gas has non-monotonic behavior. Balanced gas has monotonic behavior.

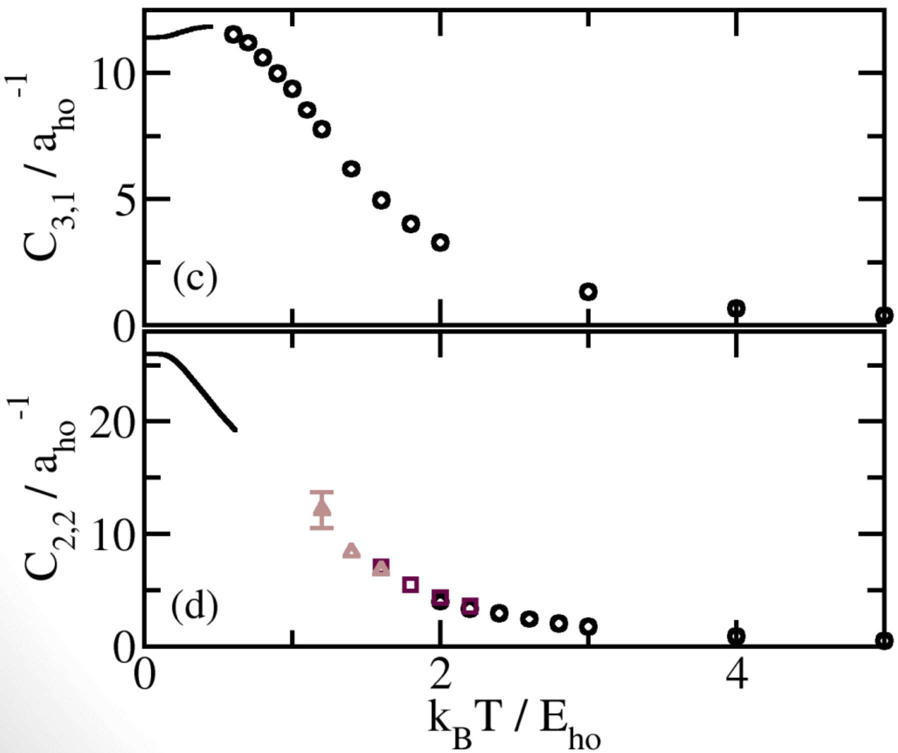
- Symbols: PIMC data for $r_0/a_{ho} = 0.06, 0.08$
- Solid lines: CG using Gaussian potential



# Contact of (3,1) & (2,2) systems

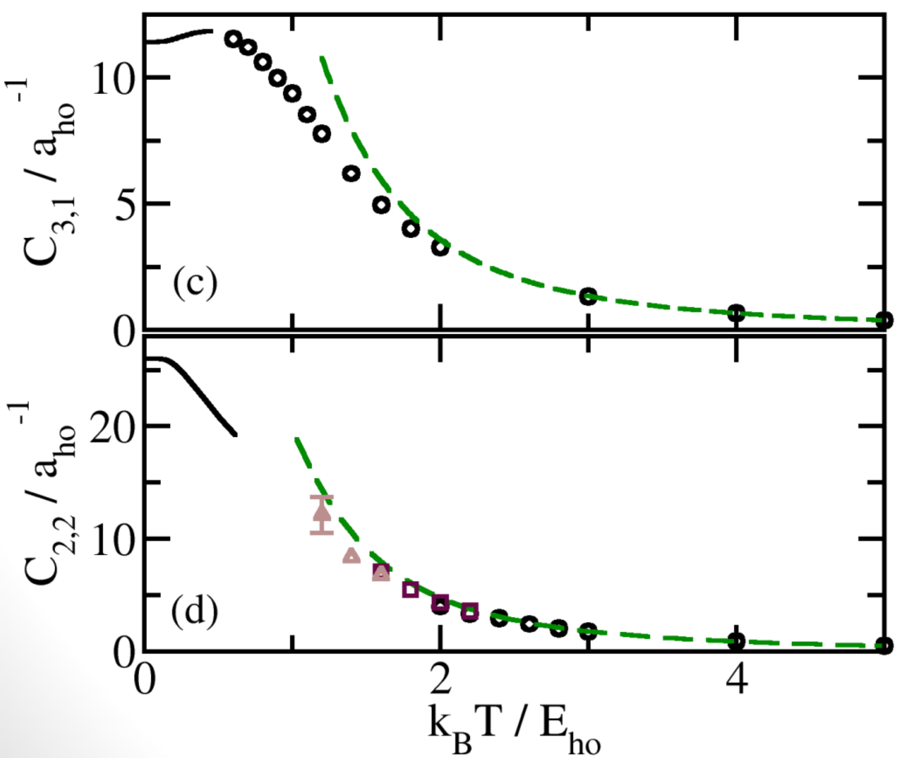
Spin-imbalanced gas has non-monotonic behavior. Balanced gas has monotonic behavior.

- Symbols: PIMC data for $r_0/a_{ho} = 0.06, 0.08, 0.1$
- Solid lines: CG using Gaussian potential



# Contact of (3,1) & (2,2) systems

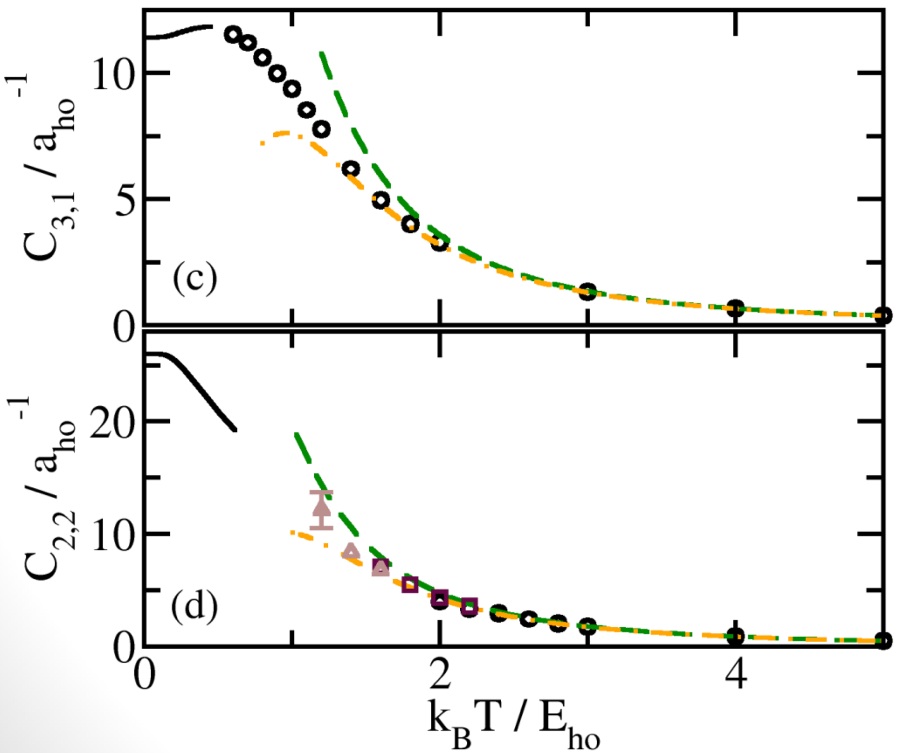
Spin-imbalanced gas has non-monotonic behavior. Balanced gas has monotonic behavior.




- Symbols: PIMC data for $r_0/a_{ho} = 0.06, 0.08, 0.1$
- Solid lines: CG using Gaussian potential
- High T cluster expansion $C_{3,1} \approx 3C_{1,1}, C_{2,2} \approx 4C_{1,1}$

# Contact of (3,1) & (2,2) systems

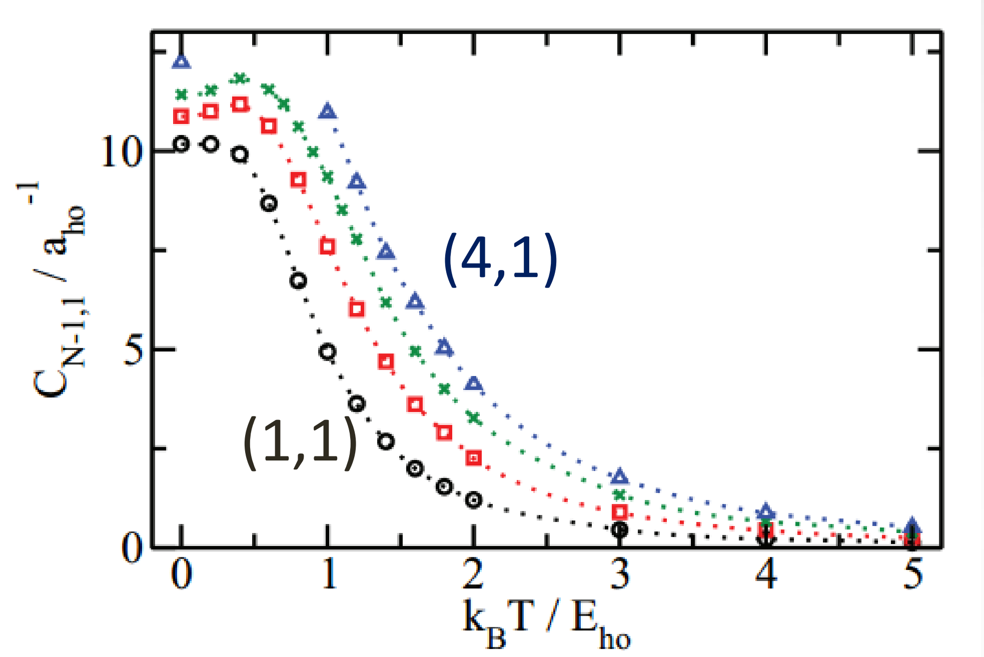
Spin-imbalanced gas has non-monotonic behavior. Balanced gas has monotonic behavior.




- Symbols: PIMC data for $r_0/a_{ho}$ = 0.06, 0.08, 0.1
- Solid lines: CG using Gaussian potential
- High T cluster expansion $C_{3,1} \approx 3C_{1,1}, C_{2,2} \approx 4C_{1,1}$
- Higher order cluster expansion:
  $C_{3,1} \approx 3C_{1,1} + 3(C_{2,1} - 2C_{1,1})$
  $C_{2,2} \approx 4C_{1,1} + 4(C_{2,1} - 2C_{1,1})$.

# Summary: Two-Component Fermi Gas

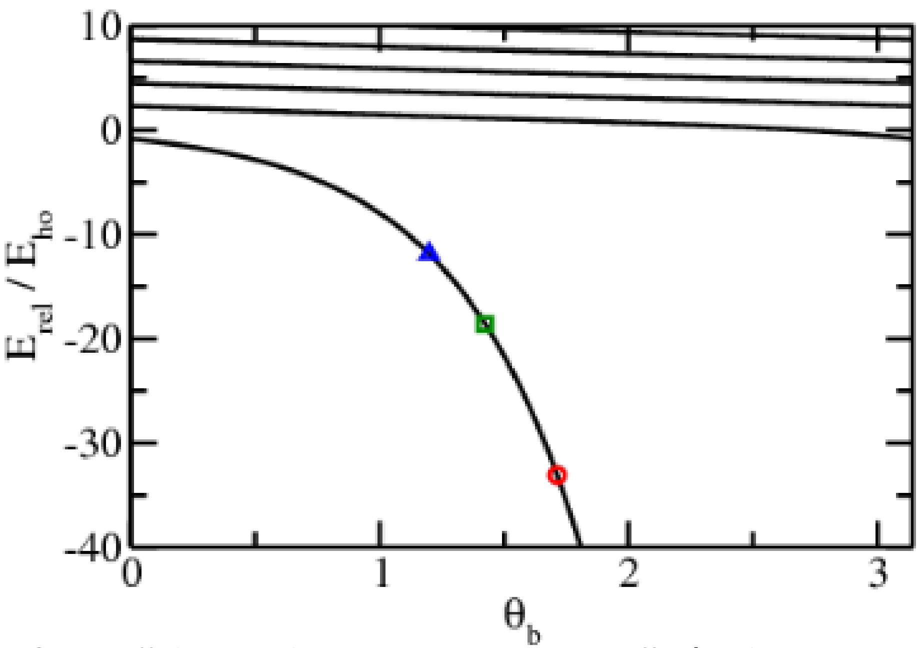
- Fermi sign problem beaten (small N).
- Accurate results for few-body systems.
- Low T:
  - Non-monotonic behavior  for spin-imbalanced system.
- High T:
  - Cluster expansion for canonical ensemble.



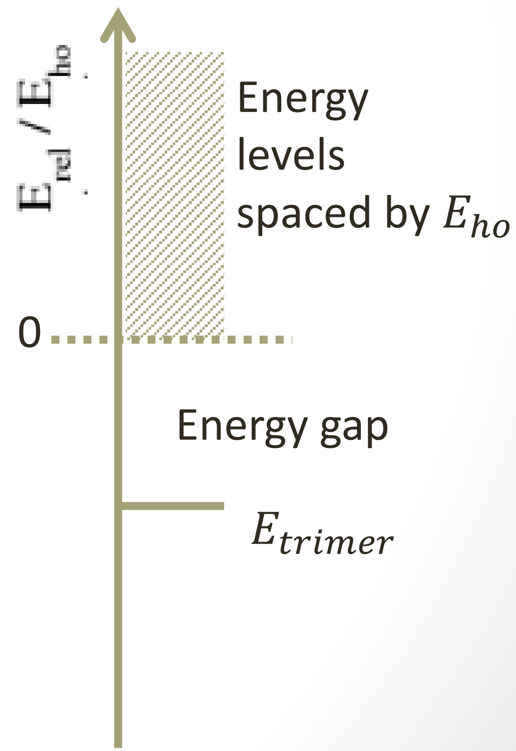

So far, fermions have been discussed.
What about bosons?

# Three identical Bosons with zero range interaction at unitarity

- Analytically solvable.
  - Partition function can be obtained from sum over states.
  - Energy can be determined as a function of temperature.

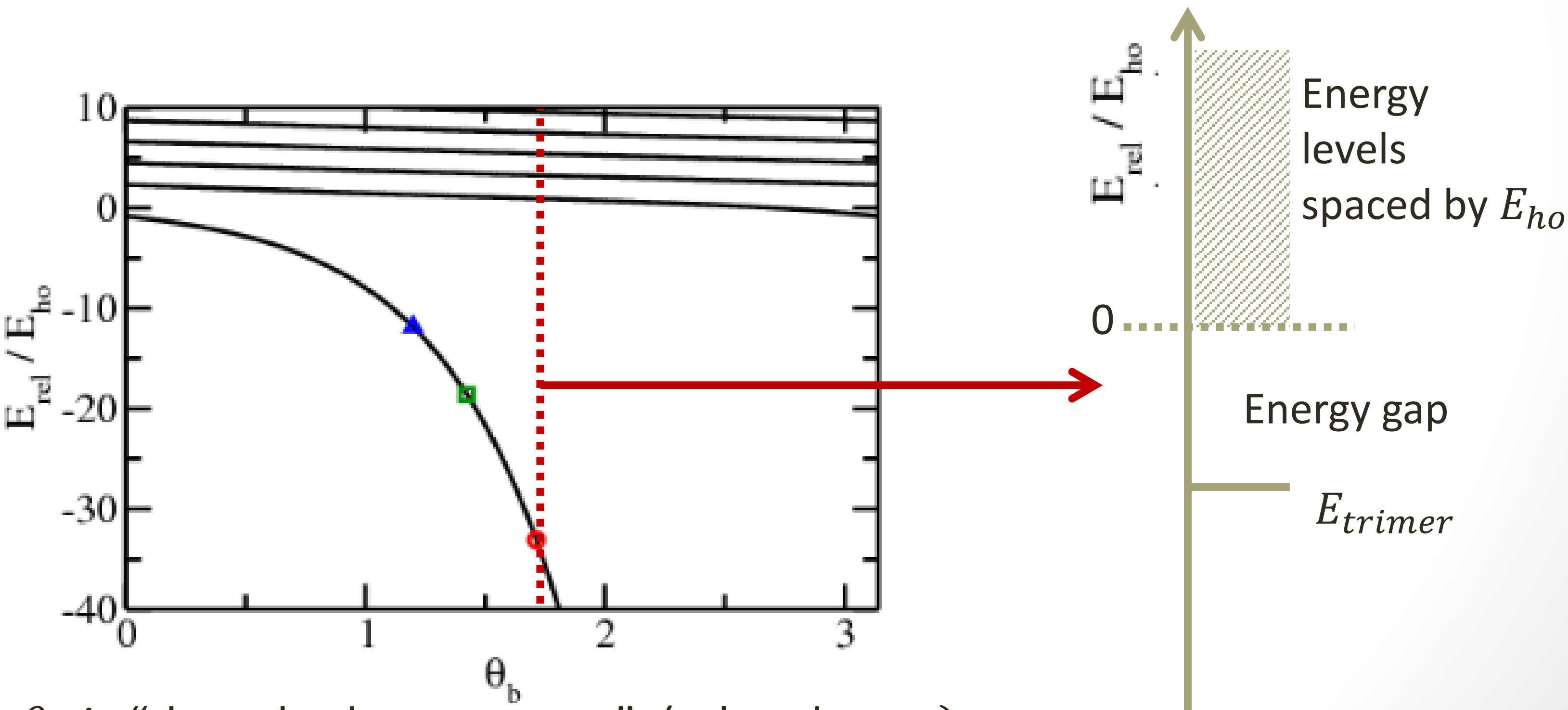



$\theta_b$ is "three-body parameter" (related to $\kappa_*$)



# Three identical Bosons with zero range interaction at unitarity

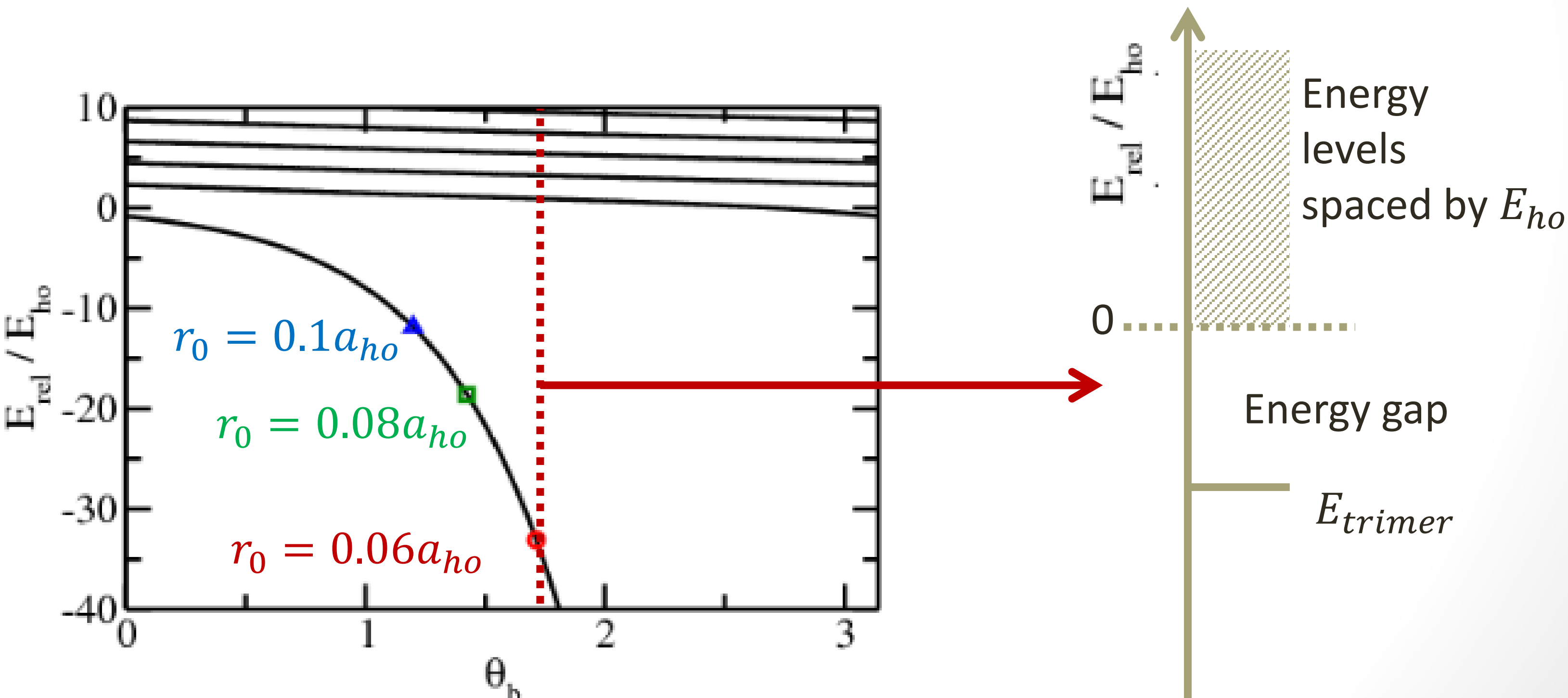
- Analytically solvable.
  - Partition function can be obtained from sum over states.
  - Energy can be determined as a function of temperature.




$\theta_b$ is “three-body parameter” (related to $\kappa_*$)

# Three identical Bosons with zero range interaction at unitarity

- Analytically solvable.
  - Partition function can be obtained from sum over states.
  - Energy can be determined as a function of temperature.

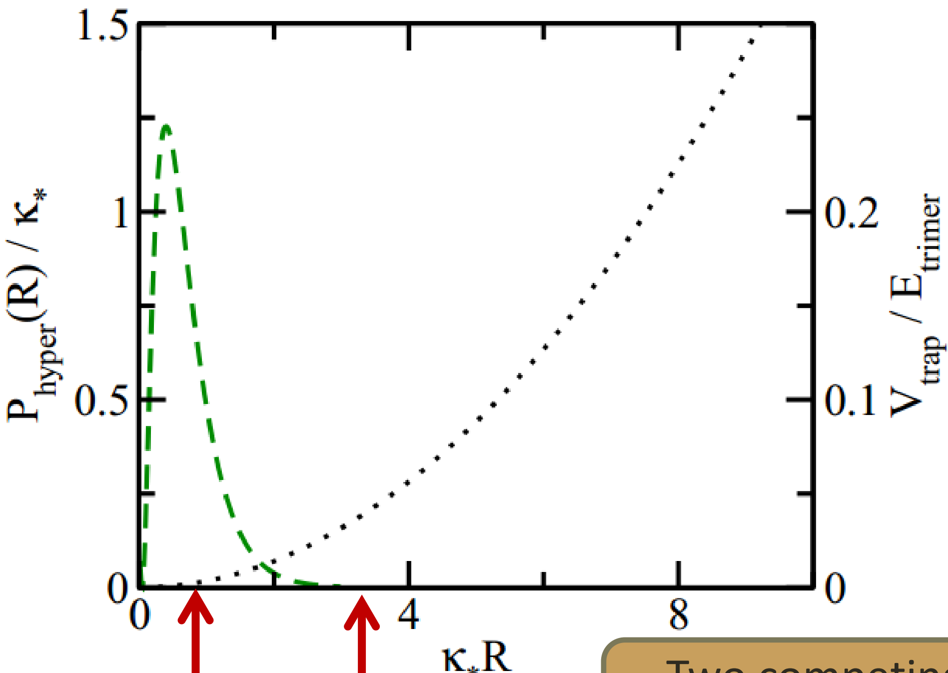



$\theta_b$ is “three-body parameter” (related to $\kappa_*$)

# Trimer state for zero-range model

Trimer energy is significantly larger than harmonic trap energy:

$E_{trimer}/E_{ho} \approx 11$ For Cs, this corresponds to $\omega \approx 2\pi * 13\text{kHz}$ (large frequency).




To fit two trimers into trap, trapping frequency has to be reduced by 515, i.e., $\omega \approx 2\pi * 25\text{Hz}$

$R_{trimer}$

$R = a_{ho}$

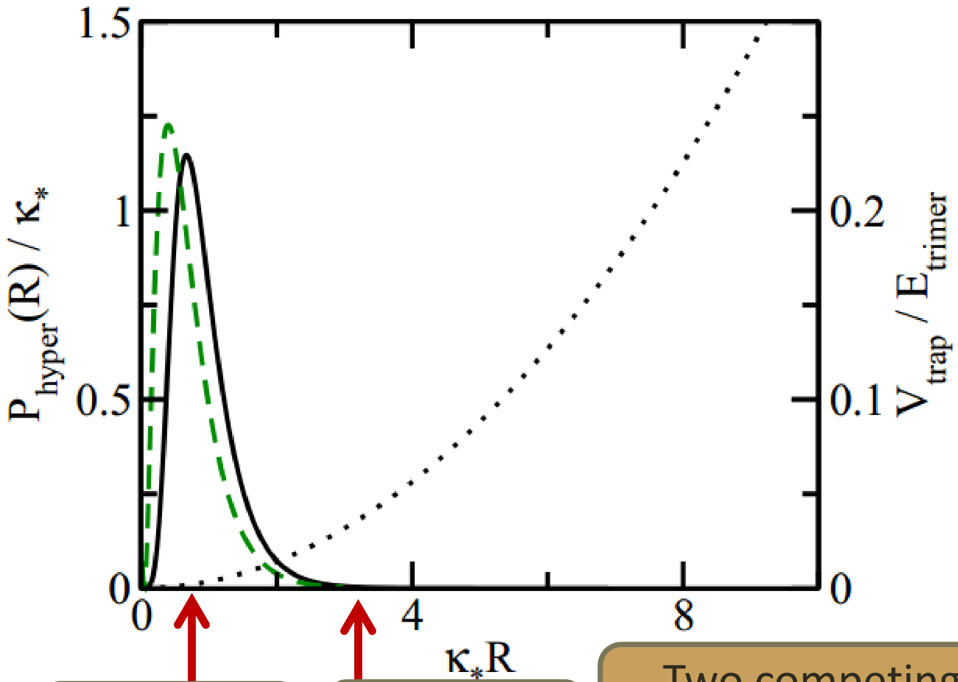
Two competing length scales

$22.7 R_{trimer}$

# Trimer state for Gaussian interaction

Trimer energy is significantly larger than harmonic trap energy:

$E_{trimer}/E_{ho} \approx 11$ For Cs, this corresponds to $\omega \approx 2\pi * 13$kHz (large frequency).



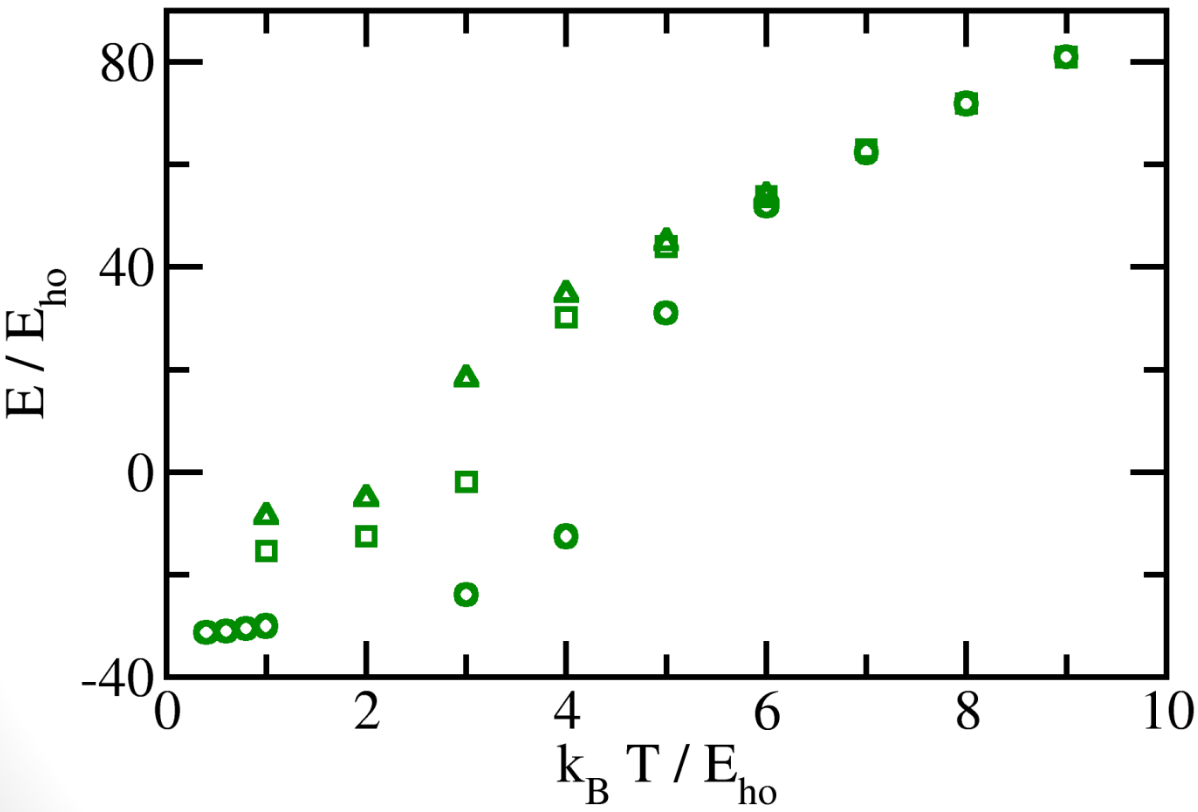

$R_{trimer}$

$R = a_{ho}$

Two competing length scales

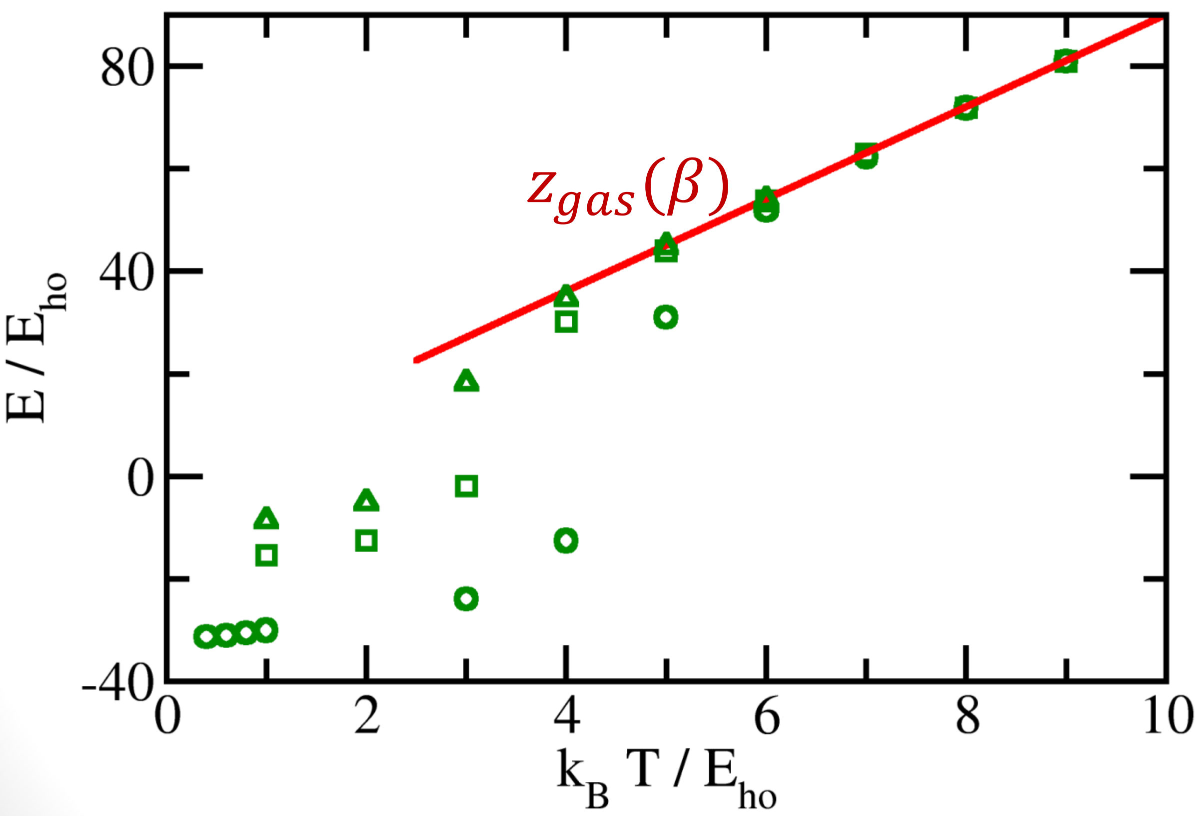
In free space, the energy ratios for series of trimers are $\frac{E^{(0)}}{E^{(1)}} \approx 23.0$ and $\frac{E^{(1)}}{E^{(2)}} \approx 22.7$.
Not fully universal but "Efimov-like".

# N=3: PIMC energy as a function of T



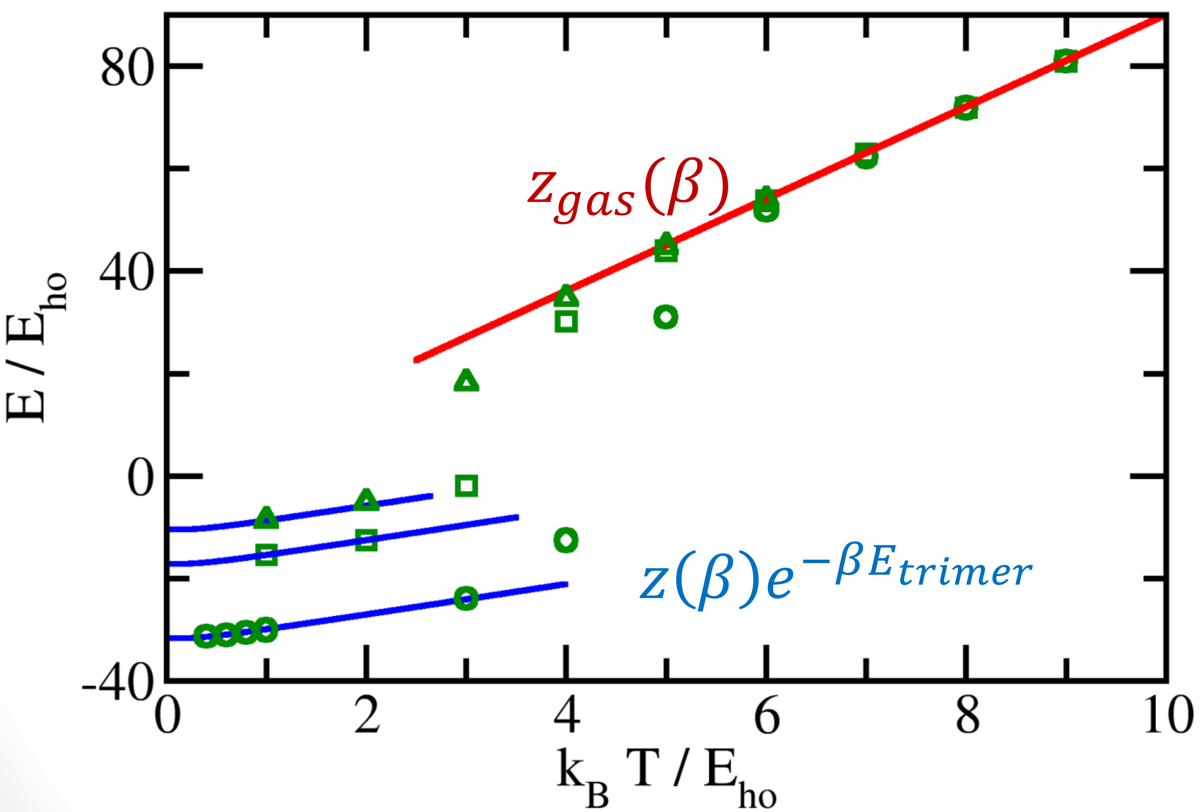

- Symbols: PIMC data for different ranges.

# N=3: PIMC energy as a function of T



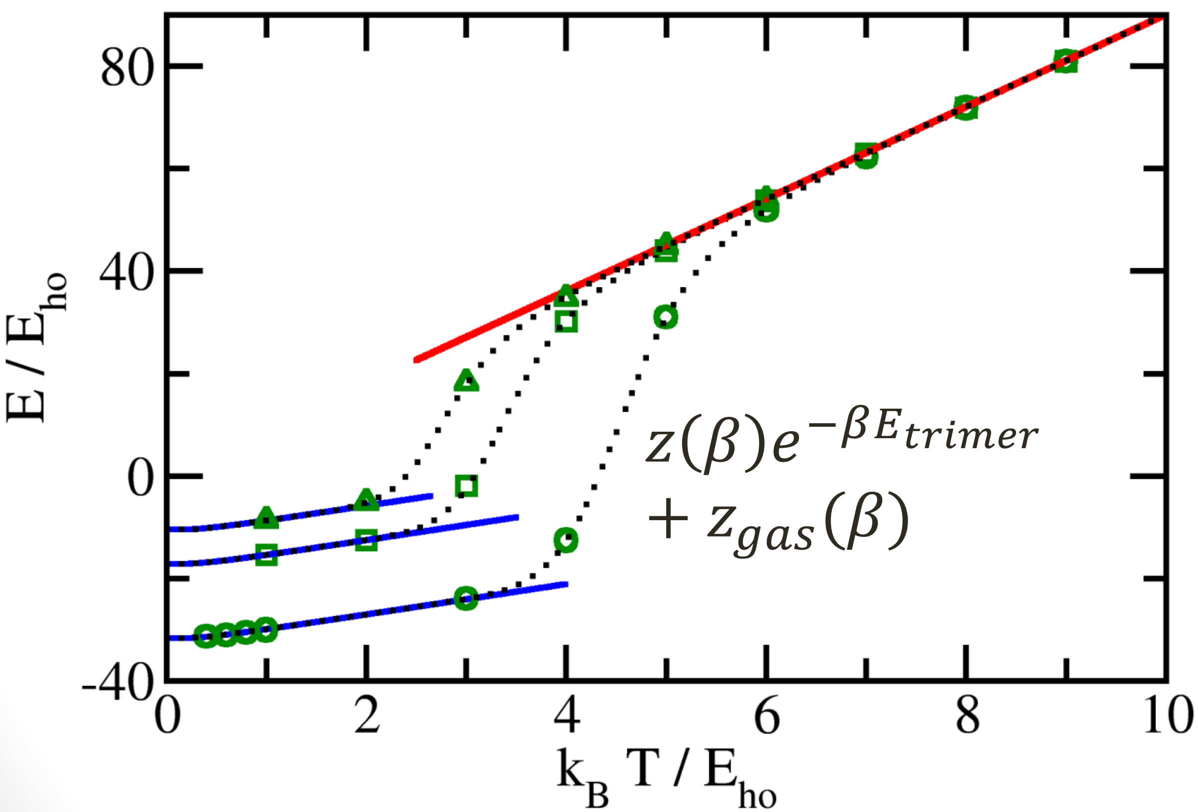

- Symbols: PIMC data for different ranges.
- Solid line: three non-interacting identical bosons.

# N=3: PIMC energy as a function of T




- Symbols: PIMC data for different ranges.
- Solid line: three non-interacting identical bosons.
- Solid line: "frozen trimer" plus center of mass excitations.

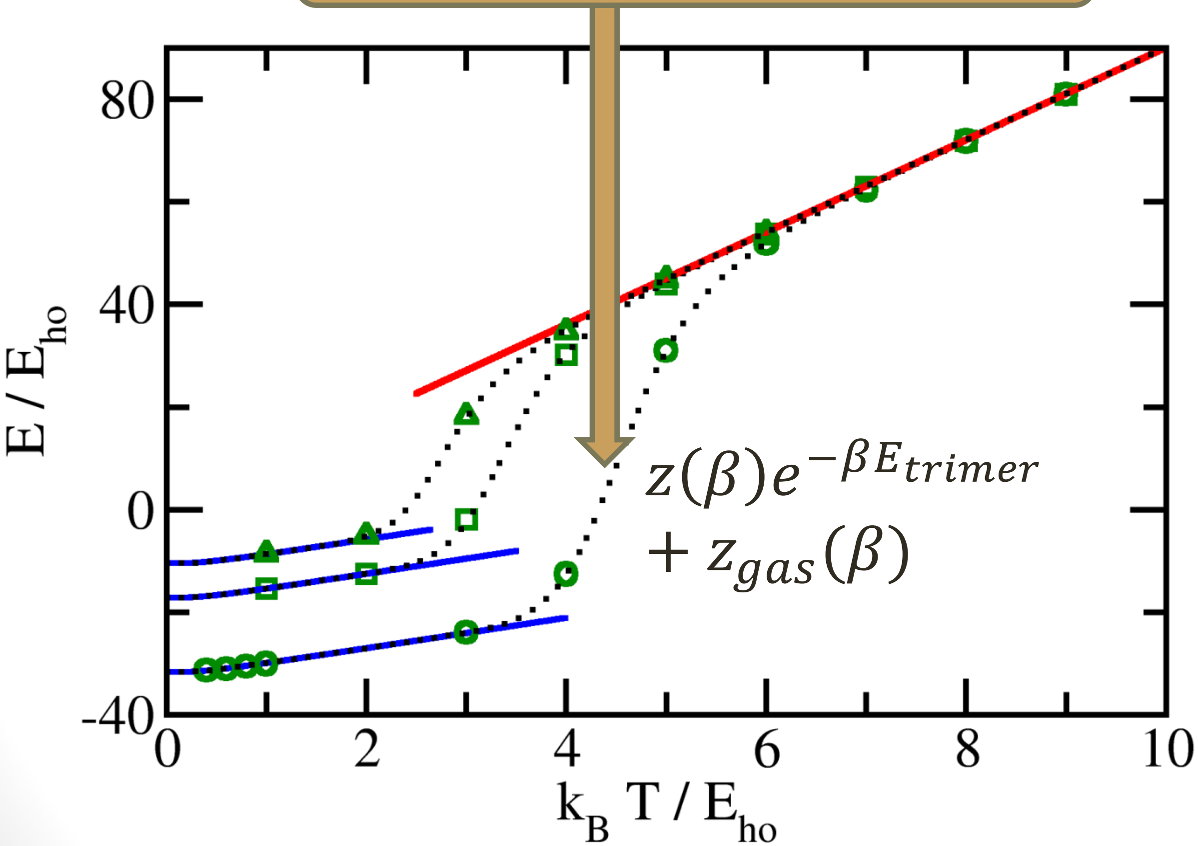
# N=3: PIMC energy as a function of T




- Symbols: PIMC data for different ranges.
- Solid line: three non-interacting identical bosons.
- Solid line: “frozen trimer” plus center of mass excitations.
- Dotted line: combined model.

# N=3: PIMC energy as a function of T

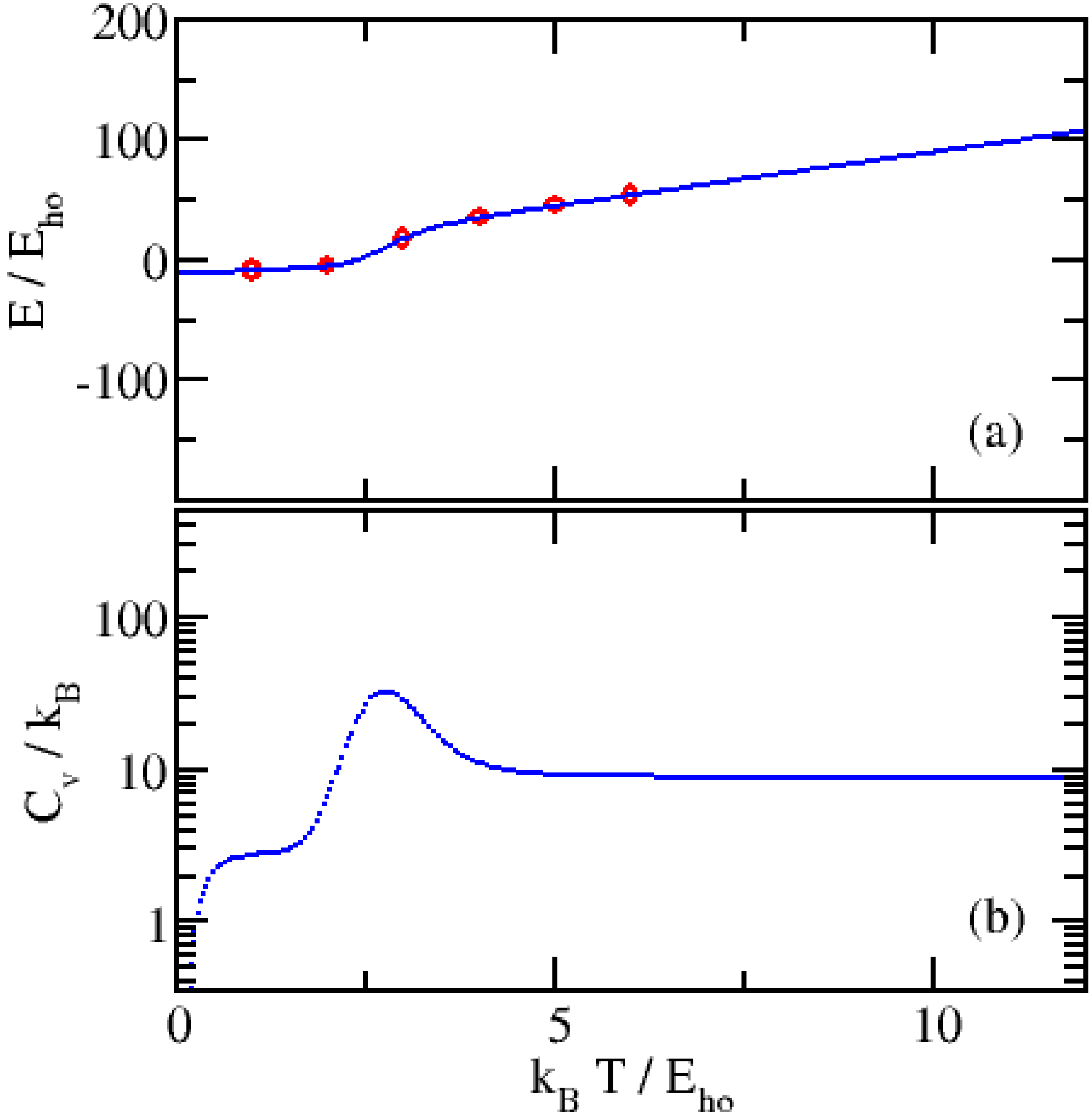
Phase transition like feature




$E_{trimer}$ determines the full curve

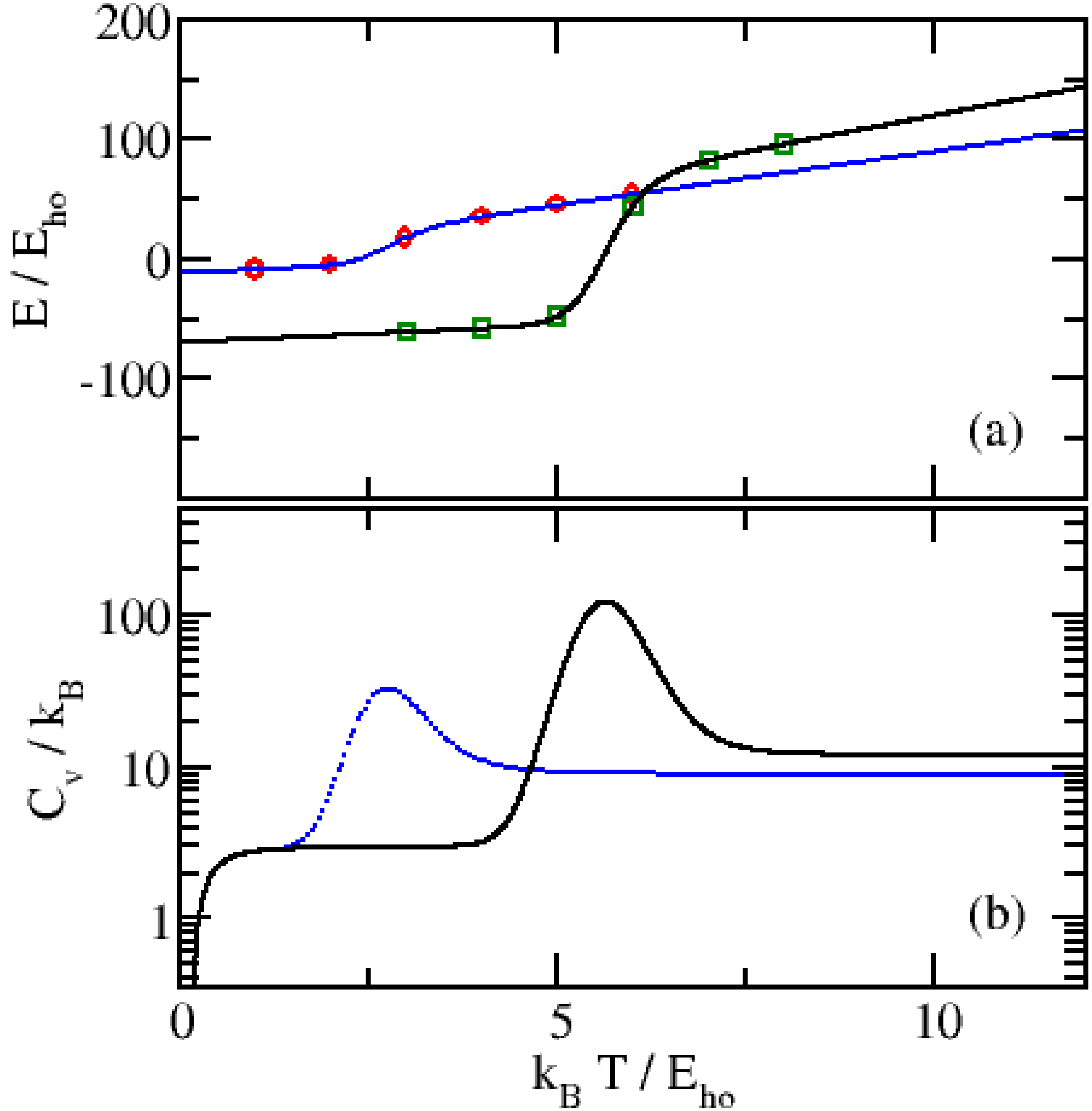
- Symbols: PIMC data for different ranges.
- Solid line: three non-interacting identical bosons.
- Solid line: “frozen trimer” plus center of mass excitations.
- Dotted line: combined model.

# Heat capacity $C_v = \partial E / \partial T$ for N=3



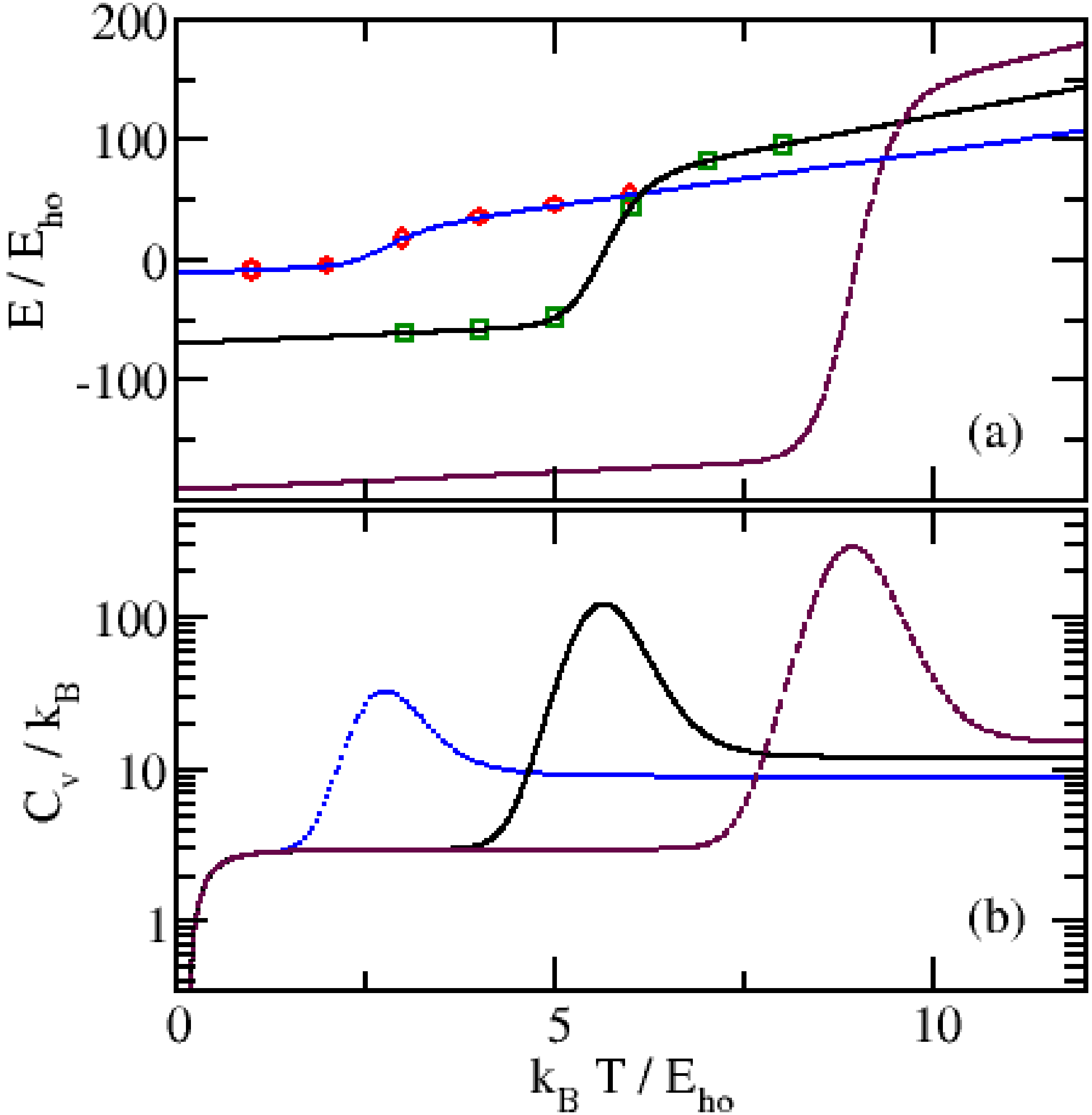

- Heat capacity resembles a lambda shape.

# Heat capacity $C_v = \partial E/\partial T$ for N=3, 4



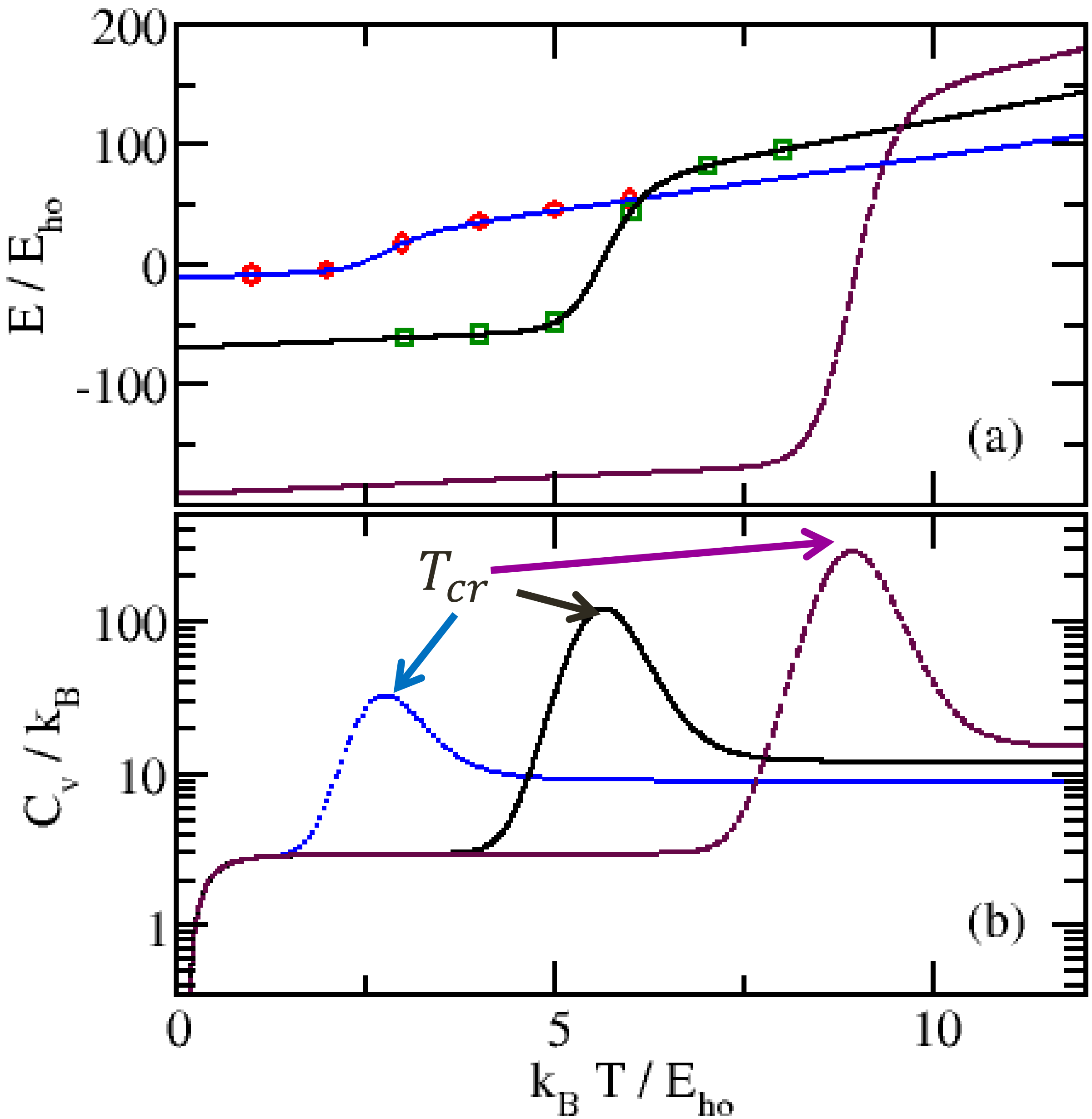

- Heat capacity resembles a lambda shape.
- For N=4, only energy of tetramer is needed.

# Heat capacity $C_v = \partial E/\partial T$ for N=3, 4, 5




- Heat capacity resembles a lambda shape.
- For N=4, only energy of tetramer is needed.
- Same for N=5

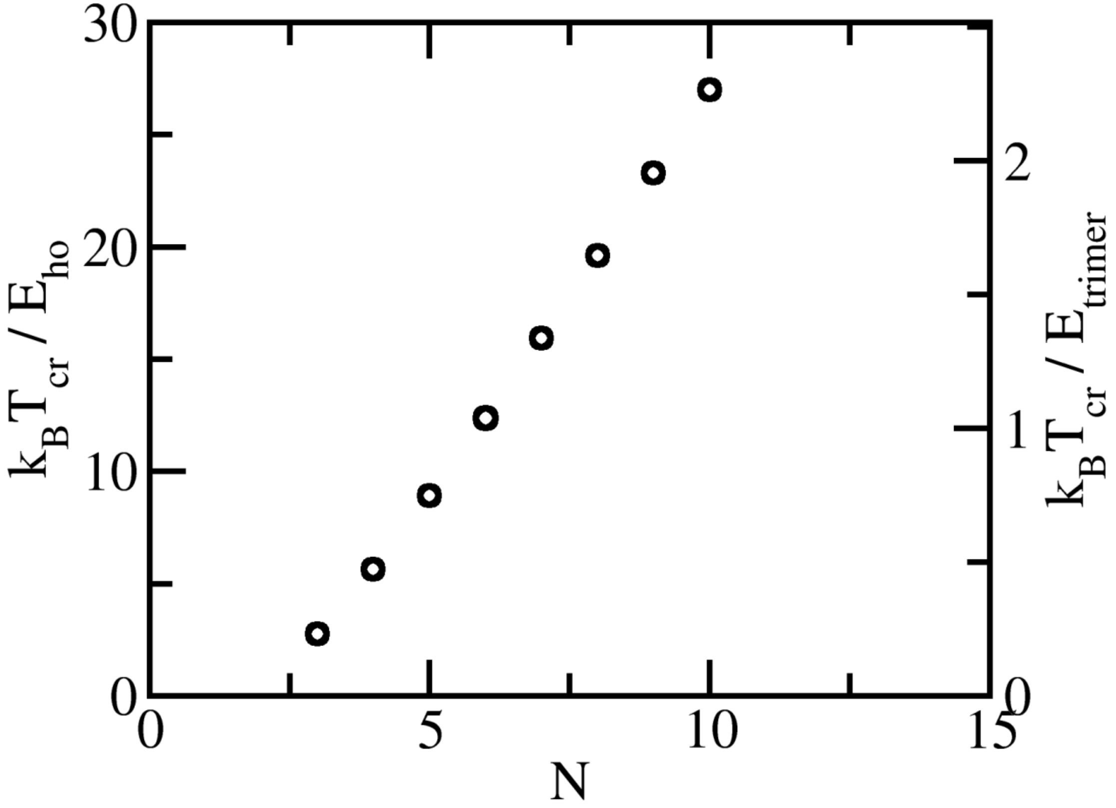
# Heat capacity $C_v = \partial E/\partial T$ for N=3, 4, 5




- Heat capacity resembles a lambda shape.
- For N=4, only energy of tetramer is needed.
- Same for N=5

# Transition temperature

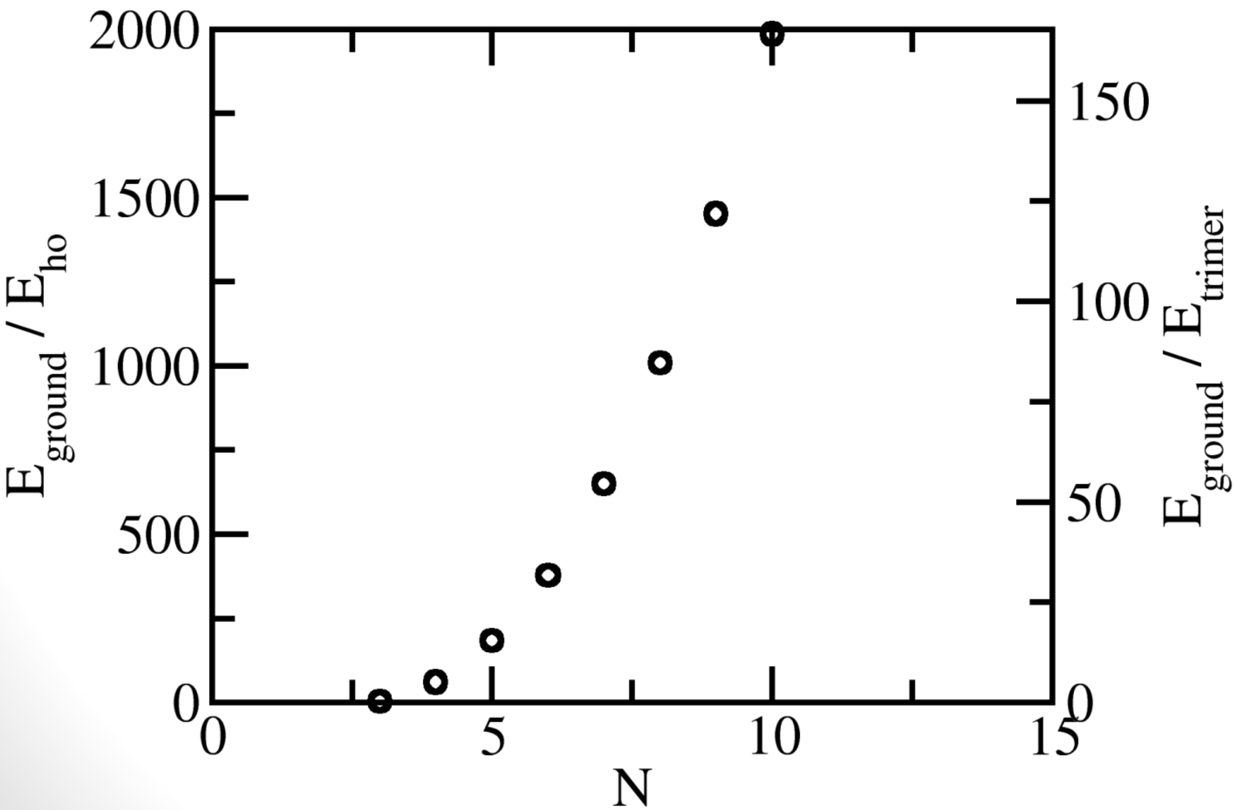
Critically depends on $E_{droplet}$




- Feed "number of particles" and "droplet state energy" into the combined model.
- $T_{cr} \sim N$

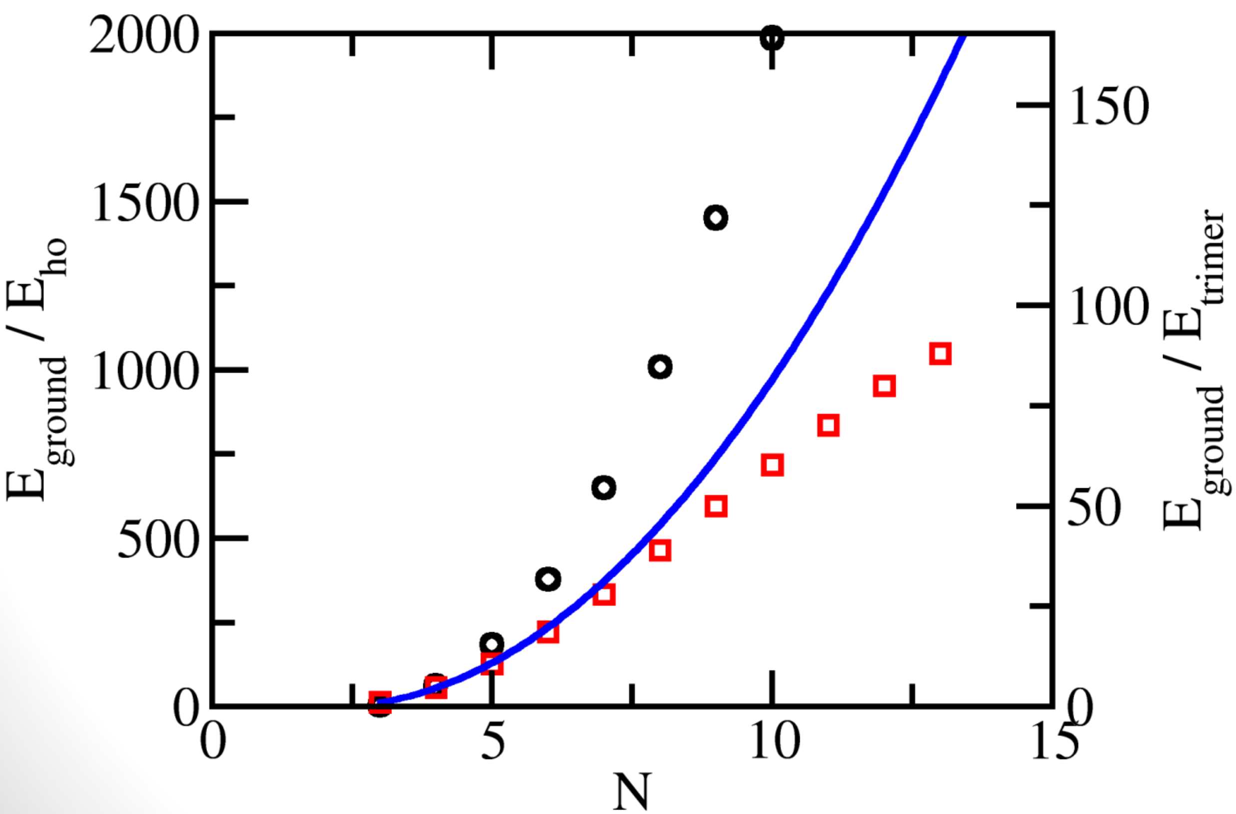
# Energy of droplet state tied to Efimov trimer

$E_{gauss} \sim N^2$



# Energy of droplet state tied to Efimov trimer

Large finite range effect?
Lack of repulsive core?

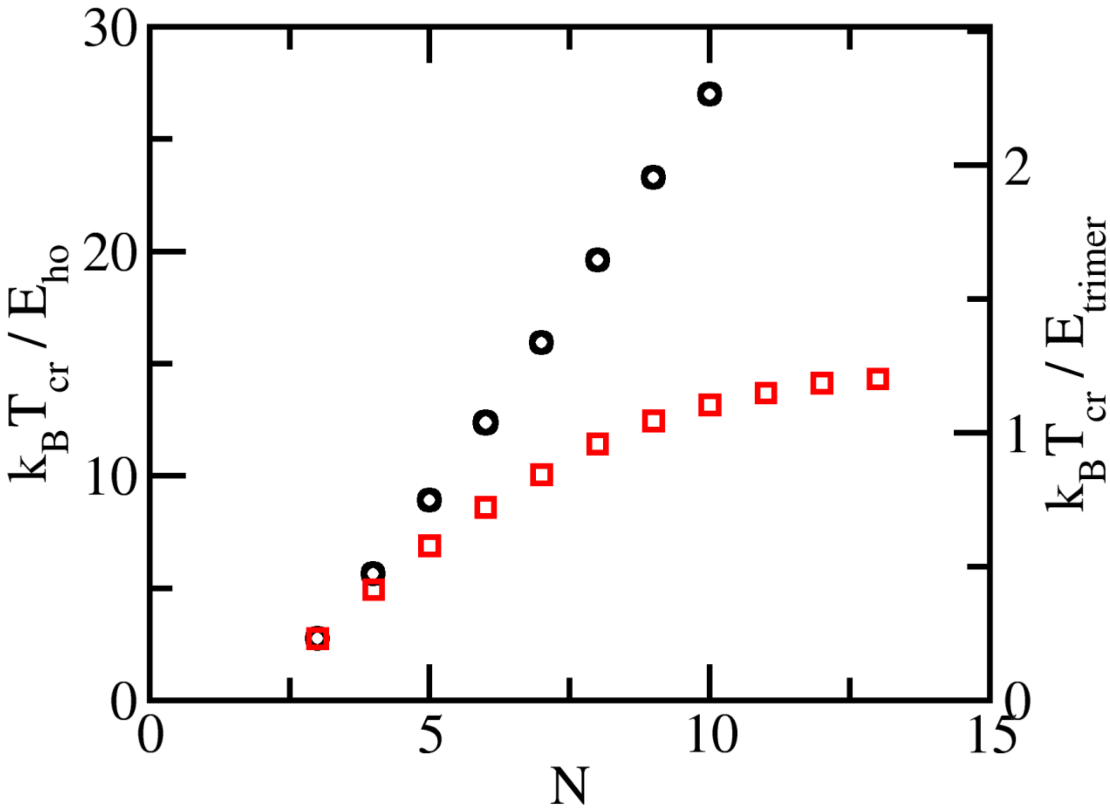



$E_{gauss} \sim N^2$

$E_{[1]} \sim N$ ([1] von Stecher, JPB (2010); a universal prediction)

$E_{[2]} \sim N^2$([2] Gattobigio and Kievsky, arXiv (2013); another universal prediction)

# Transition temperature




$E_{gauss} \sim N^2$ (non-universal for large N)

$E_{[1]} \sim N$ ([1] von Stecher, JPB (2010); a universal prediction)

For N=100, see Piatecki and Krauth, Nature Comm. (2014)

# Summary of single component Bose gas

- Combined model describes phase transition like feature from droplet state at low T to gas like state at high T.
- Possible experimental realization for few particles in trap?
- A step towards understanding unitary Bose gas?
- We assumed $|E_{trimer}| \gg E_{ho}$, what would happen if $|E_{trimer}| \approx E_{ho}$?

# Outlook

- For Bose gas:
  - Superfluid fraction (already calculated).
  - Larger N.
  - Include three-body force: go closer to universal Efimov regime (underway).
  - Condensate fraction (to be implemented).
- For Fermi gas:
  - Superfluidity (see arXiv:1312.4470).
  - Larger N?

Thank you for your attention!