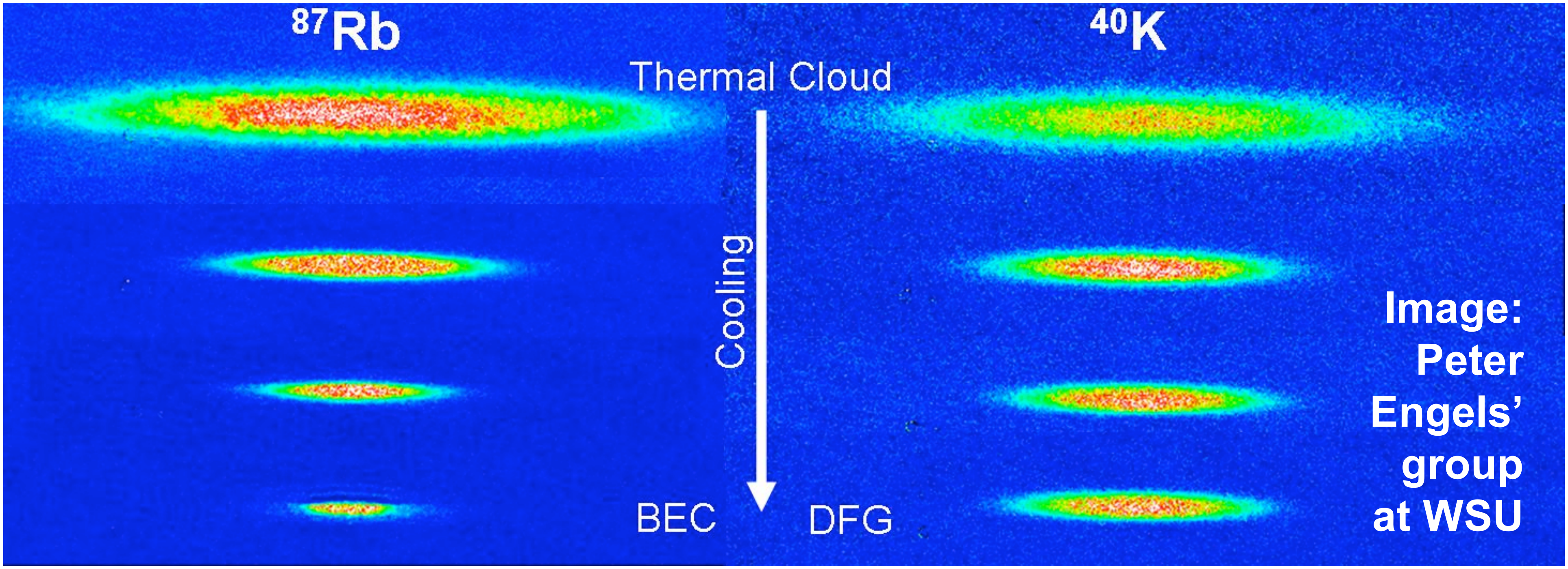


Small Trapped s-Wave Interacting Fermi Gases: How to Quantify Correlations?

Doerte Blume and Kevin M. Daily
Dept. of Physics and Astronomy, Washington State University, Pullman

Supported by NSF and ARO.

Outline of This Talk

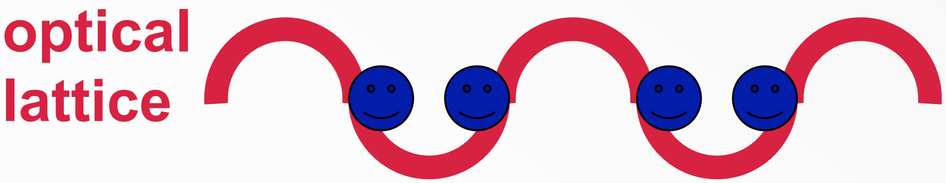
- **Introduction:**
  - **BCS-BEC (Bardeen-Cooper-Schrieffer) crossover (s-wave interacting “up” and “down” atoms).**
- **Techniques employed:**
  - **Semi-stochastic variational approach.**
  - **(Monte Carlo techniques.)**
  - **(Semi-analytical perturbative approach.)**
- **A few examples of our trapped few-fermion studies:**
  - **Universality throughout crossover and at unitarity.**
  - **Pair distribution functions.**
  - **Momentum distributions.**
- **Summary**

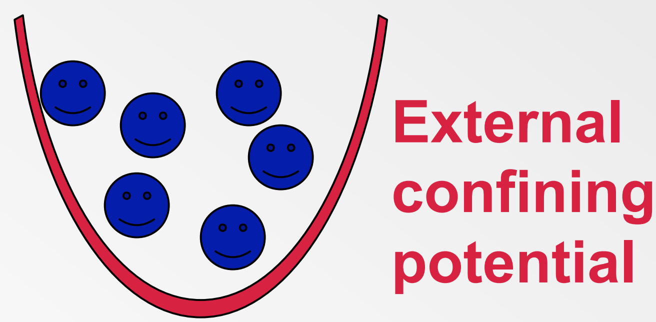
Our General Philosophy: From Few to Many

- Microscopic to macroscopic:

- Other examples:
  - Doped helium clusters: Molecular rotations, microscopic superfluidity,...
  - Metal clusters: conductivity, designing materials,...

- What is special about dilute atomic Fermi systems?
  - Controllable system (scattering length, trap geometry,…)
  - Universal behavior.



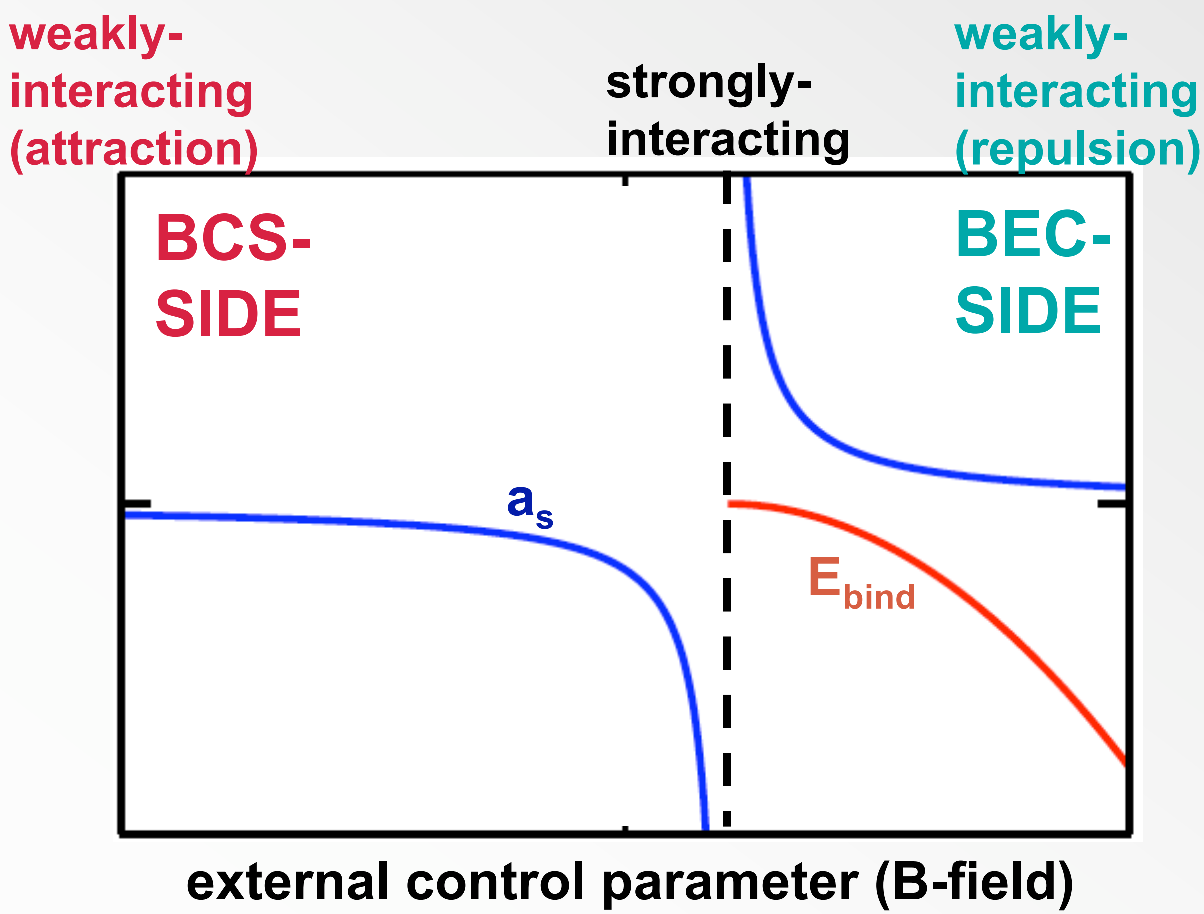


"Up" - "Down" Interactions: Two-Body s-Wave Scattering Length

At low temperature, the details of the atom-atom potential are irrelevant:

Positive s-wave scattering length: Effective repulsive interaction.

Negative s-wave scattering length: Effective attractive interaction.

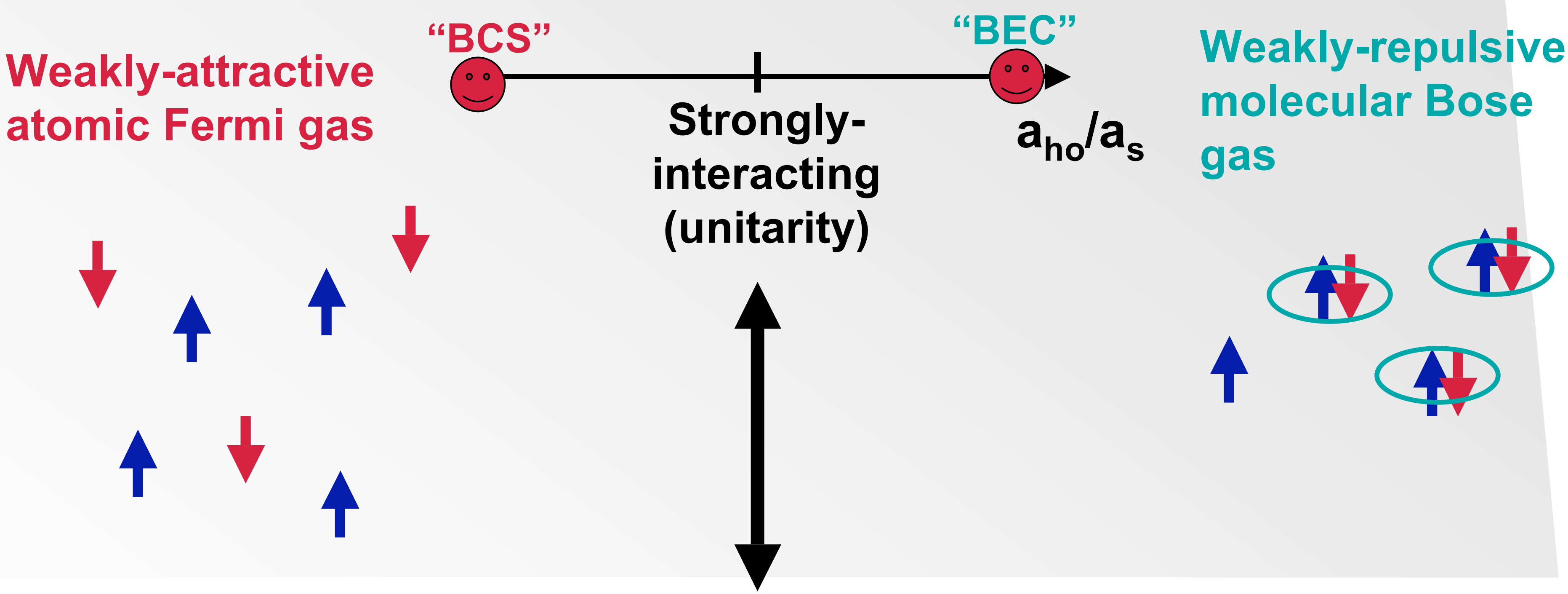


$$a_s = \lim_{k \to 0} - \frac{\tan(\delta_s)}{k}$$

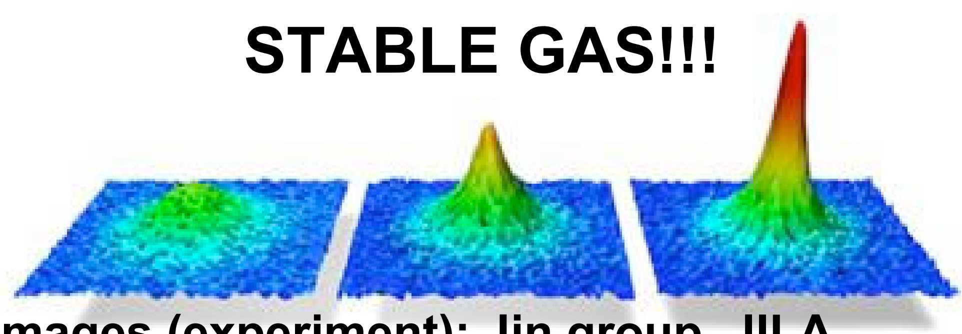
Dilute gas:
$r_0 \ll a_{ho}$, a_s or $n(0) r_0^3 \ll 1$.

Similarities with nuclear matter, condensed matter/ Cooper pairs.

BCS-BEC Crossover with Cold Two-Component Atomic Fermi Gas



STABLE GAS!!!



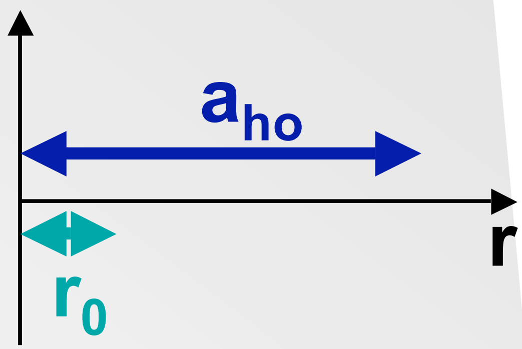
Images (experiment): Jin group, JILA.

Beyond N=3? Semi-Stochastic Variational Approach I

Non-relativistic system Hamiltonian:

$$H = \Sigma_i (T_i + V_{trap,i}) + \Sigma_{l<j} V_{twobody,ij} \; ; \quad V_{twobody} = V_0 \exp[-(0.5r/r_0)^2]$$

- $V_{trap,i}$ → Spherically symmetric.
- $V_{twobody,ij}$ → Sum over unlike spin pairs.
- $V_{twobody}$ → Short-range. Simple. Independent of spin and angular momentum.



Idea:

Use basis set expansion approach that involves Gaussian of different widths in interparticle distances.

Method first introduced to cold atom community for bosons by Sorensen, Fedorov and Jensen, AIP Conf. Proc. No. 777, p. 12 (2005). Our work inspired by work on fermions by von Stecher and Greene, PRL 99, 090402 (2007). For details see: Suzuki and Varga (Springer, 1998); von Stecher, Greene, Blume, PRA 77, 043619 (2008).

Beyond N=3? Semi-Stochastic Variational Approach II

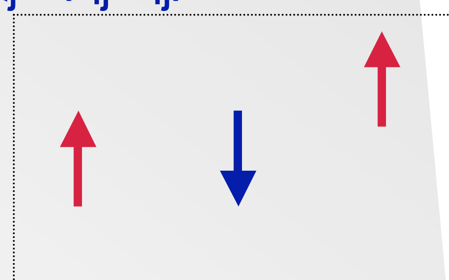
Idea:

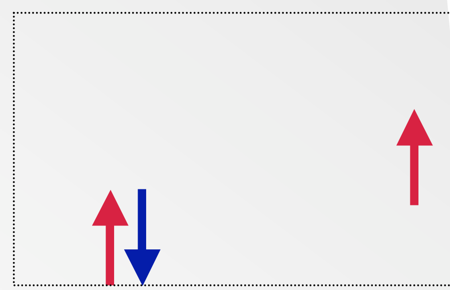
Use basis set expansion approach that involves correlated Gaussian.

- **Symmetrized basis function** $\Psi = \Sigma_{Np} |\underline{v}|^L Y_{LM}(\hat{\underline{v}}) \exp(-\underline{x}^T A \underline{x}/2)$

Determines angular momentum: L distributed with "weight" u_i among the Jacobi vectors $\underline{\rho}_i$

Sum over interparticle distances: $\Sigma_{i<j} -(r_{ij}/d_{ij})^2 / 2$





- **$\underline{x}$ collectively denotes N-1 Jacobi coordinates.**
- **$\underline{v} = \underline{u} \cdot \underline{x}$**
- **A denotes (N-1)x(N-1) dimensional parameter matrix.**
- **$\underline{u}$ denotes N-1 dimensional parameter vector.**

Beyond N=3? Semi-Stochastic Variational Approach III

Hamiltonian matrix can be evaluated analytically.

Rigorous upper bound for energy (“controlled accuracy”).

Basis functions with good angular momentum and parity (unnatural parity states must be treated differently…).

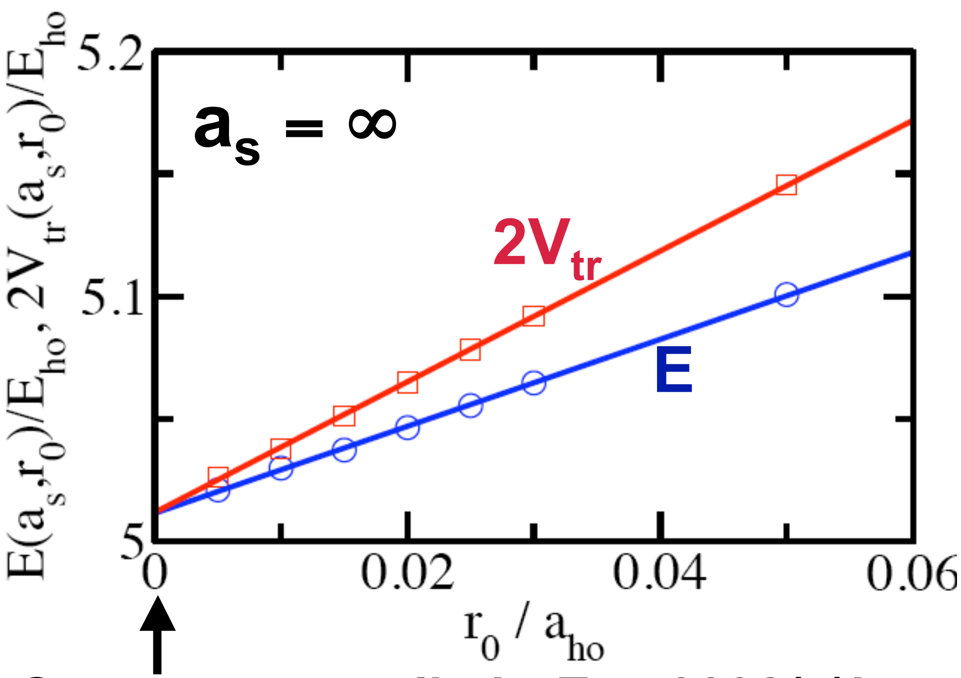
Matrix elements for structural properties and momentum distribution can be calculated analytically.

Linear dependence of basis functions needs to be watched carefully.

Computational effort increases with N:

- Evaluation of Hamiltonian matrix elements involves diagonalizing (N-1)x(N-1) matrix.
- More degrees of freedom require more basis functions.
- Permutations N_p scale nonlinearly (N_p=2,4,12,36 for N=3,4,5,6).

Extrapolation of Four-Body "Ground State Energy" to $r_0 \rightarrow 0$ Limit (L_{rel}=0)

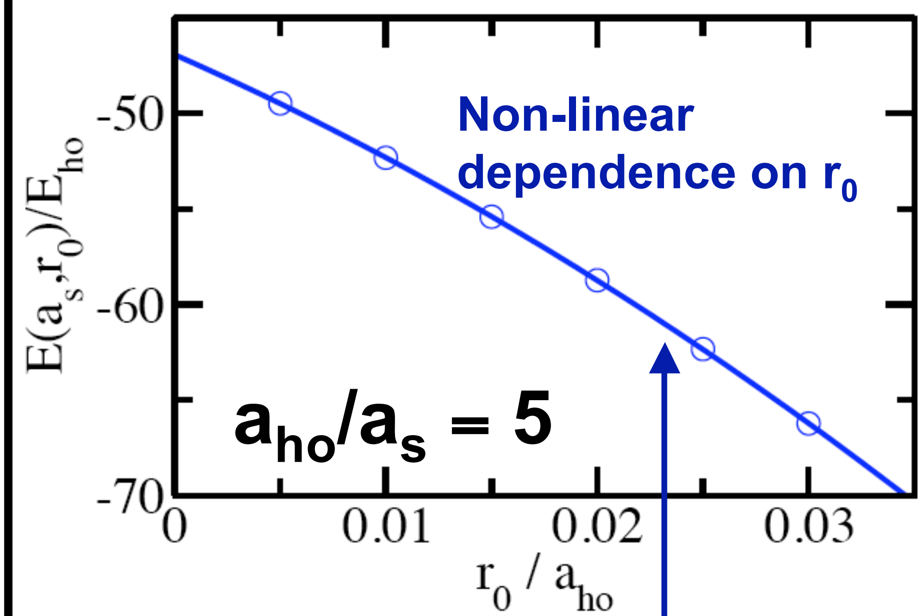


Our zero-range limit: E=5.0092(5)hν [uncertainty arises from fit]. Effective interaction theory: E=5.050(24)hν.

[Alhassid et al., PRL 100, 230401 (2008)].

Confirmation of virial theorem at unitarity: $E(\infty, 0) = 2V_{tr}(\infty, 0)$.

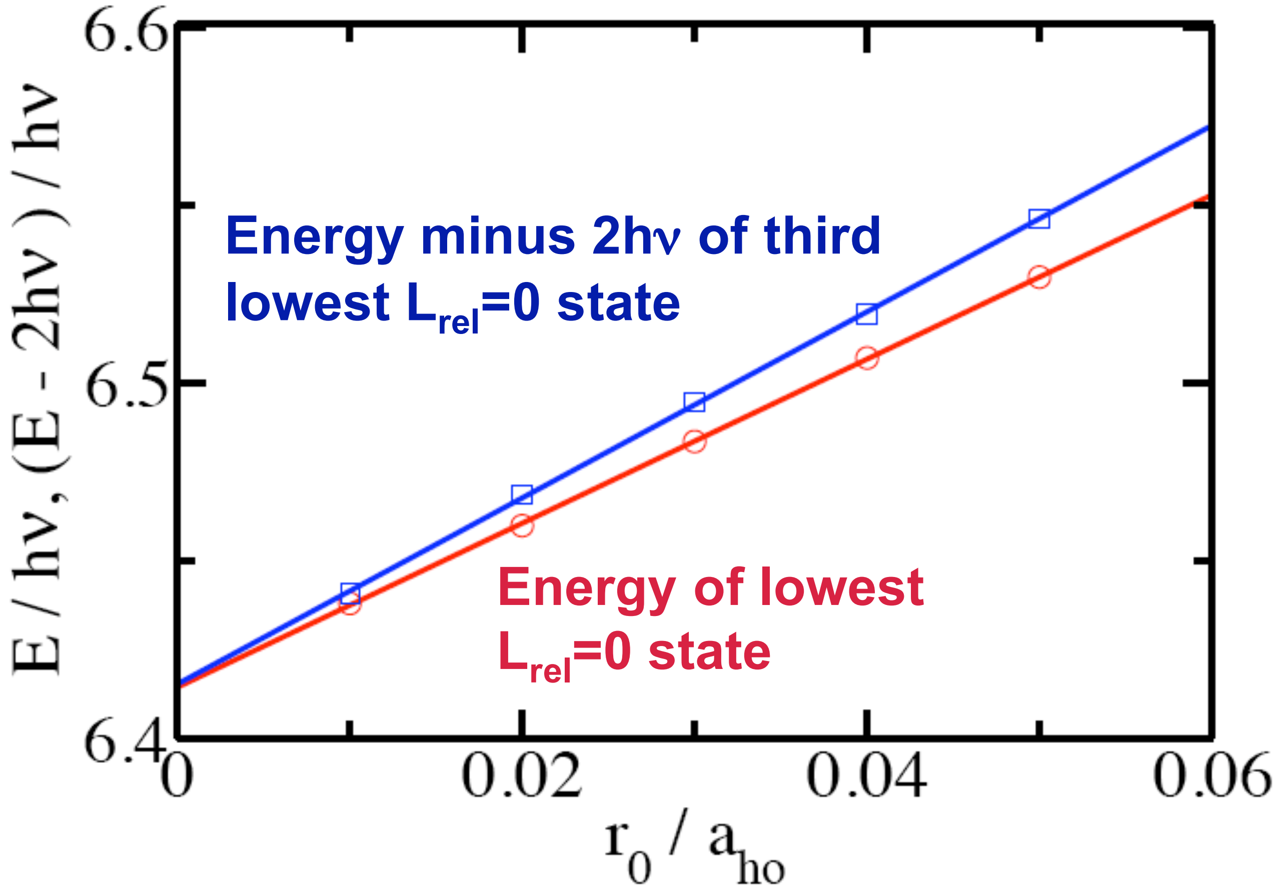
[e.g.: Thomas et al., PRL 95, 120402 (2005)]



In this case, it is better to first subtract the energy of two dimers and to then extrapolate.

Example for N=5 ($N_\uparrow$=3, $N_\downarrow$=2): 2hν Spacing in Zero-Range Limit

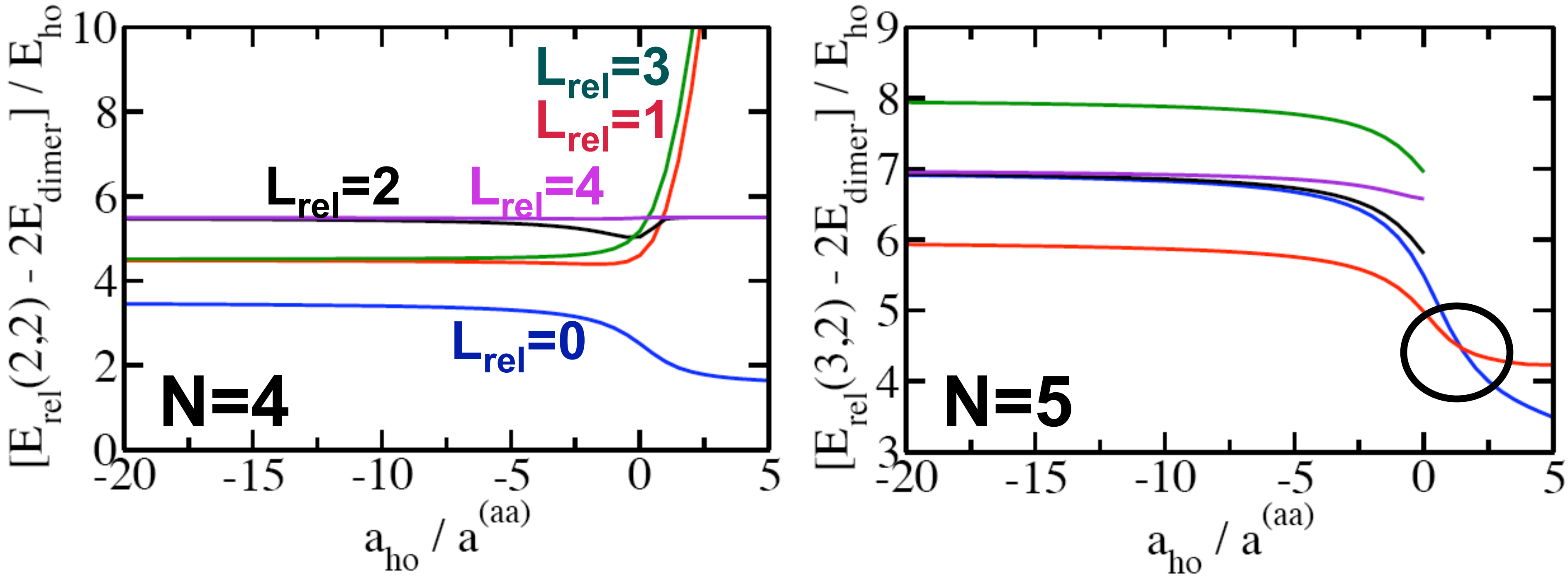
$1/a_s=0, L_{rel}=0$ (symbols: CG; lines: fit)



For ZR interactions, universal states have been predicted to have 2nhν energy spacing [e.g., Werner et al., PRA 74, 053604 (2006)]: Hyperangular and hyperradial degrees of freedom separate.

Analytical predictions can be used to assess accuracy of numerics.

Energy Crossover Curves for Few-Fermion System (Natural Parity States)

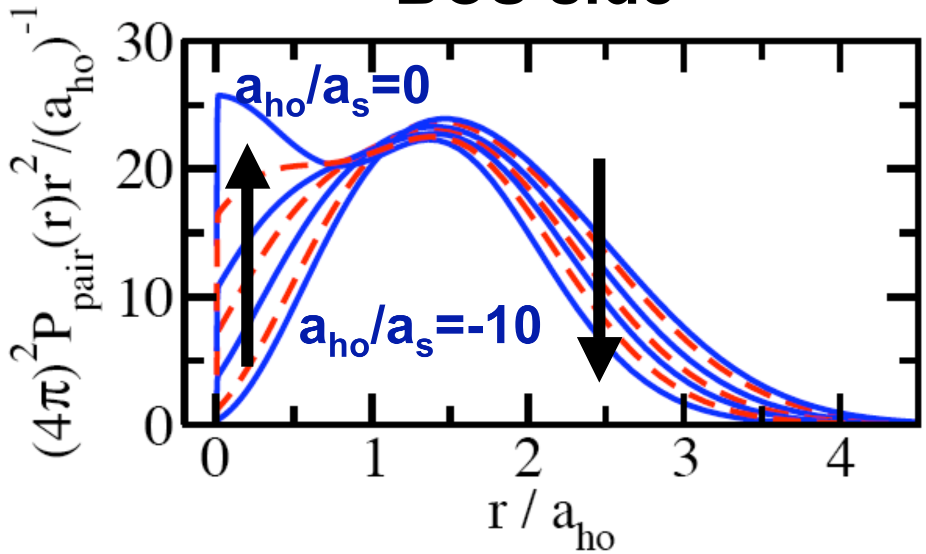


- **Benchmark for approximate numerical and analytical approaches:**
  - **Monte Carlo (see later).**
  - **Effective low-energy theories: Four-body problem is becoming tractable** (Stetcu et al., PRA 76, 063613 (2007); Alhassid et al., PRL 100, 230401 (2008); Hammer et al.).

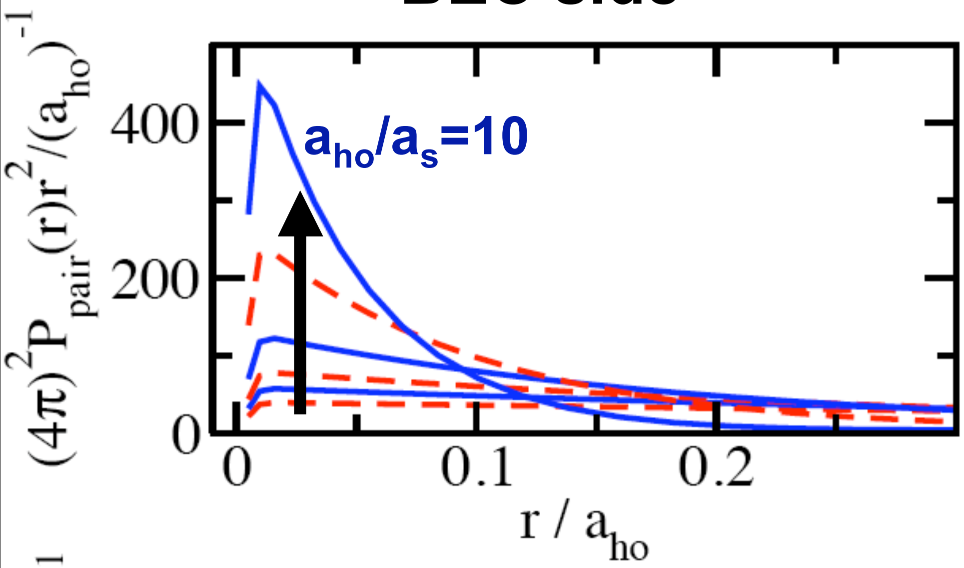
- **Next:**
  - **Focus on N=4, L_{rel}=0 system and quantify correlations.**

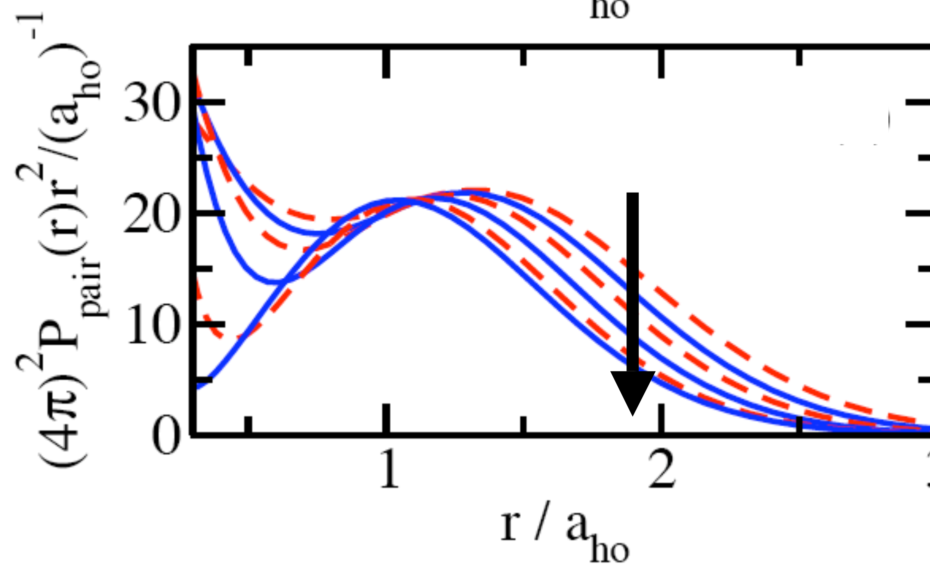
Structural Correlations (N=4): Pair Distribution Functions for $r_0=0.005a_{ho}$

"BCS side"

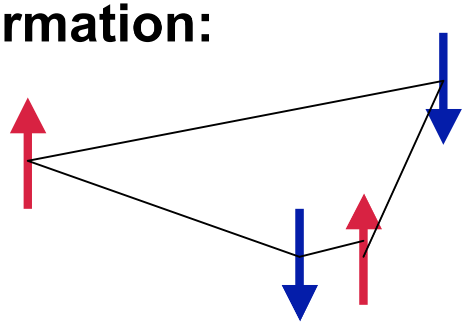


"BEC side"



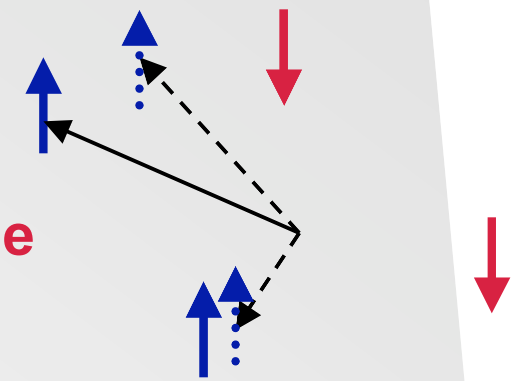


Development of two-peak structure indicates pair formation:



More Correlations: One-Body Density Matrix and Natural Orbitals

- **One-body density matrix:**
  $\rho(\underline{r}',\underline{r}) = N_{\uparrow} \int\ldots\int \Psi^*(\underline{r}',\underline{r}_2,\ldots,\underline{r}_N)\Psi(\underline{r},\underline{r}_2,\ldots,\underline{r}_N)d\underline{r}_2\ldots d\underline{r}_N$



- **Alternatively:**
  $\rho(\underline{r}',\underline{r}) = \langle\psi^+(\underline{r}')\psi(\underline{r})\rangle$, **where** $\psi^+(\underline{r}')$ **and** $\psi(\underline{r})$ **are field operators that create and destroy a particle at position** $\underline{r}$ **and** $\underline{r}'$.

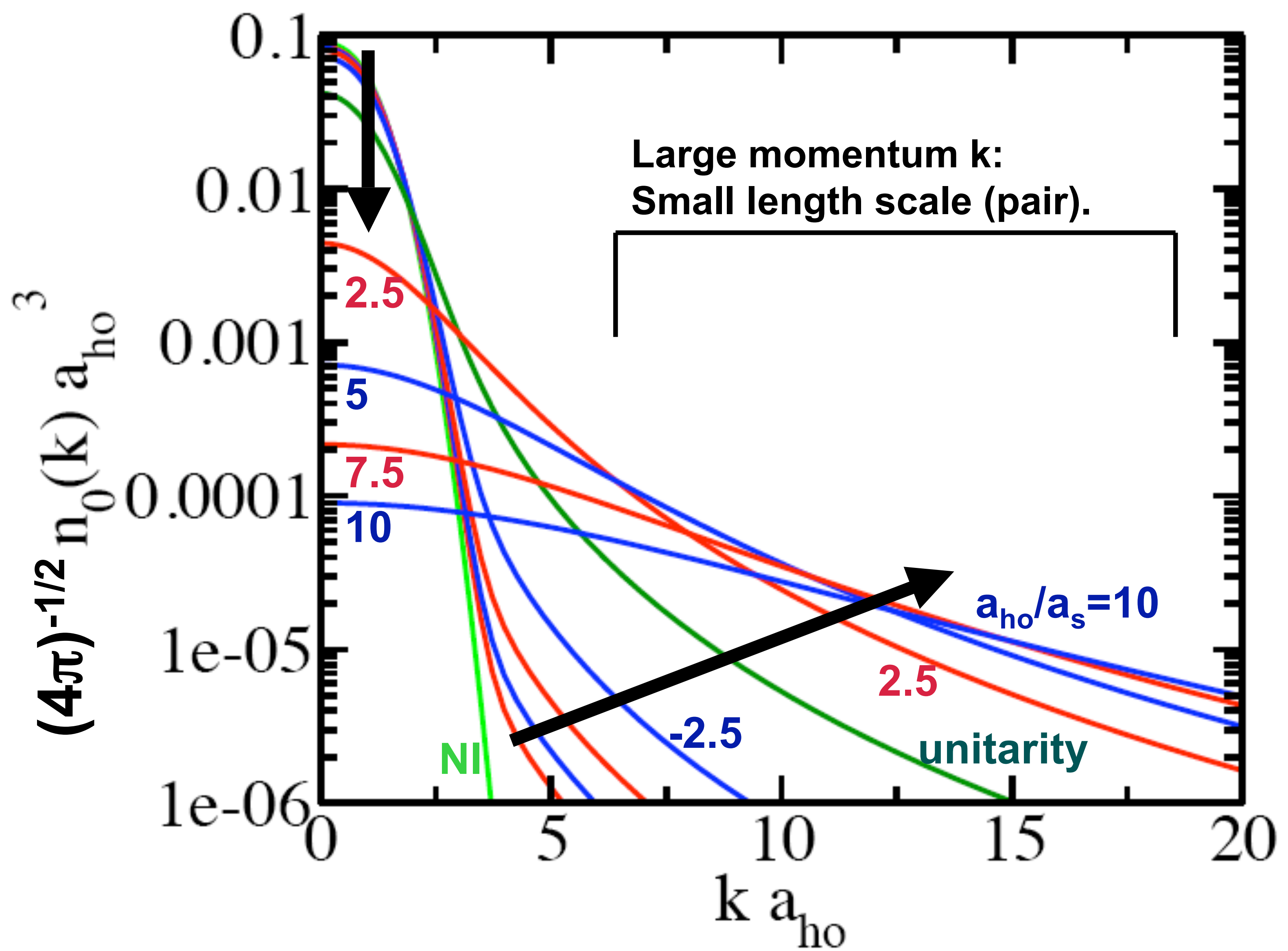
- **It follows:** $n(\underline{k}) = (2\pi)^{-3} \iint \exp[i\underline{k}\cdot(\underline{r}-\underline{r}')]\rho(\underline{r}',\underline{r})\, d\underline{r}d\underline{r}'$.

- **Partial wave decomposition:**
  $n(\underline{k}) = \Sigma_{lm}\, n_l(k)\, Y_{lm}(\theta_k,\varphi_k)$.

- **Then:** $\int n(\underline{k})d\Omega_k = (4\pi)^{1/2}\, n_0(k)$

Shown on next slide for N=4

l=0 Projection of Momentum Distribution for N=4



Universal Relations for ZR Interactions throughout Crossover due to Tan

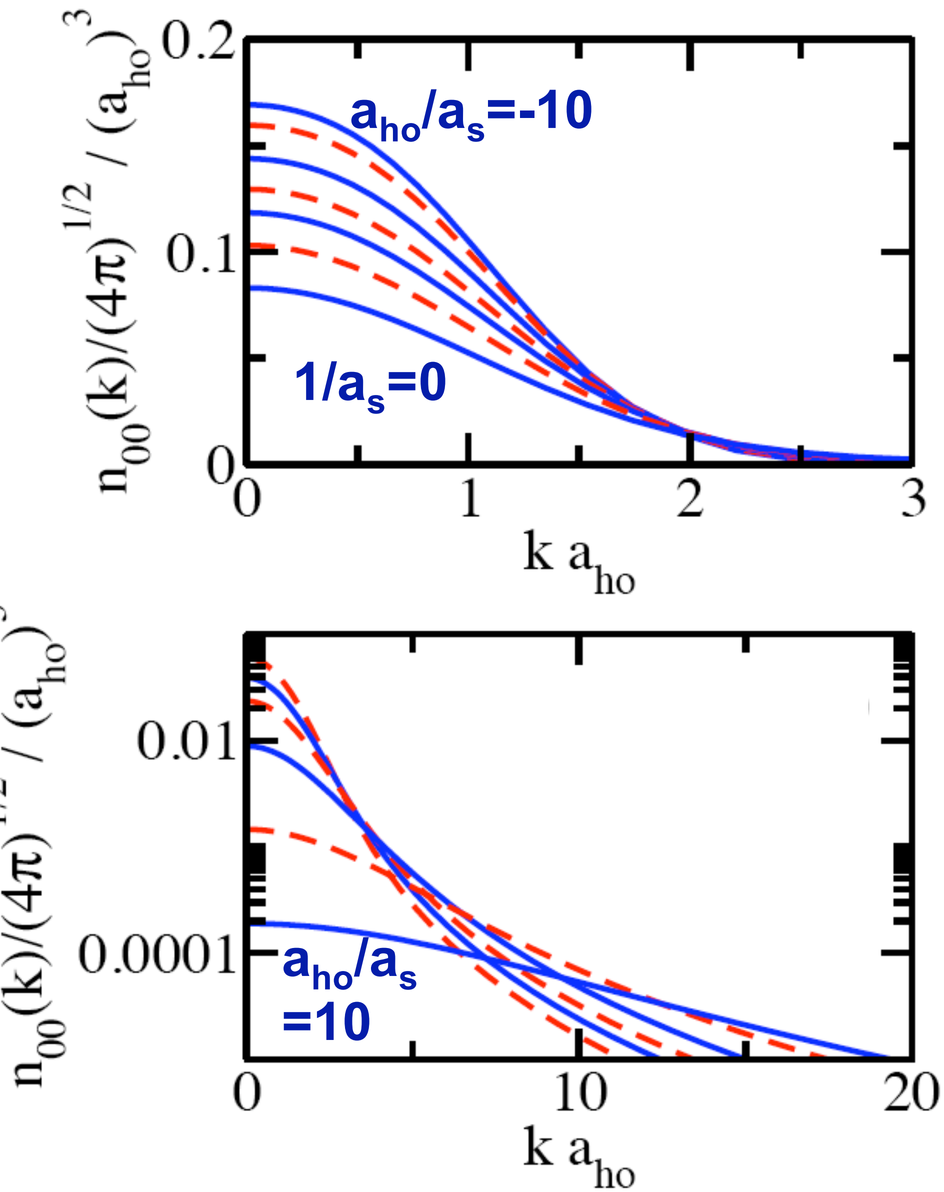
Quantitative relation between distinctly different quantities such as change of energy, trap energy, pair distribution function and momentum distribution, inelastic two-body loss rate,...

"Integrated contact intensity" $I(a_s)$ defined through momentum relation [Tan, Annals of Physics ('08)]: $I_k(a_s) = \lim_{K\to\infty} \pi^2 K N_{atom}(k>K)$.

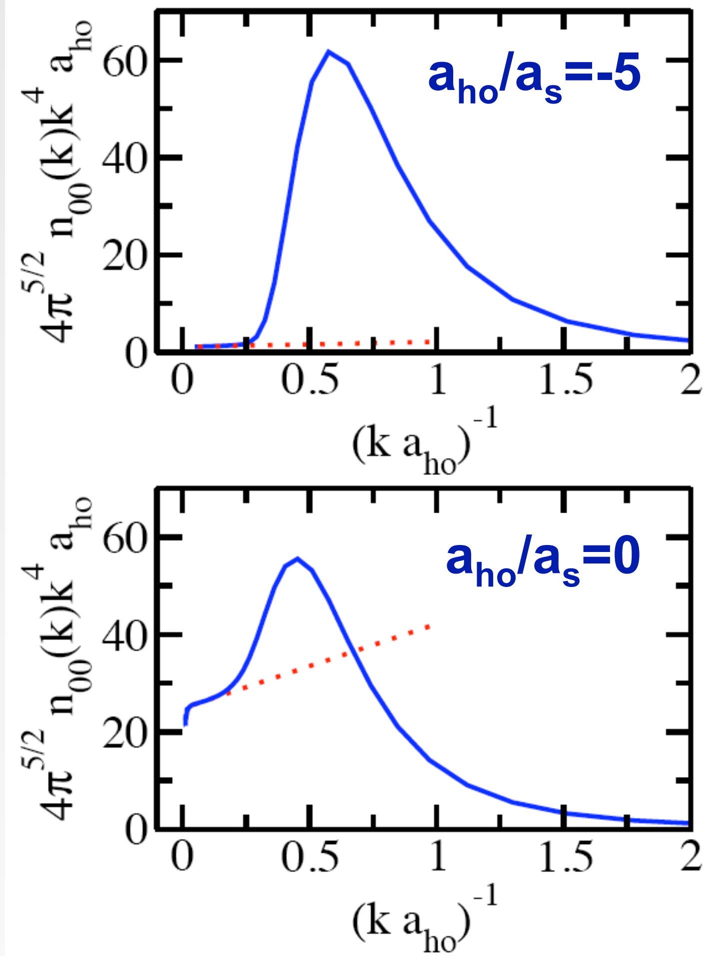
- It then follows:
  - Adiabatic relation: $\partial E(a_s,0)/\partial a_s = h^2/(16\,\pi^3 m a_s^2)\, I_{adia}(a_s)$.
  - Virial theorem: $E(a_s,0) = 2 \langle V_{trap}(a_s,0)\rangle - h^2/(32\pi^3 m a_s)\, I_{virial}(a_s)$.
  - Pair relation: $I_{pair}(a_s) = \lim_{s\to 0} 4\pi\, N_{pair}(r<s) / s$.

As a check, use all four relations to obtain $I(a_s)$.

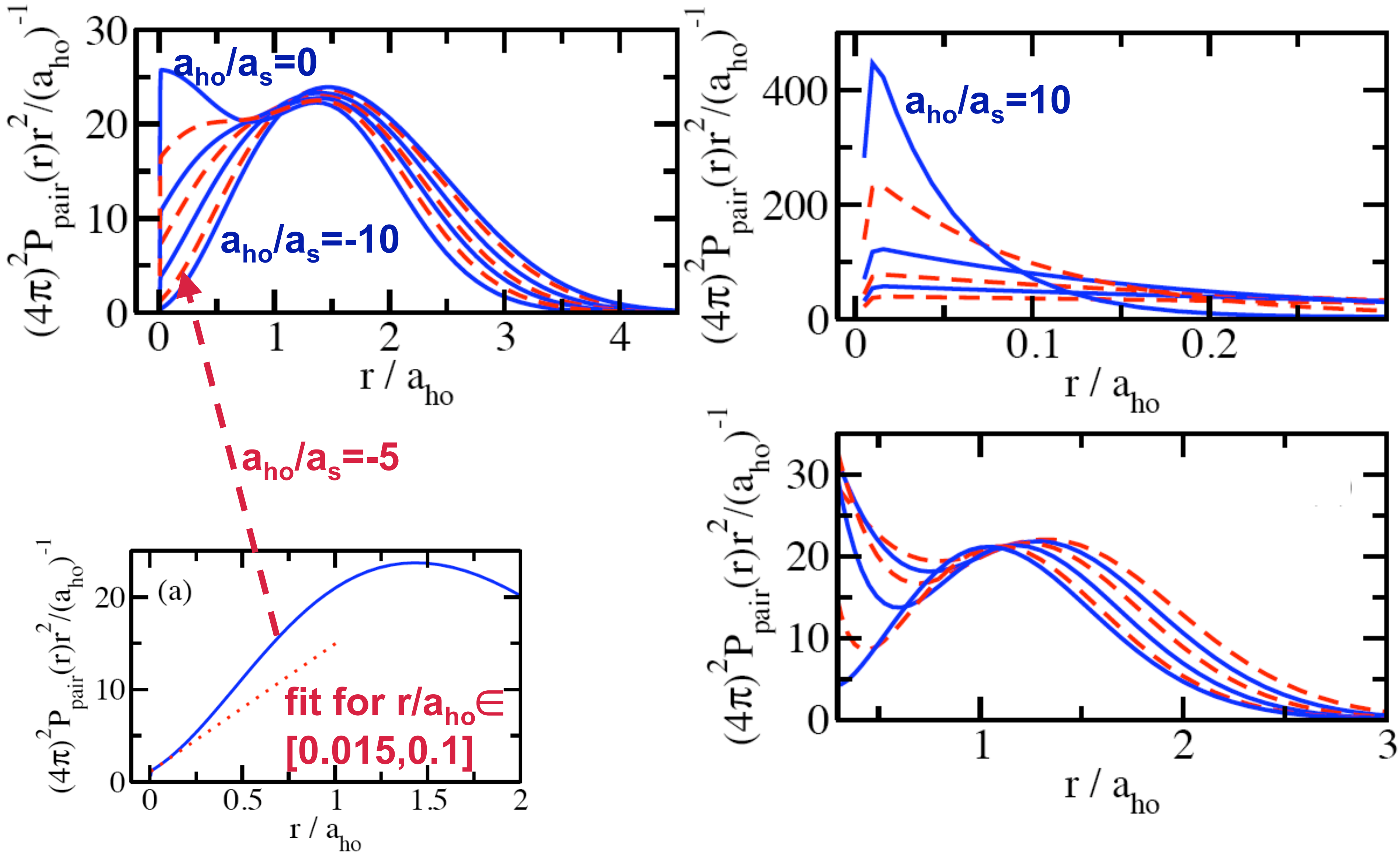
Lowest Partial Wave Projection of Momentum Distribution



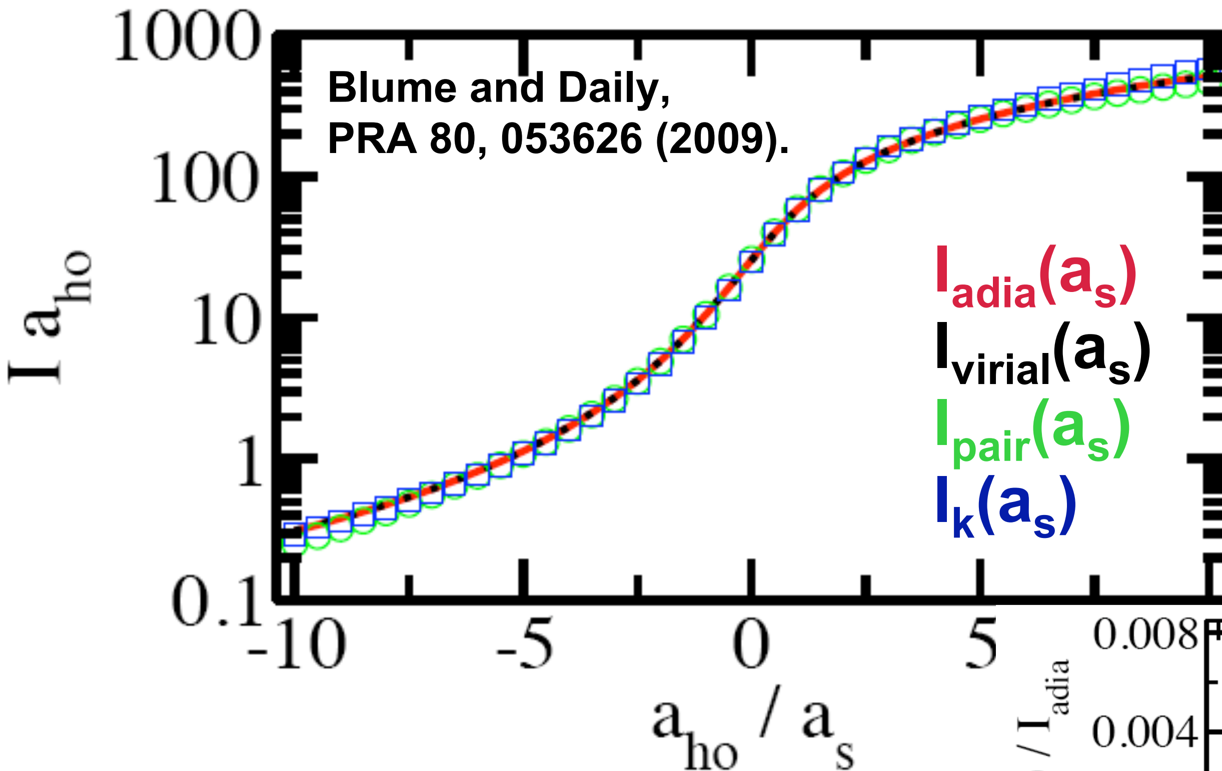
$I_{k,\uparrow}(a_s)$ =
$\lim_{1/k \to 0} 4\pi^{5/2} n_{00,\uparrow}(k) k^4$



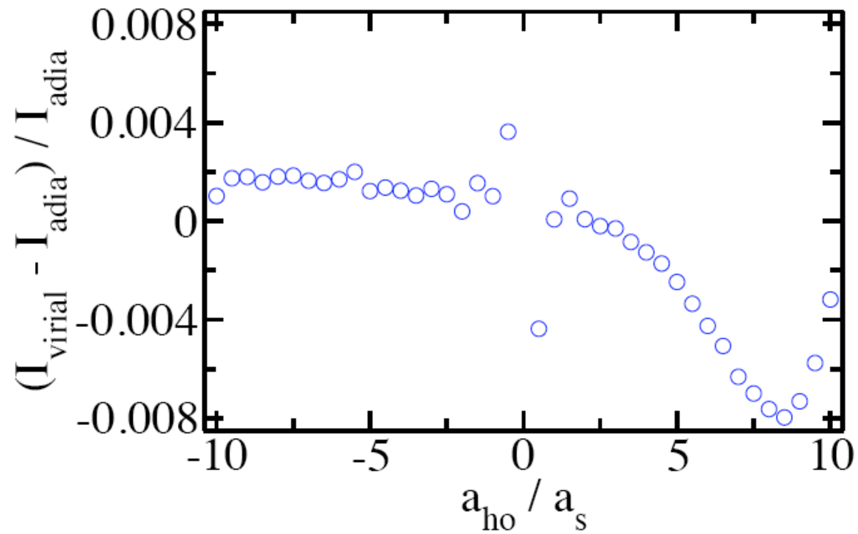
Pair Distribution Functions for N=4 ($r_0=0.005a_{ho}$)



Integrated Contact for Energetically Lowest Gas-Like State of N=4 System

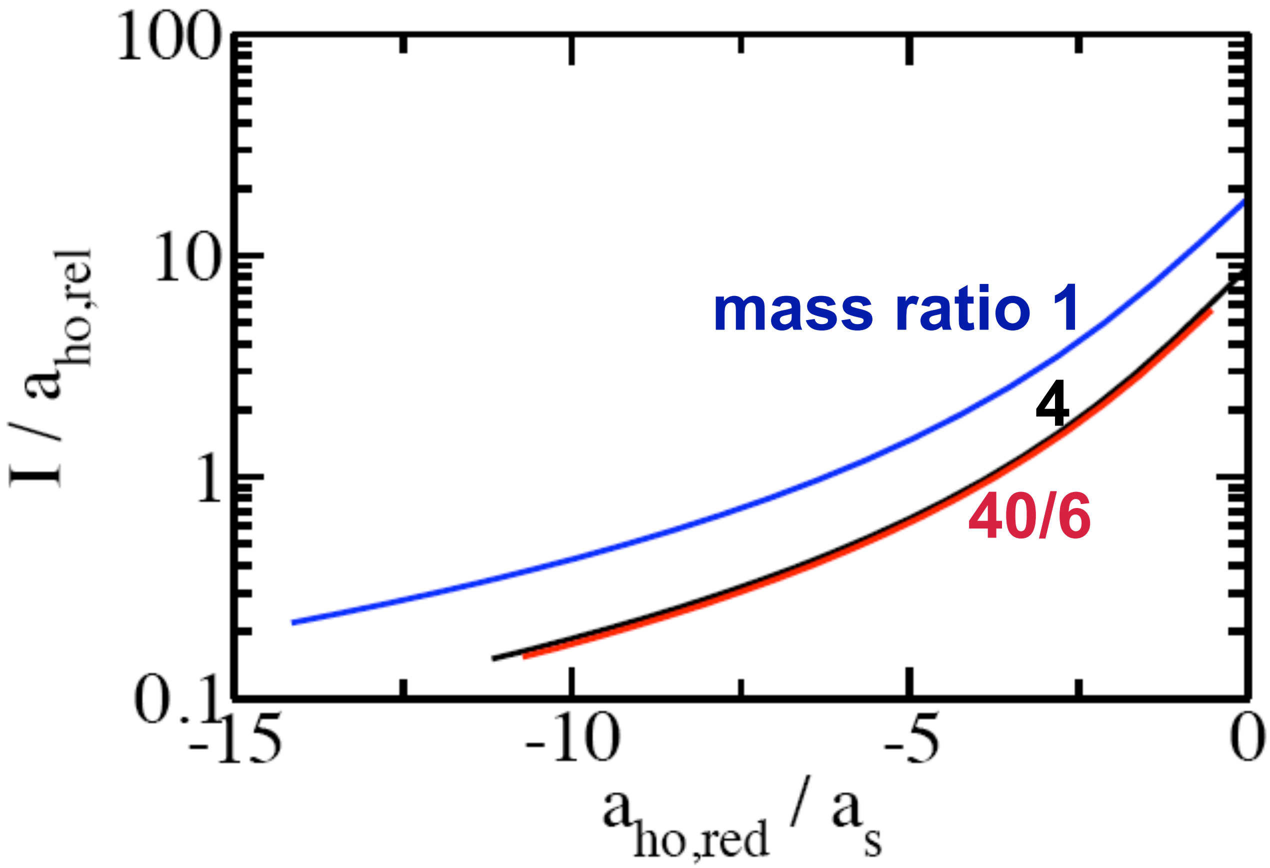


Recent experiments:
Hu et al., arXiv:1001.3200.
Stewart et al., arXiv:1002.1987.
Earlier work:
Partridge et al., PRL 95, 020404 (2005).



$I(a_s)$ changes by about three orders of magnitude throughout crossover.
Very good agreement among the four "different" $I(a_s)$.

Extension to Unequal-Mass Two-Component Fermi Gas: N=4 ($\omega_1=\omega_2$)



- Contact obtained from virial theorem.
- In good agreement with adiabatic relation and pair relation.
- We have not yet analyzed momentum distribution tail.

Question raised by Braaten et al., Werner/Castin,…:
Can these concepts be extended to regimes where Efimov trimers exist? The-day-before-yesterday's answer, probably yes.

Condensate Fraction on BEC Side

Astrakharchik et al., PRL 230405 (2005).

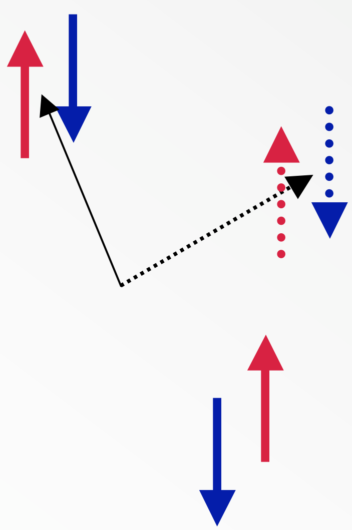
- Number of pairs: $\langle \Psi^{+}(\underline{r}_1')\Psi^{+}(\underline{r}_2')\Psi(\underline{r}_1)\Psi(\underline{r}_2)\rangle$

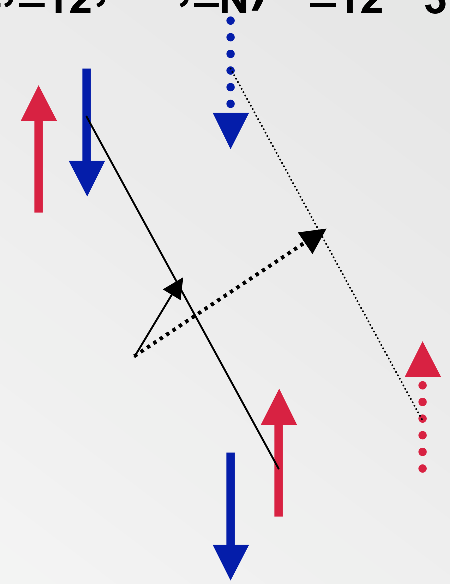
up-down position vectors

- Pair density matrix:

$$\rho(\underline{R}',\underline{R}) = (N/2)\int\ldots\int\Psi^{*}(\underline{R}',\underline{r}_{12},\ldots,\underline{r}_N)\Psi(\underline{R},\underline{r}_{12},\ldots,\underline{r}_N)d\underline{r}_{12}d_3\ldots d\underline{r}_N$$

CM of up-down pair



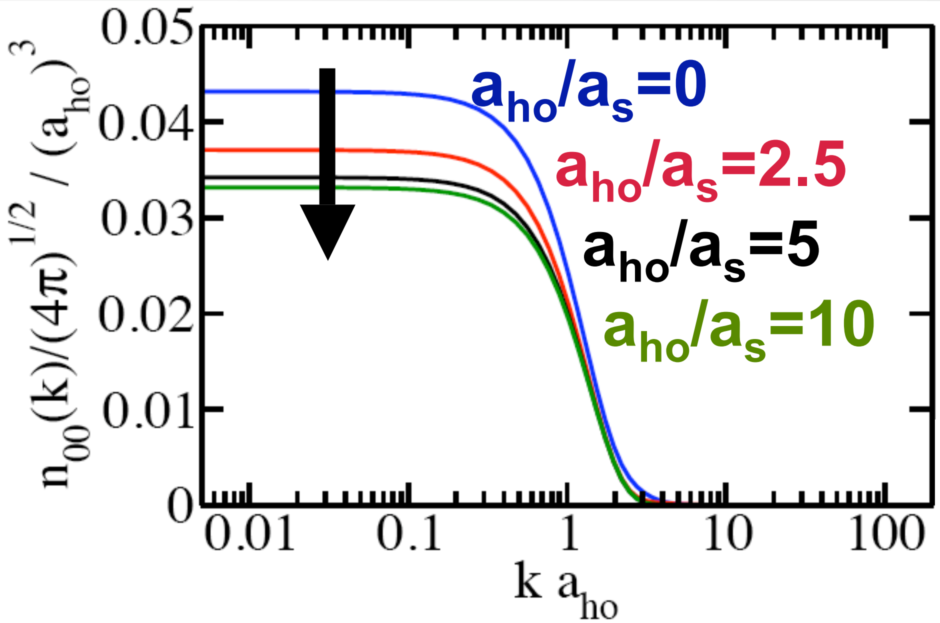


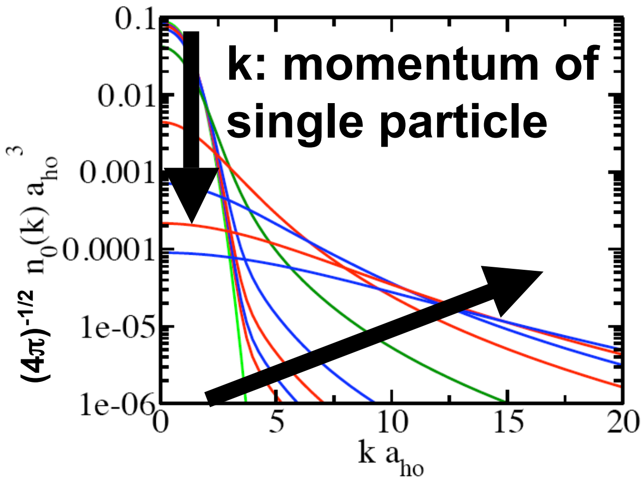
Pair remains "in tact": "good CM vector". $\rho(\underline{R}',\underline{R})$ has notable amplitude for all R' and R inside trap.

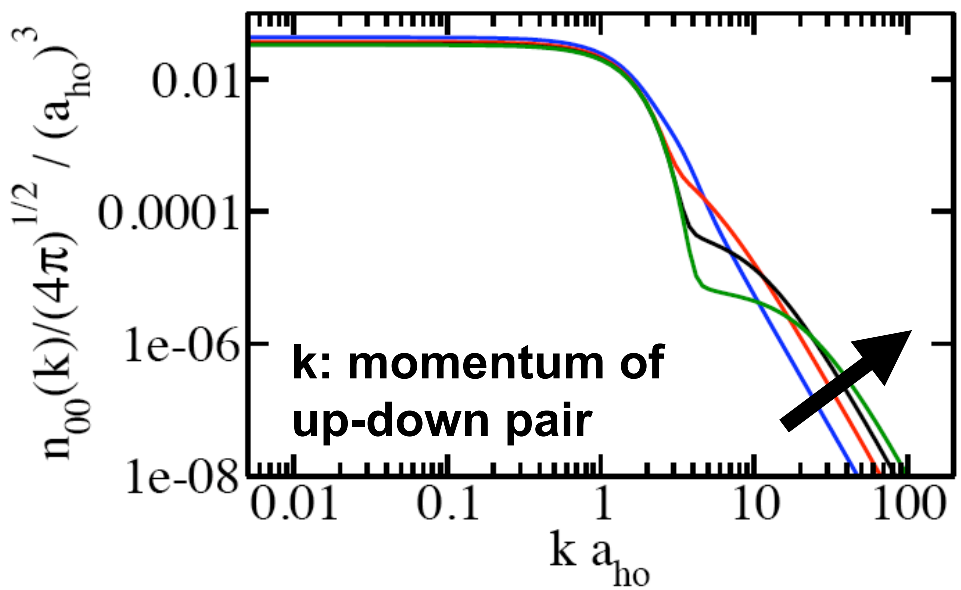
Pair "destroyed": "bad CM vector". $\rho(\underline{R}',\underline{R})$ has notable amplitude only for $\underline{R}' \sim \underline{R}$.

l=0 Projection of Momentum Distribution for CM of Pair (N=4, L_{rel}=0)

Preliminary results:







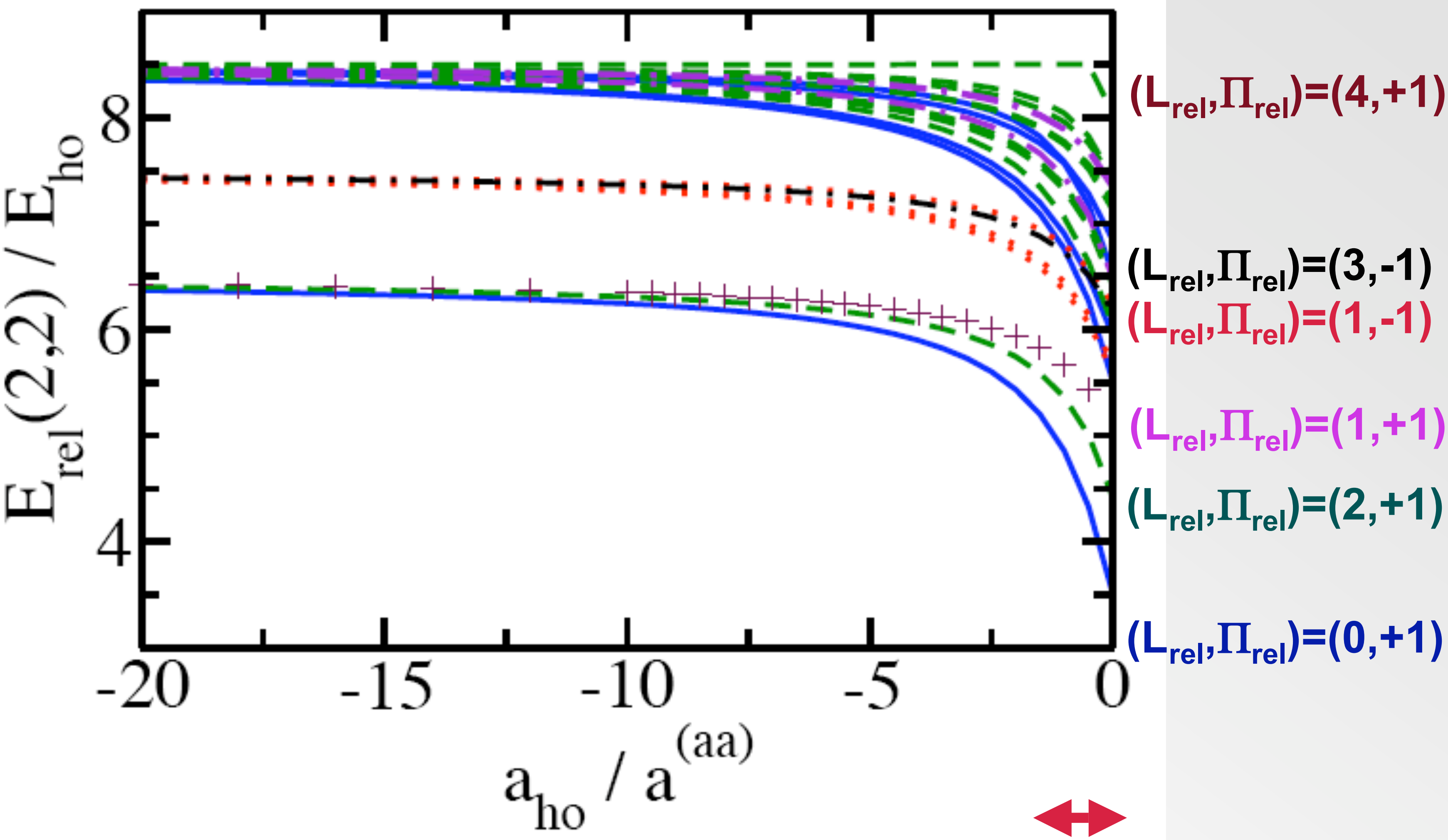
Two-peak structure: Signature of pair formation. Future: Want to quantify condensate fraction.

Two-Third Summary: Correlations of Two-Component Few-Fermion System

- Tool: Stochastic variational approach (combination of analytics and numerics).
- Examplary analysis for N=4 (L_{rel}=0):
  - Pair correlation functions.
  - Momentum distribution.

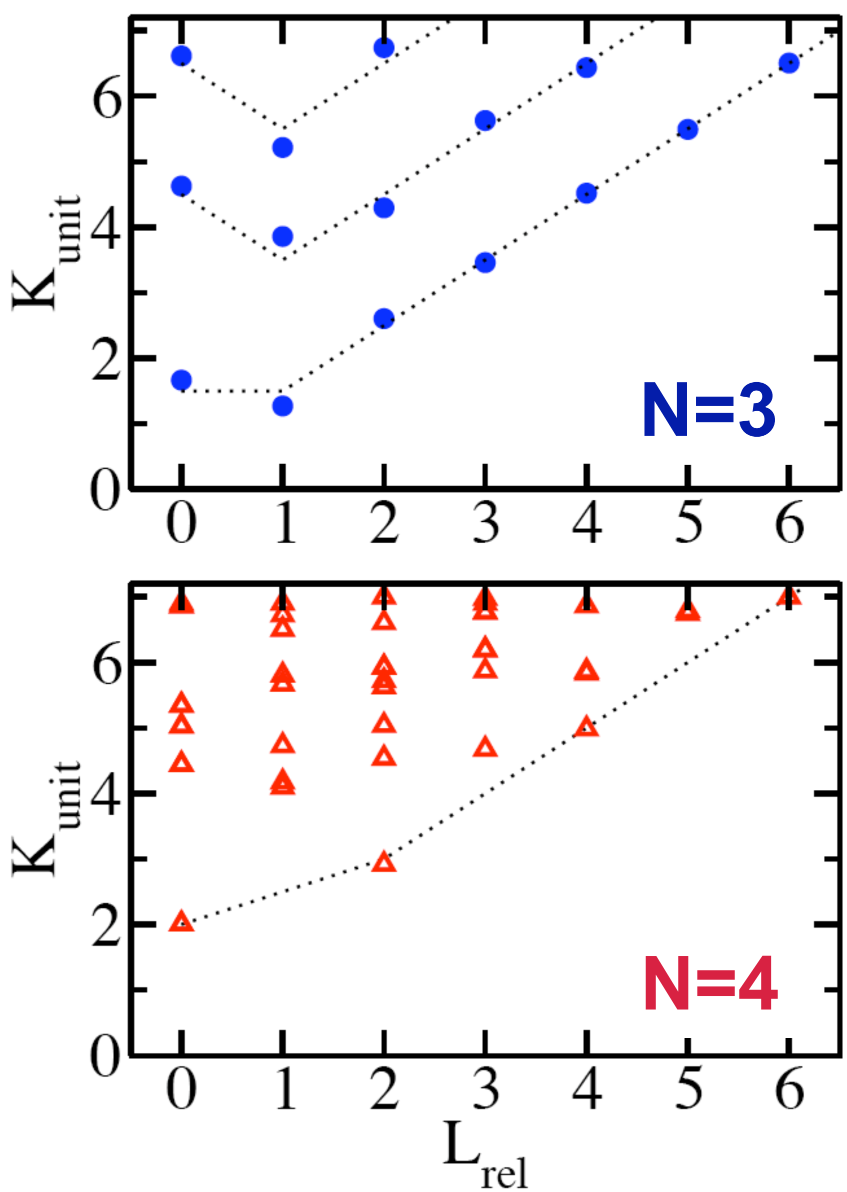
- Outlook:
  - Toward determining the entire energy spectrum of small few-fermion systems:
    - Stochastic variational approach.
    - Semi-analytical perturbative approach.
  - Monte Carlo study for larger N.

Trapped Four-Fermion Spectrum: Lowest Three Energy Manifolds



strongly-interacting (overlapping energy manifolds)

Natural Parity States at Unitarity for Three- and Four-Fermion Systems



For N=3: Werner and Castin, PRL 97, 150401 (2006); huge body of earlier work...
For N=4: Daily and Blume (submitted); L_{rel}=0: von Stecher and Greene, PRA 80, 022504 (2009).

$$E_{rel,unit} = (2q+K_{unit}+3/2)h\nu$$

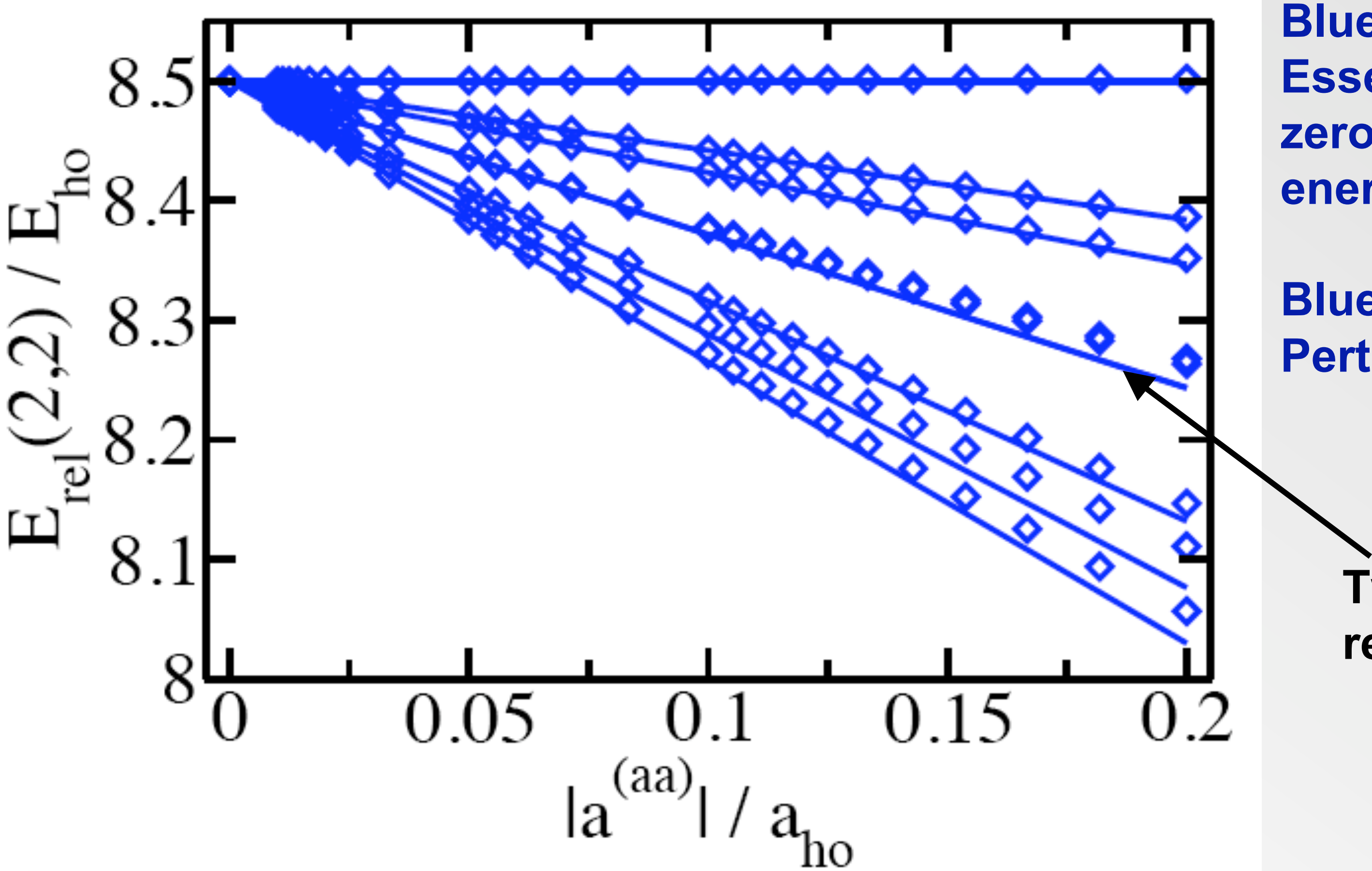
Energies of three-fermion system obtained by solving transcendental equation.

Energies of four-fermion system obtained by stochastic variational approach (extrapolation of finite-range energies to zero-range limit).

Future goal: Similar calculations for unnatural parity states of four-fermion system…

Perturbative Treatment for Weakly-Interacting Four-Fermion Gas (L_{rel}=2)

K. M. Daily and D. Blume (submitted).



Blue symbols: Essentially exact zero-range energies.

Blue lines: Perturbative results.

Current work: Determine perturbative energy shifts for large number of energy manifolds and calculate fourth-order virial coefficient (expected to be qualitatively correct up to $a_{ho}/|a^{(aa)}| \approx 2$).

Excitation Gap and Residual Oscillations at Unitarity

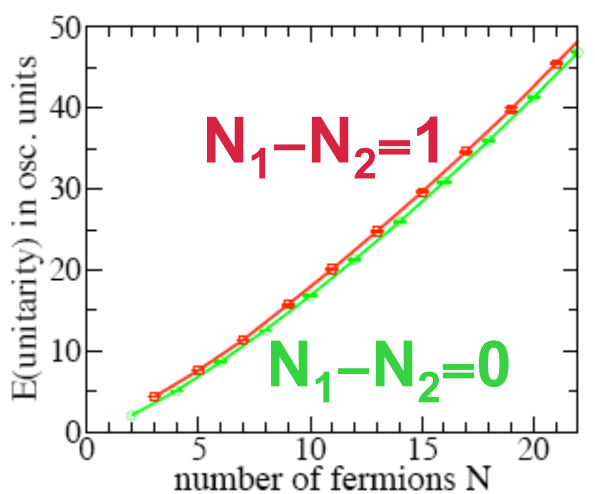
Blume/von Stecher/ Greene:
PRL 99, 233201 (2007);
PRA 77, 043619 (2008).

See also, Chang and Bertsch,
PRA 76, 021603(R) (2007).

N odd, $N=N_1+N_2$ and $N_1=N_2+1$

$$\Delta(N) = E(N_1, N_2) - \frac{1}{2}\left[E(N_1 - 1, N_2) + E(N_1, N_2 + 1)\right]$$

Fixed-node diffusion Monte Carlo



$$E_{fit}(N) = \sqrt{\xi_{tr}} E_{NI,ETF}$$