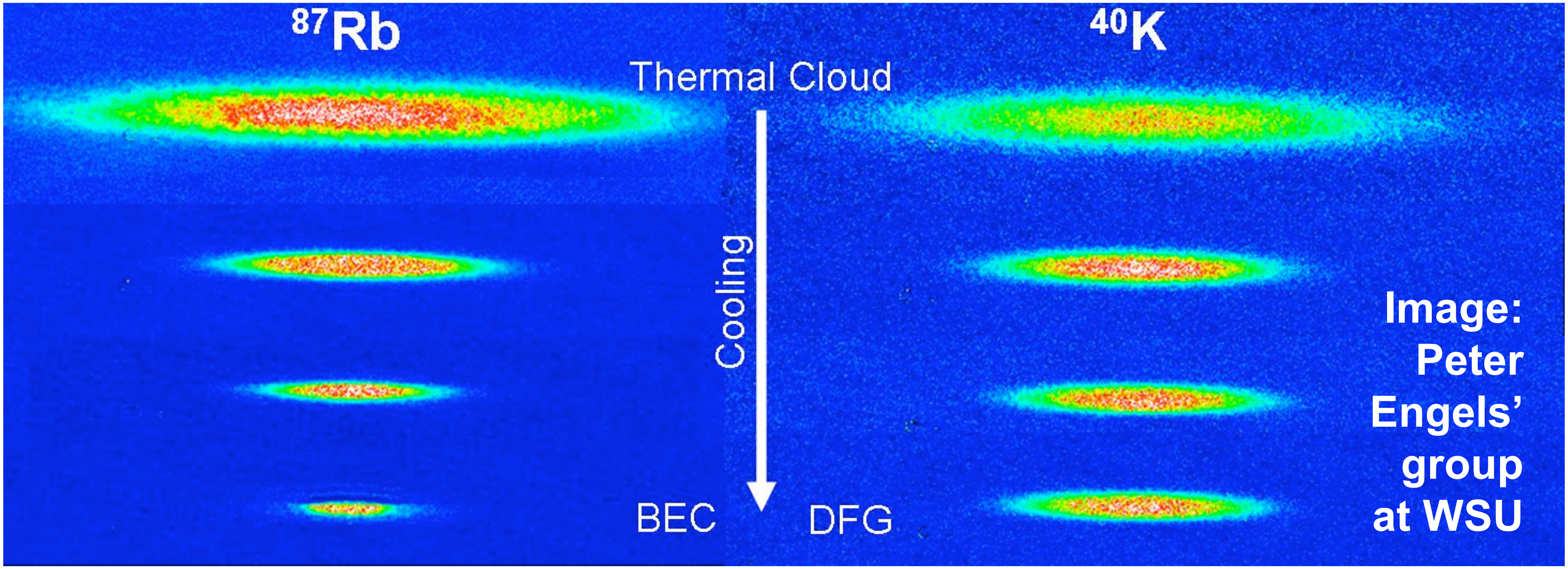

Universal Behavior of Small Two-Component Fermi Gases with Equal Masses

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At JILA: Chris Greene, Javier von Stecher, Seth Rittenhouse, John Bohn, Shai Ronen, Danielle Bortolotti.
At BEC Center in Trento: Stefano Giorgini, Grigori Astrakharchik.

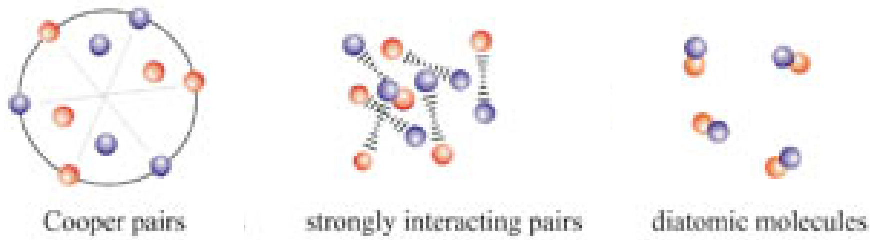
Supported by NSF and ARO.

Outline of This Talk

Graphics from JILA homepage.

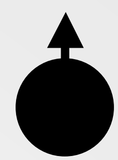
BCS **BEC**

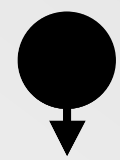
Weak attraction



Weak repulsion

- **Introduction:**
  - BCS (Bardeen-Cooper-Schrieffer) to BEC (Bose-Einstein condensation) crossover.





- **Techniques employed:**
  - Semi-analytical perturbative approach.
  - Semi-stochastic variational approach.
  - Monte Carlo techniques.

- **Examples of our trapped few-fermion studies:**
  - Universality throughout crossover and at unitarity.
  - Energetics and structure (pair distribution function and momentum distribution).

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

Weakly-attractive atomic Fermi gas

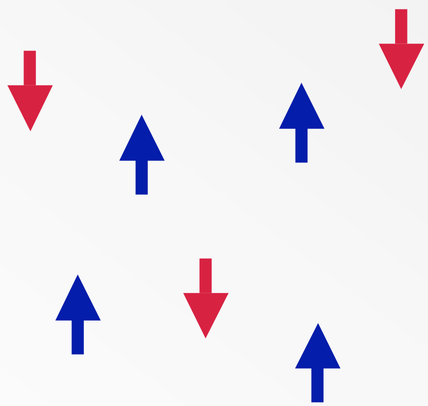
"BCS"

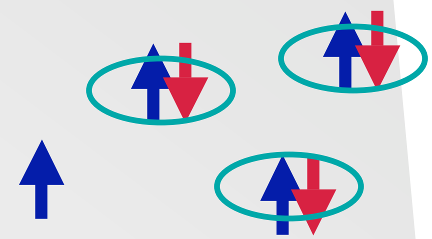
Strongly-interacting (unitarity)

"BEC"

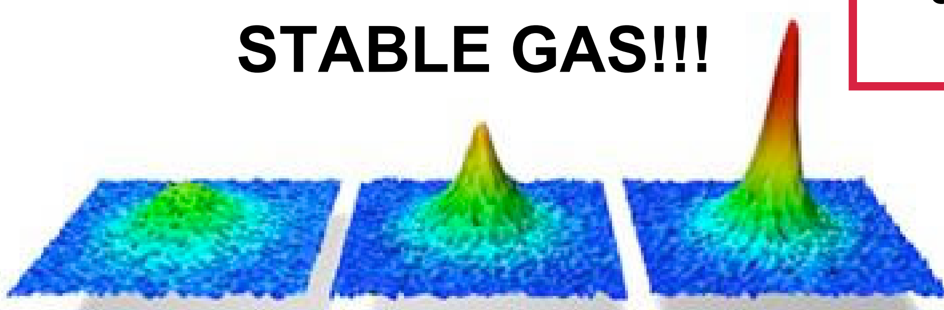
a_{ho}/a_s

Weakly-repulsive molecular Bose gas





STABLE GAS!!!



Images (experiment): Jin group, JILA.

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

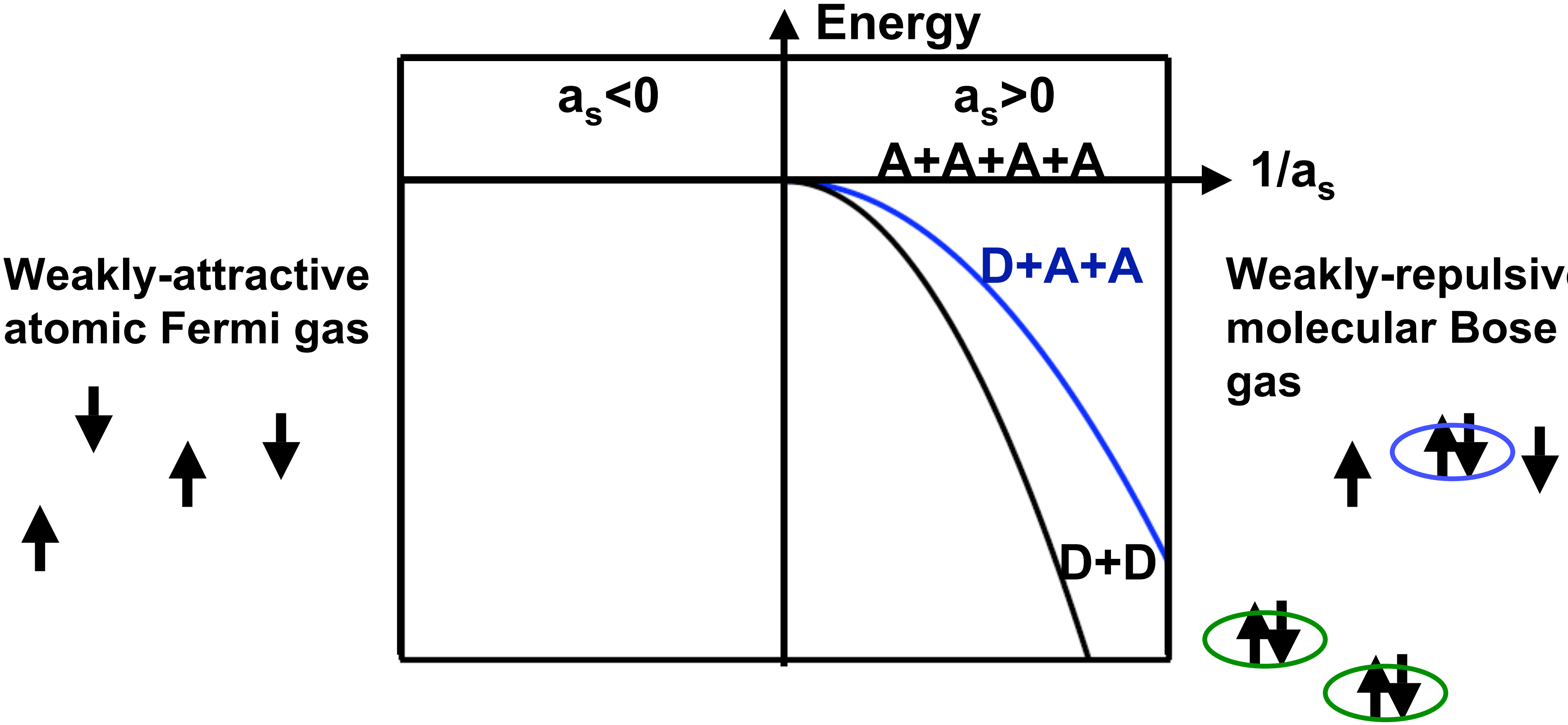
Dilute gas:

$r_0 \ll a_{ho}$, a_s or

$n(0)r_0^3 \ll 1$.

Two-Component Equal-Mass Fermi Gas: Four-Particle System in Free Space

Weakly-attractive atomic Fermi gas



Weakly-repulsive molecular Bose gas

Weakly-bound three- and four-body bound states are absent.
Atom-dimer s-wave scattering length $a_{ad} \approx 1.2a_s$.
Dimer-dimer s-wave scattering length $a_{dd} \approx 0.6a_s$.

Petrov, PRA 67, 010703 (R) (2003); Petrov, Salomon, Shlyapnikov, PRL 93, 090404 (2004).

What is Interesting about Two-Component Fermi Gases?

- Clean model system (no impurities).
- Tunability of interaction strength and confinement.
- Strongly-interacting regime can be reached.

- Realization of Yang-Gaudin model.
- Realization of polaron physics.
- Model for high-T_c superconductivity?
- Many other model Hamiltonian…

- Simple but non-trivial.
- Cross-disciplinary.

Relevance Beyond Atomic Physics: Nuclear Physics.

- Universal behavior (large scattering length a_s):
  - Nuclear: neutron-neutron a_s = -18fm (effective range 2.8fm). Desirable: low density neutron matter.
  - Atomic: Tunability of a_s near Feshbach resonance.

Experiment: Jin, Ketterle, Hulet, Thomas,… groups.

- Three-component system:
  - Nuclear: low density: nucleon = tri-quark bound state; high density: quark color superconductor.
  - Atomic: Fermi gas with three internal states.

Experiment: Jochim, O'Hara groups.

- Efimov effect/physics:
  - Nuclear: 2n-rich halo nuclei, ^{12}C
  - Atomic: ^4He trimer, Cs_2+Cs, K_2+K, three-body collisions.

Experiment: Grimm, Inguscio,… groups.

Microscopic Many-Body Hamiltonian of Trapped Two-Component Gas

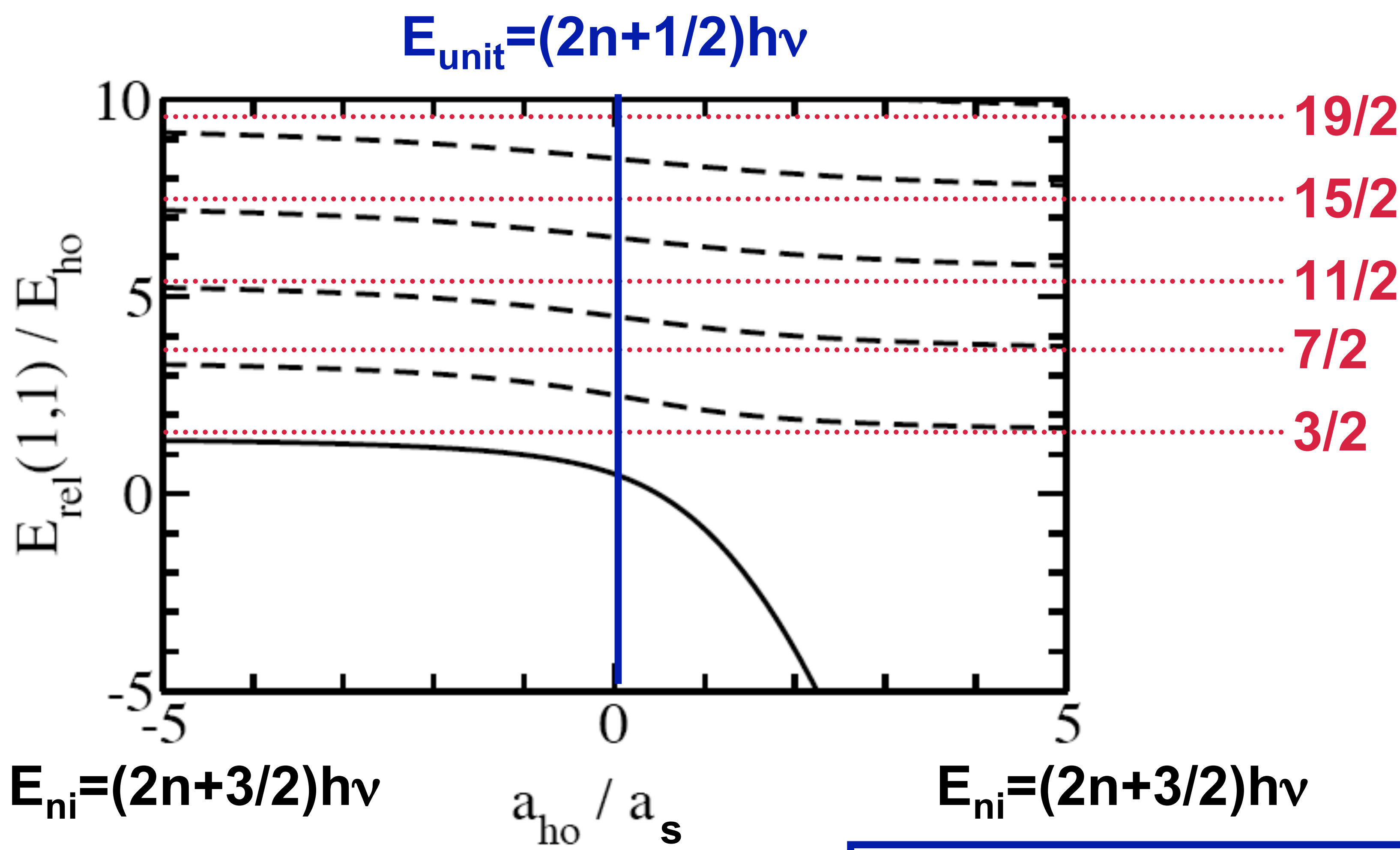
$$H = \sum_{i=1}^{N} \left[\frac{-\hbar^2}{2m} \vec{\nabla}^2_{\vec{r}_i} + \frac{1}{2} m \omega^2 \vec{r}_i^{\,2} \right] + V_{int}(\vec{r}_1, \ldots, \vec{r}_N)$$

$$V_{int}(\vec{r}_1, \ldots, \vec{r}_N) = \sum_{i=1}^{N_\uparrow} \sum_{j=N_\uparrow+1}^{N} V_{TB}(\underbrace{\vec{r}_i - \vec{r}_j}_{r_{ij}})$$

- Angular momentum L and parity π are good quantum numbers.

- V_{TB} chosen conveniently:
  - Perturbative treatment: Zero-range pseudo potential.
  - Stochastic variational treatment: Gaussian interaction.
  - Monte Carlo treatment: Square well interaction.

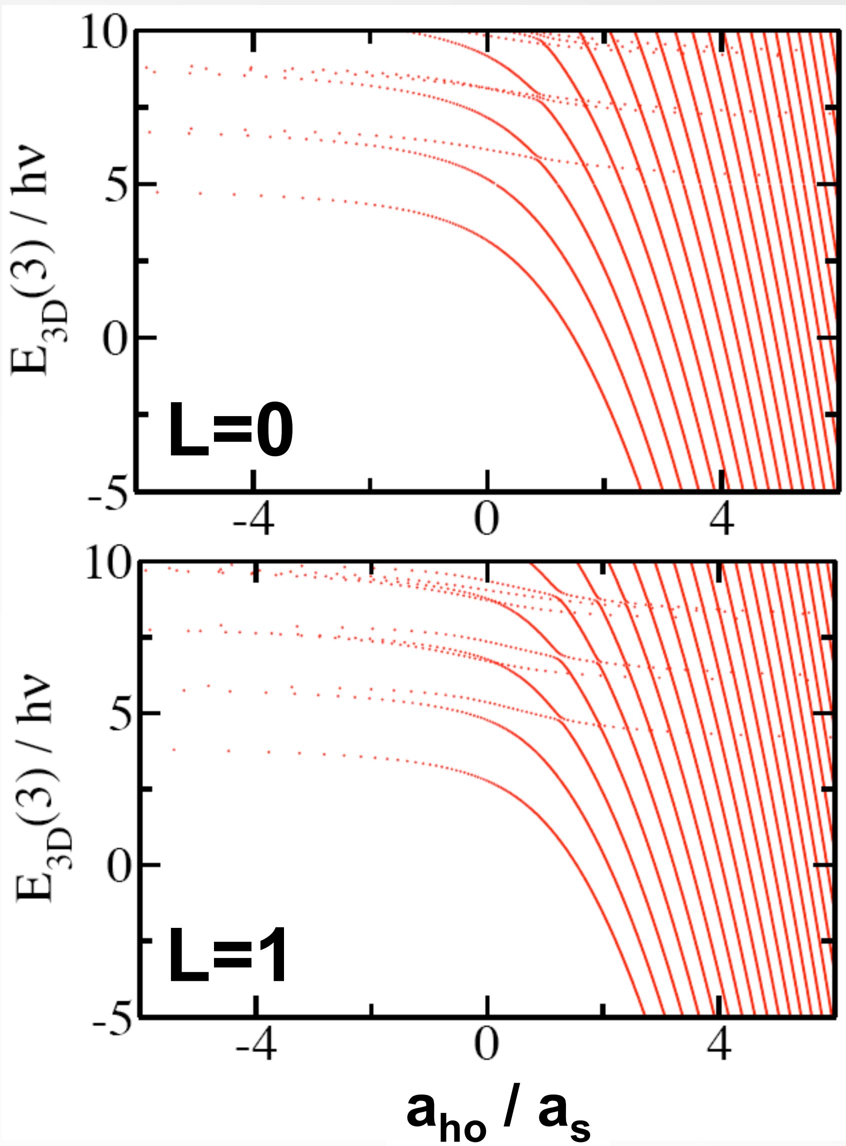
Two s-Wave Interacting Particles in External Spherically Harmonic Trap



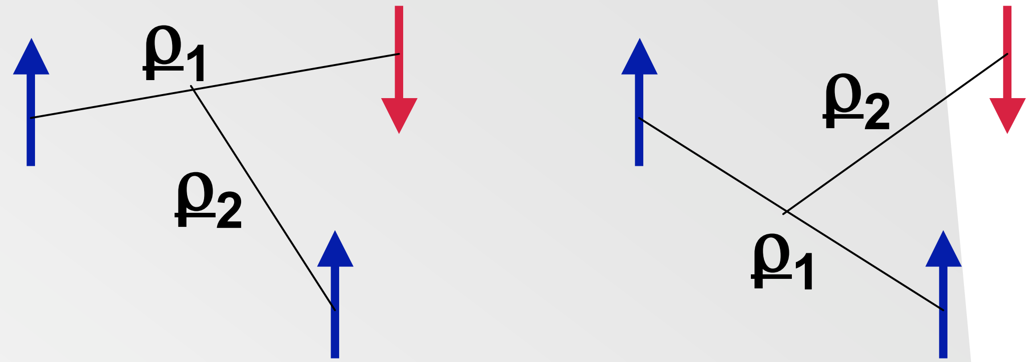
Analytical treatment:
Busch et al., Found. of Phys. (1998).

Finite angular momentum:
$E_{nl}=(2n+l+3/2)h\nu$

Three S-Wave Interacting Fermions Under Harmonic Confinement



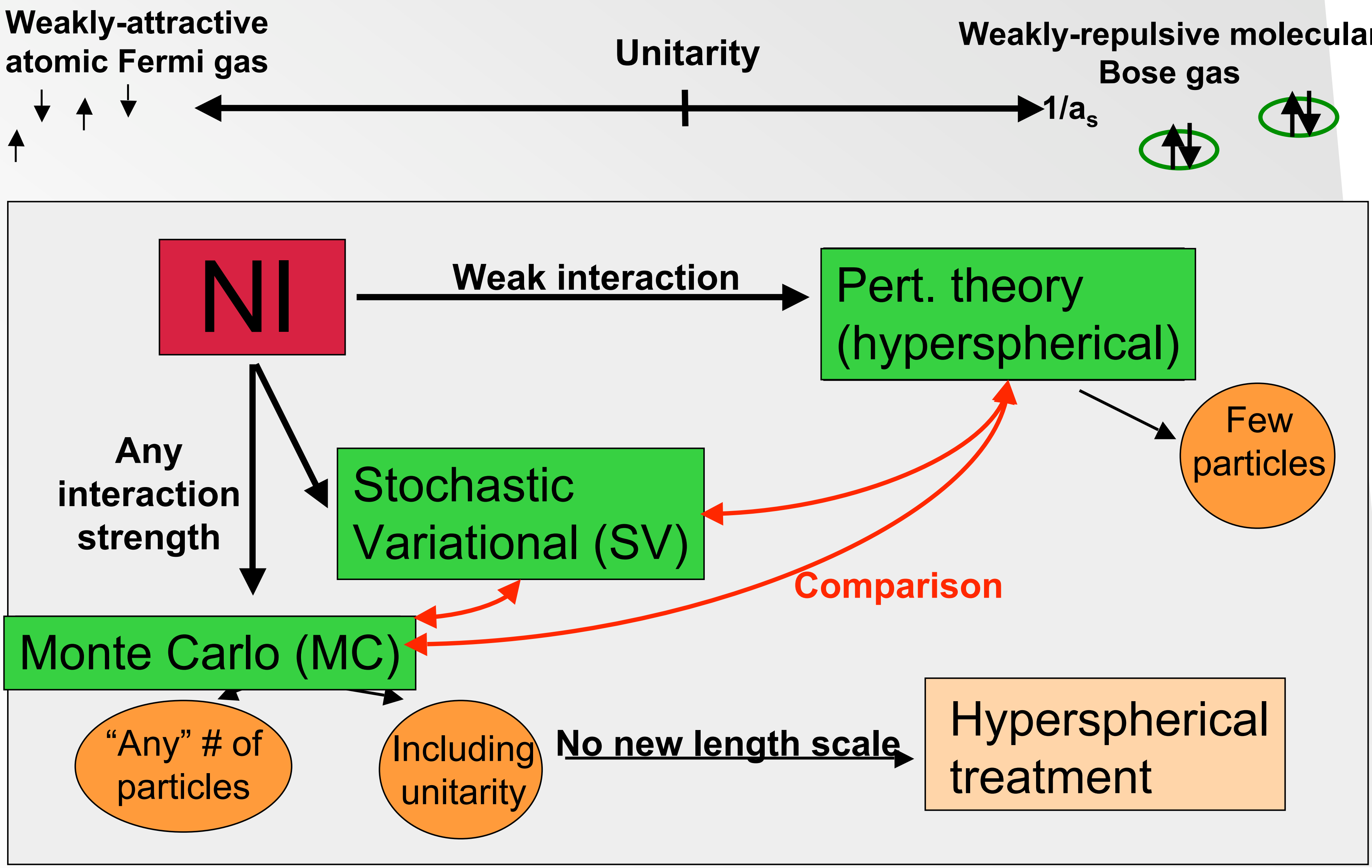
Jacobi vectors:



Questions:
How to understand mess of energy levels?
What to do with the spectra?

[calculated following Kestner and Duan, PRA 76, 033611 (2007)]:

Roadmap: Multifaceted Approach to Understanding System



Weak Interactions: First Order Degenerate Perturbation Theory

$$V_{int}(\vec{r}_1, \ldots, \vec{r}_N) = \frac{4\pi\hbar^2}{m} a_s \sum_{i=1}^{N_\uparrow} \sum_{j=N_\uparrow+1}^{N} \delta(\vec{r}_{ij})$$

For a degenerate subspace, must diagonalize V_{jk} matrix:

$$V_{jk} =< \Psi^j_{NI}(\vec{r_1} \ldots \vec{r_N})|V_{int}|\Psi^k_{NI}(\vec{r_1}, \ldots, \vec{r_N}) >$$

- Cartesian coordinates (brute force approach):
  - Ψ_{NI} readily constructed (product of two Slater determinants).
  - Ψ_{NI} not eigenstates of L^2, L_z, π.

- Hyperspherical coordinates (smarter approach):
  - CM degrees of freedom separated off.
  - Ψ_{NI} constructed to be eigenstates of L^2, L_z, π.

Construction of NI Wave Function in Hyperspherical Coordinates

$$M = Nm$$

$$R^2 = \frac{1}{N}\sum_{i=1}^{N}(\vec{r}_i - \vec{R}_{CM})^2$$

$$\Psi_{NI}(\vec{r}_1, \ldots, \vec{r}_N) = G(\vec{R}_{CM})F(R)\Phi(\vec{\Omega})$$

$$E_{\nu n}^{NI} = \left(2n + \nu + \frac{3}{2}\right)\hbar\omega + E_{CM}$$

$$H_{NI} = H_{CM} - \frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial R^2} + \frac{3N-4}{R}\frac{\partial}{\partial R}\right) + \frac{\Lambda^2}{2MR^2} + \frac{1}{2}M\omega^2R^2$$

$$H_{CM} = \frac{-\hbar^2}{2M}\vec{\nabla}^2_{CM} + \frac{1}{2}M\omega^2R^2_{CM}$$

$$E_{CM} = (2n_{CM} + l_{CM} + 3/2)\hbar\omega$$

Reduce deg. of freedom.
Remove CM energy spectrum.

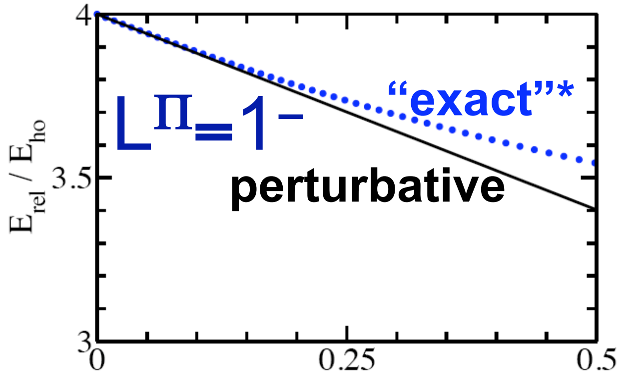
$$\Lambda^2\Phi_{\lambda,\mu}(\vec{\Omega}) = \hbar^2\lambda(\lambda + 3N-5)\Phi_{\lambda,\mu}(\vec{\Omega})$$

Anti-symmetrization.

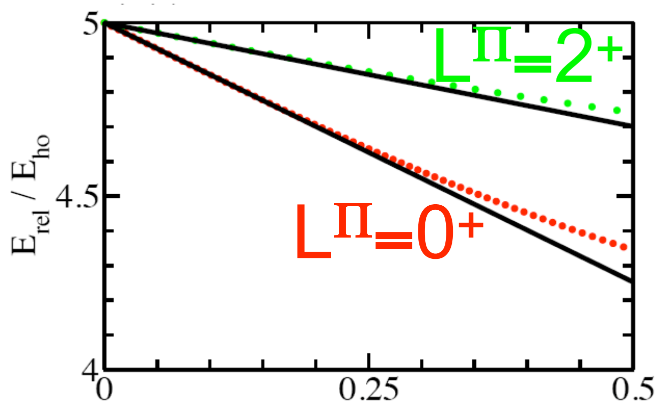
$$H_R = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2} + \frac{\hbar^2\nu(\nu+1)}{2MR^2} + \frac{1}{2}M\omega^2R^2$$

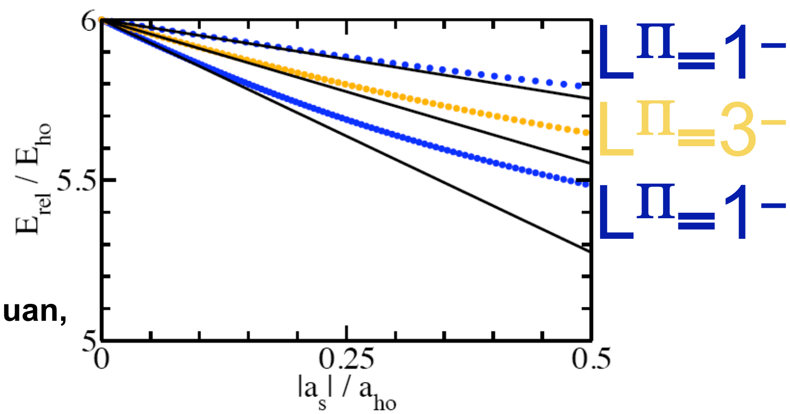
ν(λ,N) - non-integer.
Simple HO solution.

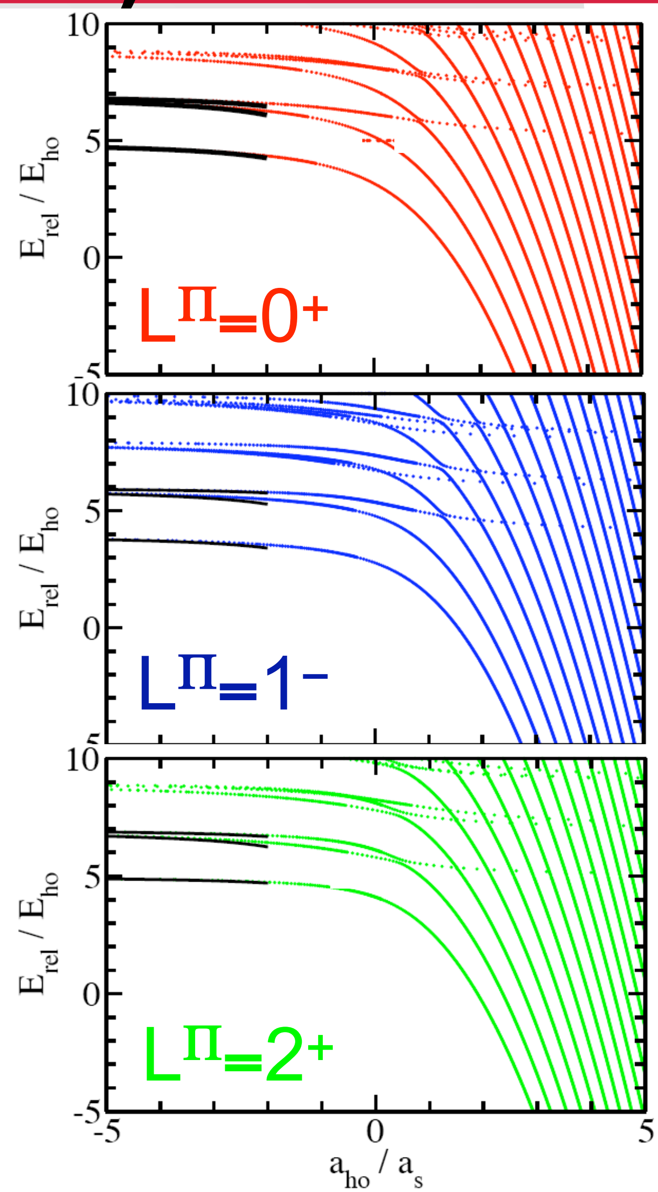
Energy Spectrum for N=3: Perturbative Treatment (Weak Attraction)



$E^{(1)} \approx E^{(0)} + \Delta E^{(1)}$
(diagonalize $\langle \Psi^{(0)} | V_{int} | \Psi^{(0)} \rangle$;
potential matrix elements evaluated analytically)



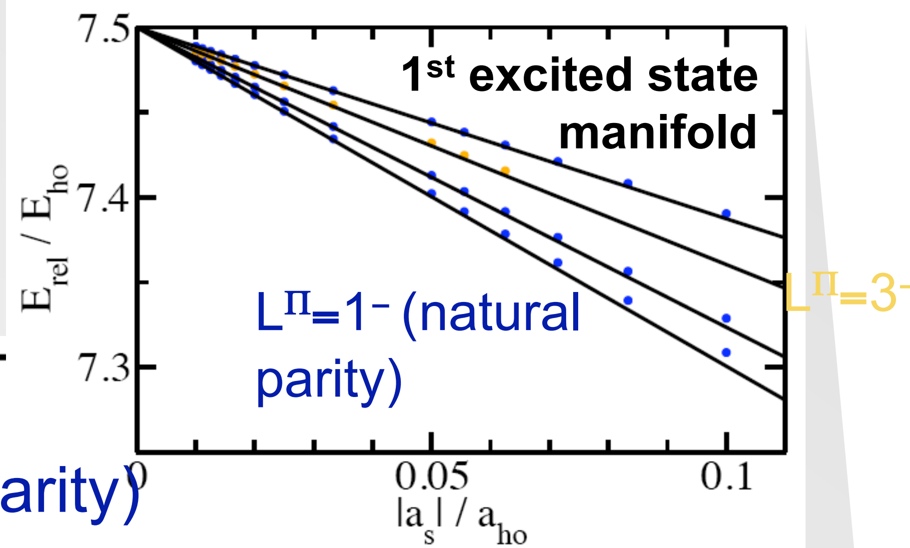


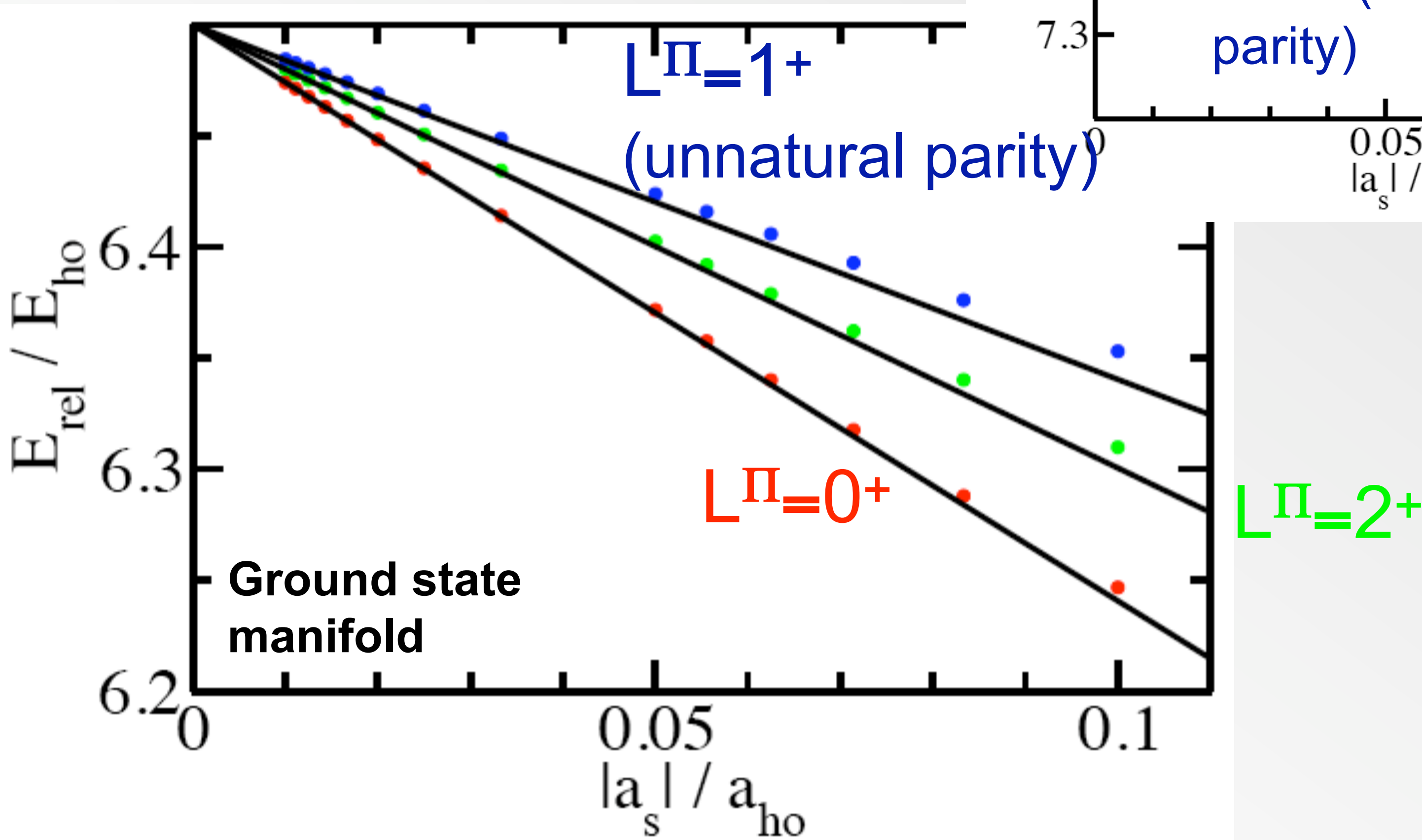


*method of Kestner and Duan, PRA 76, 033611 (2007)

Perturbative Treatment for N=4: Weak Attraction

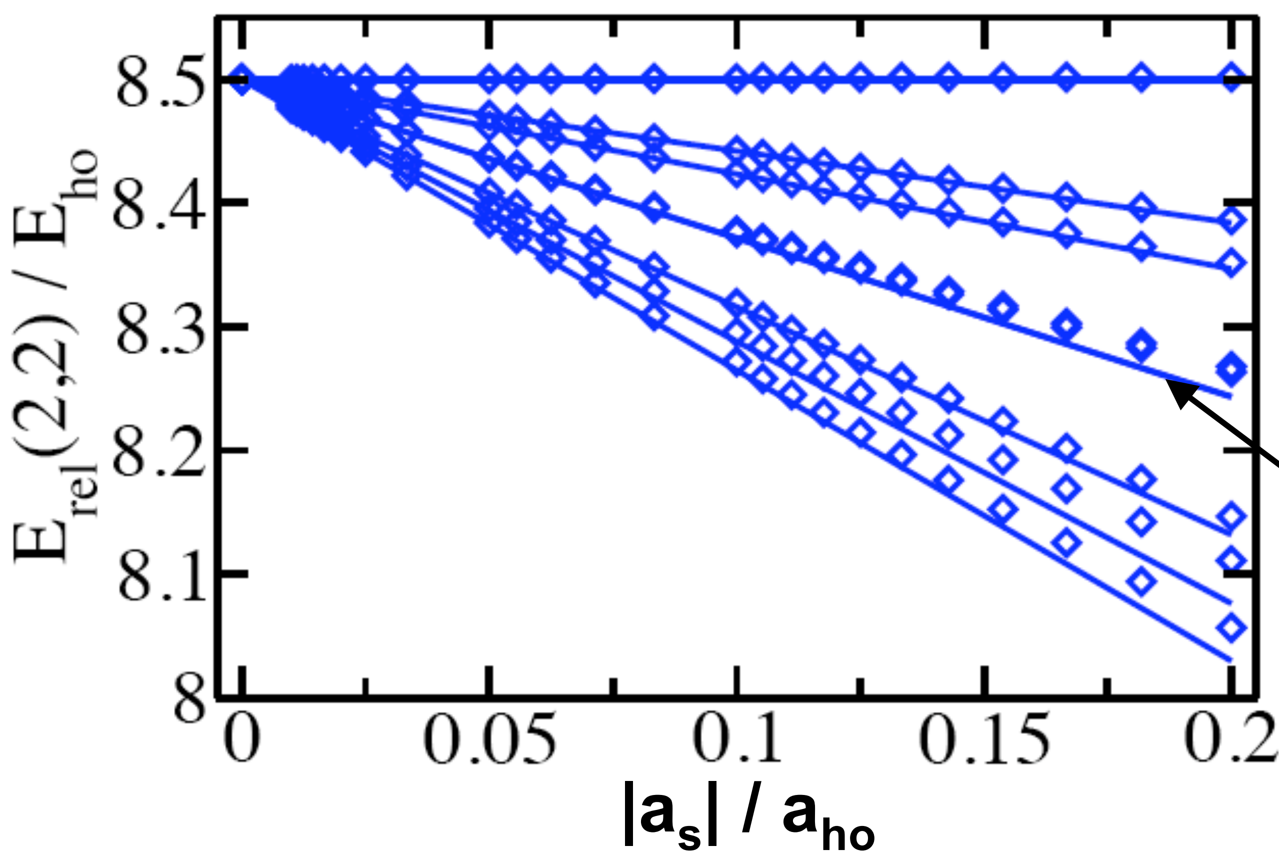
Black solid lines: Perturbative.
Colored symbols: "exact" (stochastic variational approach; see later in talk).





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

K. M. Daily and D. Blume (PRA accepted).



Blue symbols: Essentially exact zero-range energies.

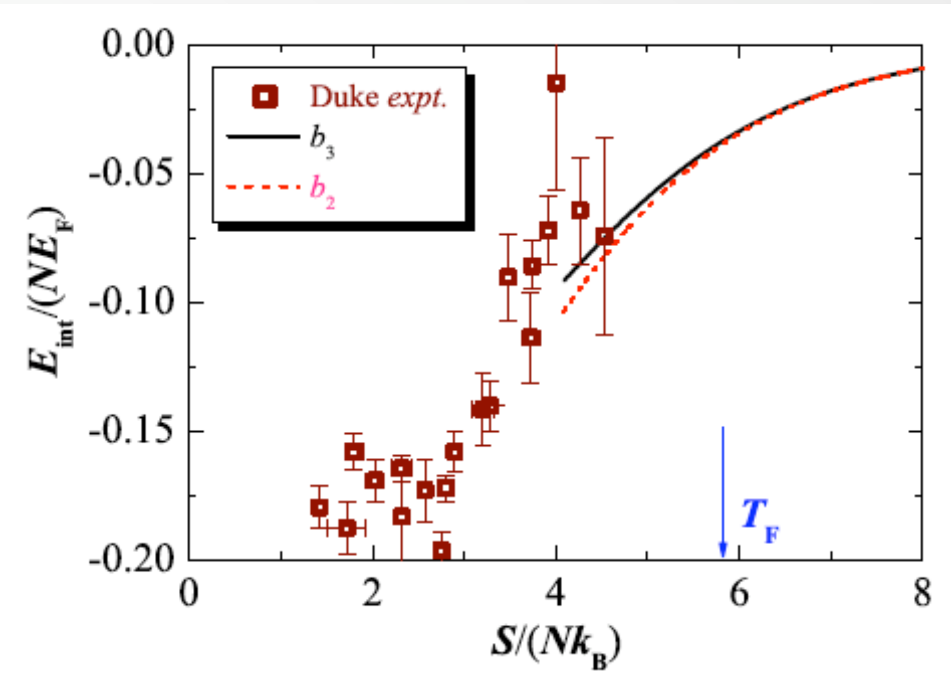
Blue lines: Perturbative results.

Two well resolved states.

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 $a_{ho}/|a_s| \approx 2$).

Virial Expansion for Fermi Gas Based on Two- and Three-Fermion Spectra

"High-T" thermodynamics in trap (virial coefficients calculated from two- and three-body energies):



Liu et al., PRL 102, 160401 (2009)

Idea:

Start with grand partition function:
$Z = Tr[-(H-\mu N)/(k_B T)]$

Perform cluster expansion:
$Z = 1 + zQ_1 + z^2Q_2 + \ldots$

where $Q_n = Tr_n[\exp(-H_n/(k_B T))]$;
fugacity $z = \exp[\mu/(k_B T)] << 1$.

Thermodynamic potential Ω:
$\Omega = -k_B T \ln(Z)$
$\Omega = -k_B T\, Q_1\, (z + b_2 z^2 + b_3 z^3 + \ldots)$
$b_i = b_i(Q_1,\ldots,Q_i)$

How Can Hyperspherical Framework be Applied to Unitary Fermi Gas?

Werner and Castin, PRA 74, 053604.

- **Unitary and NI system have same number of length scales.**
- **Wave function at unitarity separates just as in NI case:**

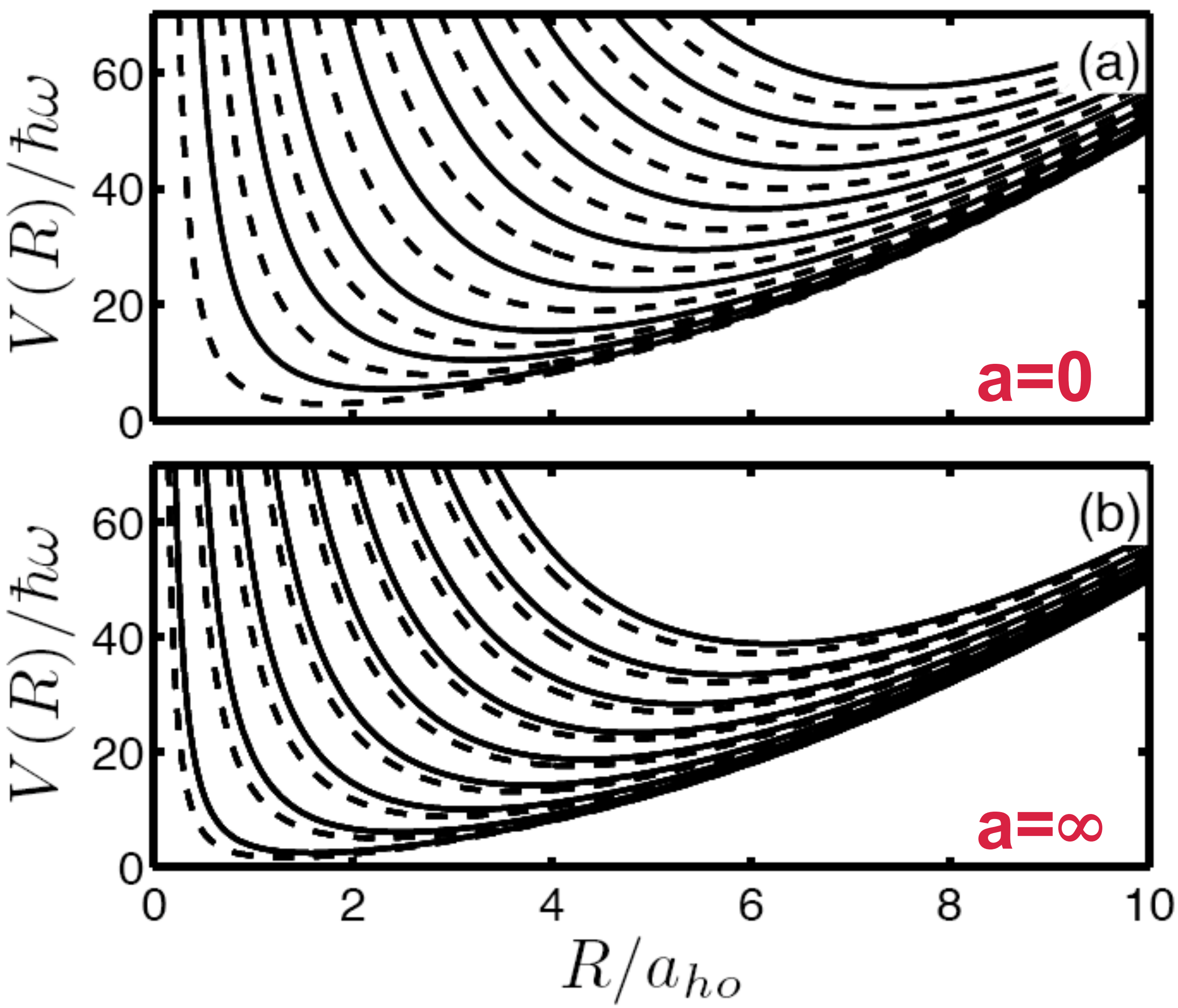
$$\Psi(\vec{r}_1, \ldots, \vec{r}_N) = G(\vec{R}_{CM})F(R)\Phi(\vec{\Omega})$$

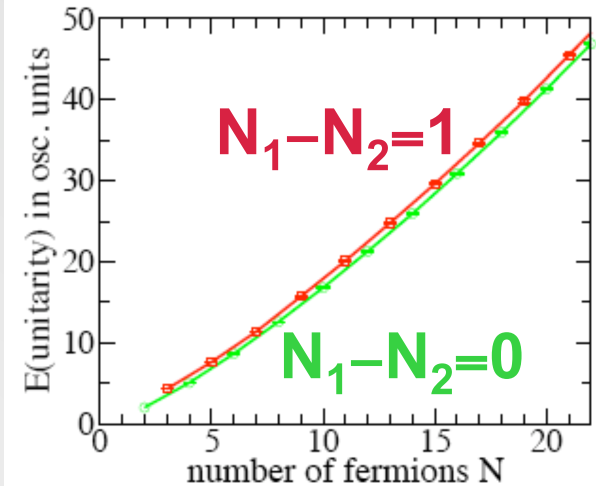
- **It follows:**

$$E_{\text{unit}} = \left(2n + \nu + \frac{3}{2}\right)\hbar\omega + E_{CM}$$

- **ν obtained from hyperangular equation (with interactions).**
- **Ladder of states separated by 2hν.**
- **Alternatively: Calculate E_{unit} and "back out ν"**

Hyperspherical Potential Curves for N=3-20: Non-Interacting and Unitarity





Odd-even oscillations:
Odd-N curves pushed up compared to even-N curves.

Odd-even oscillations usually interpreted in terms of excitation gap Δ(N) → see later.

How Do We Obtain Solutions? Semi-Stochastic Variational Approach I

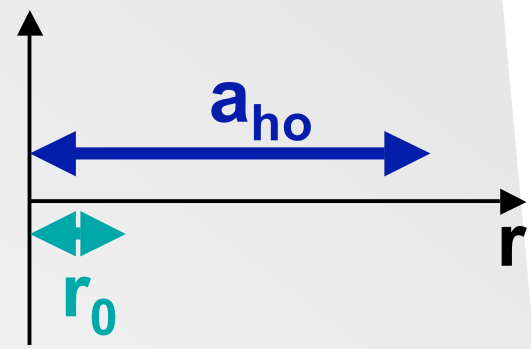
Non-relativistic system Hamiltonian:

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

Spherically symmetric.

Sum over unlike spin pairs.

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).

How to Treat Interacting System? Semi-Stochastic Variational Approach II

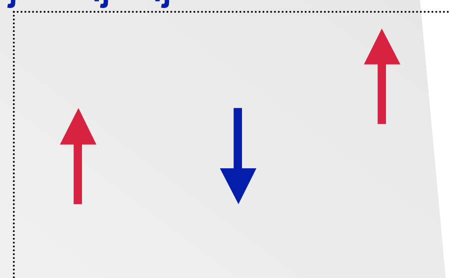
Idea:

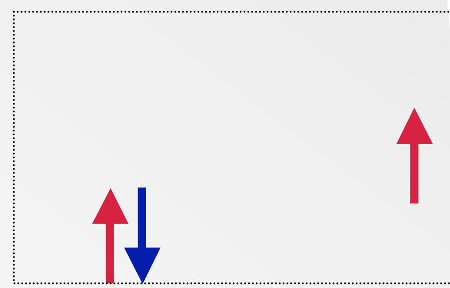
Use basis set expansion approach that involves correlated Gaussian.

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

How to Treat Interacting System? 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…).

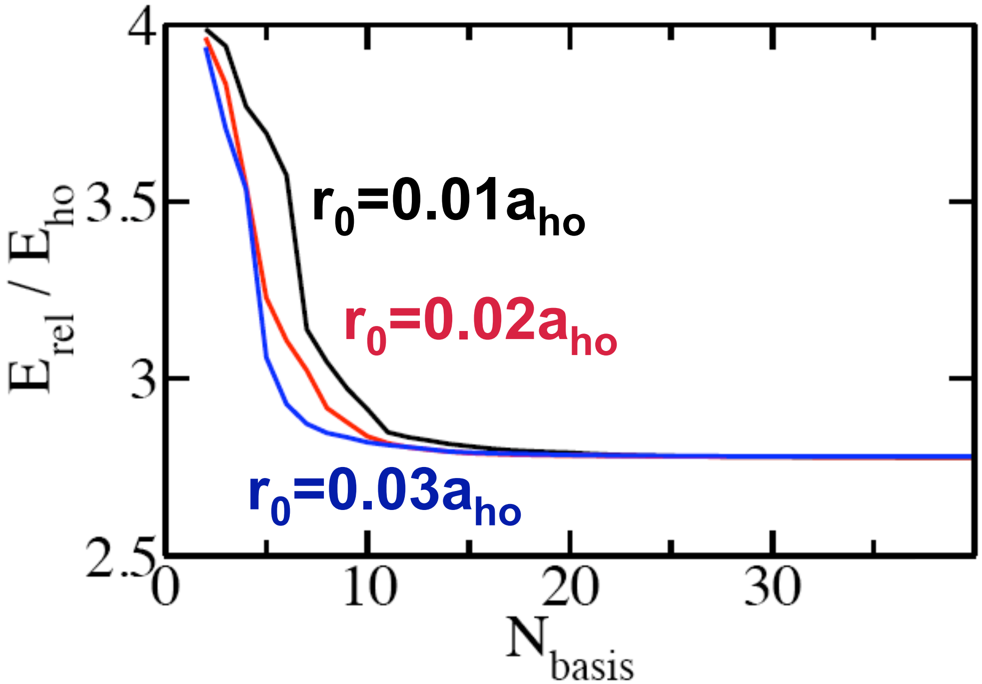
Matrix elements for structural properties and momentum distribution can be calculated analytically.

Linear dependence of basis functions needs to be watched carefully.

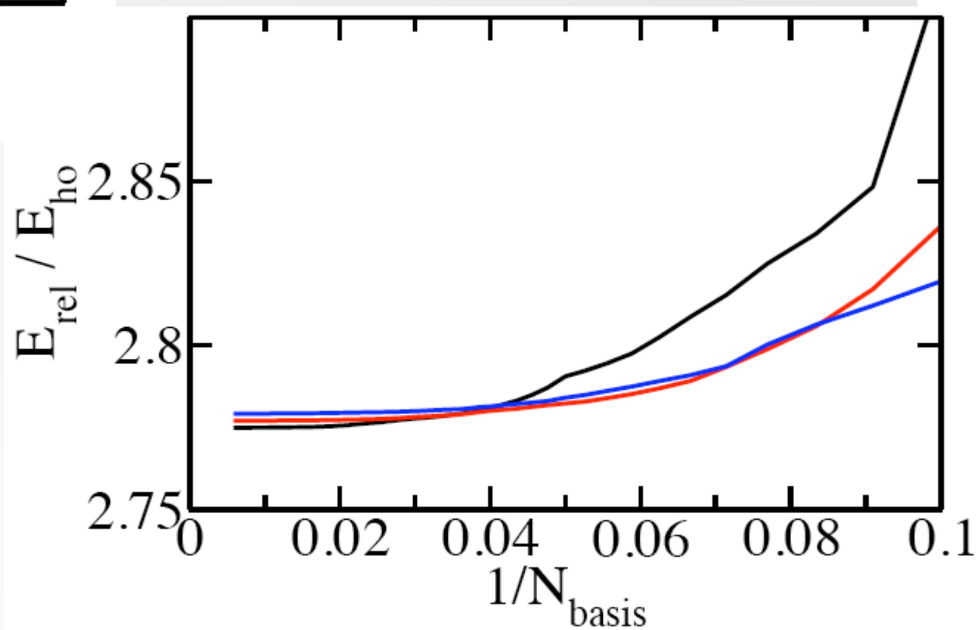
Computational effort increases with N:

- 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).

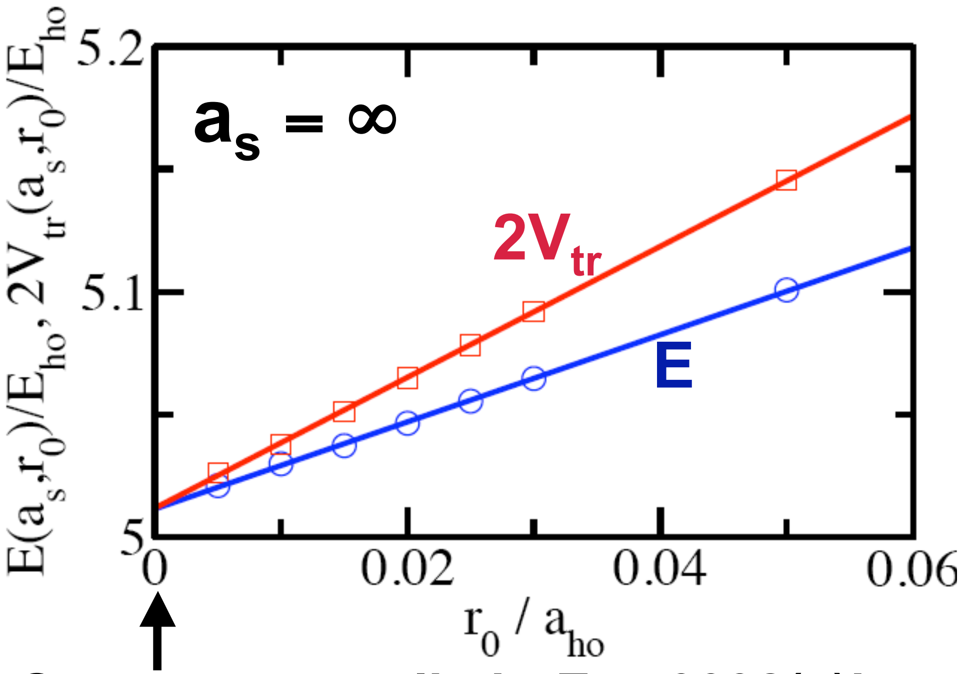
SV Approch at Unitarity: Illustration of Convergence for N=3



Larger range:
Faster convergence.



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

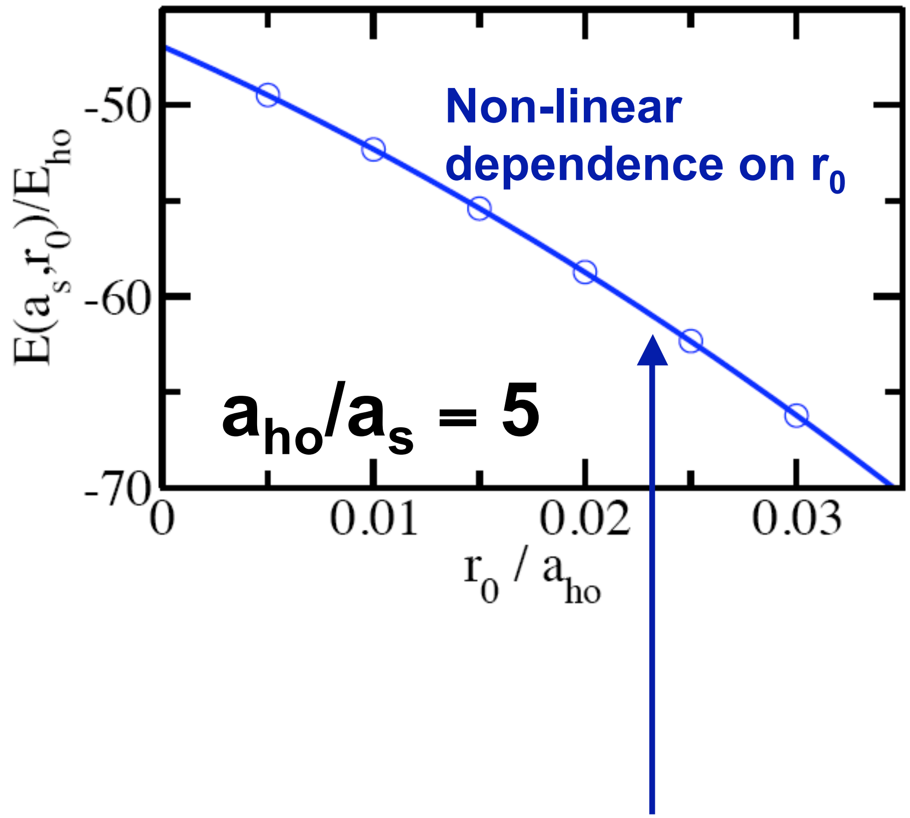


Our zero-range limit: E=5.0092(5)hν [uncertainty arises from fit]. Effective interaction theory: E=5.050(24)hν.

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

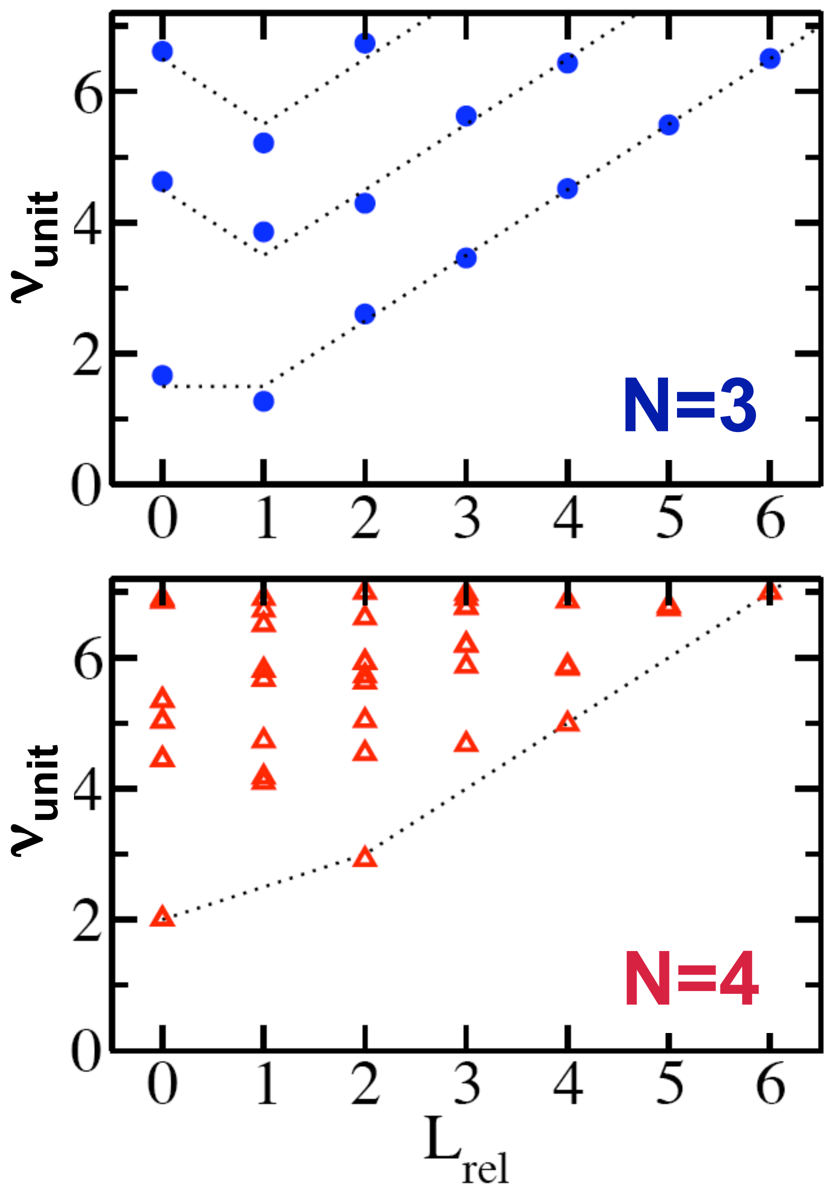
Confirmation of virial theorem at unitarity: $E(\infty, 0) = 2V_{tr}(\infty, 0)$.

[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.

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 (PRA, 2010); L_{rel}=0: von Stecher and Greene, PRA 80, 022504 (2009).

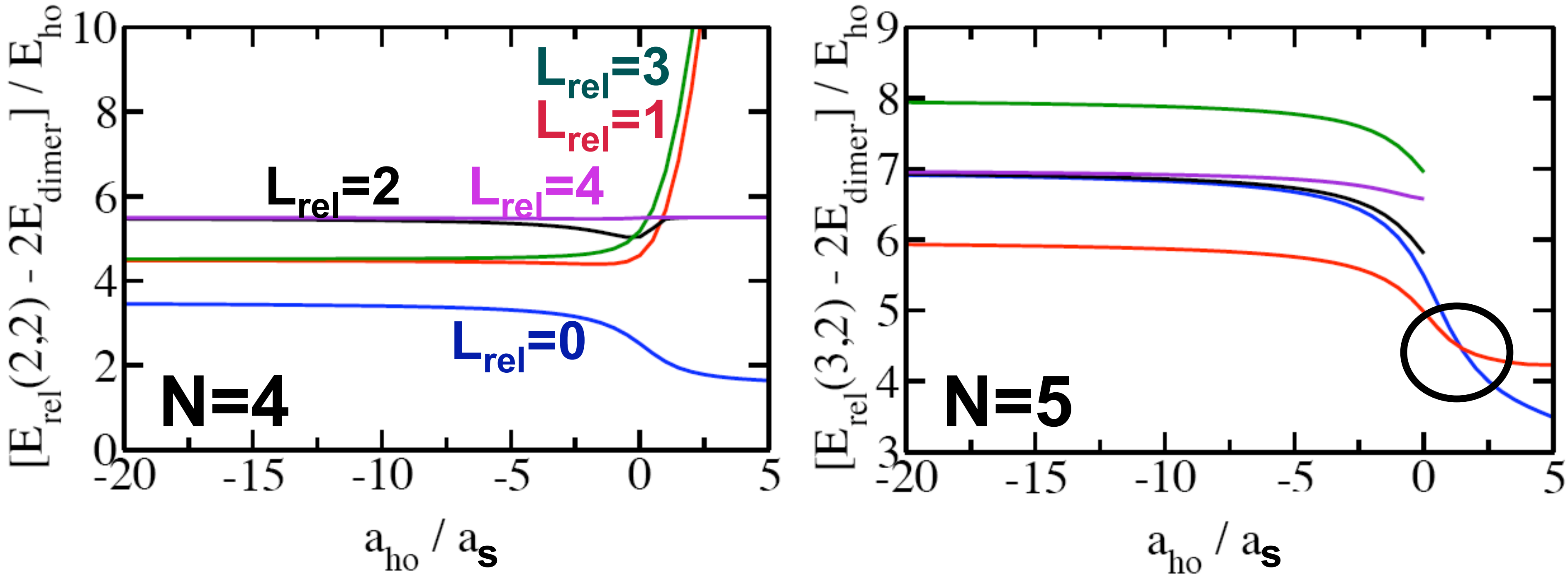
$E_{rel,unit} = (2n+\nu_{unit}+3/2)h\nu$; n=0,1,2,…

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…

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.**

Universal "Tan" Relations for ZR Interactions throughout Crossover

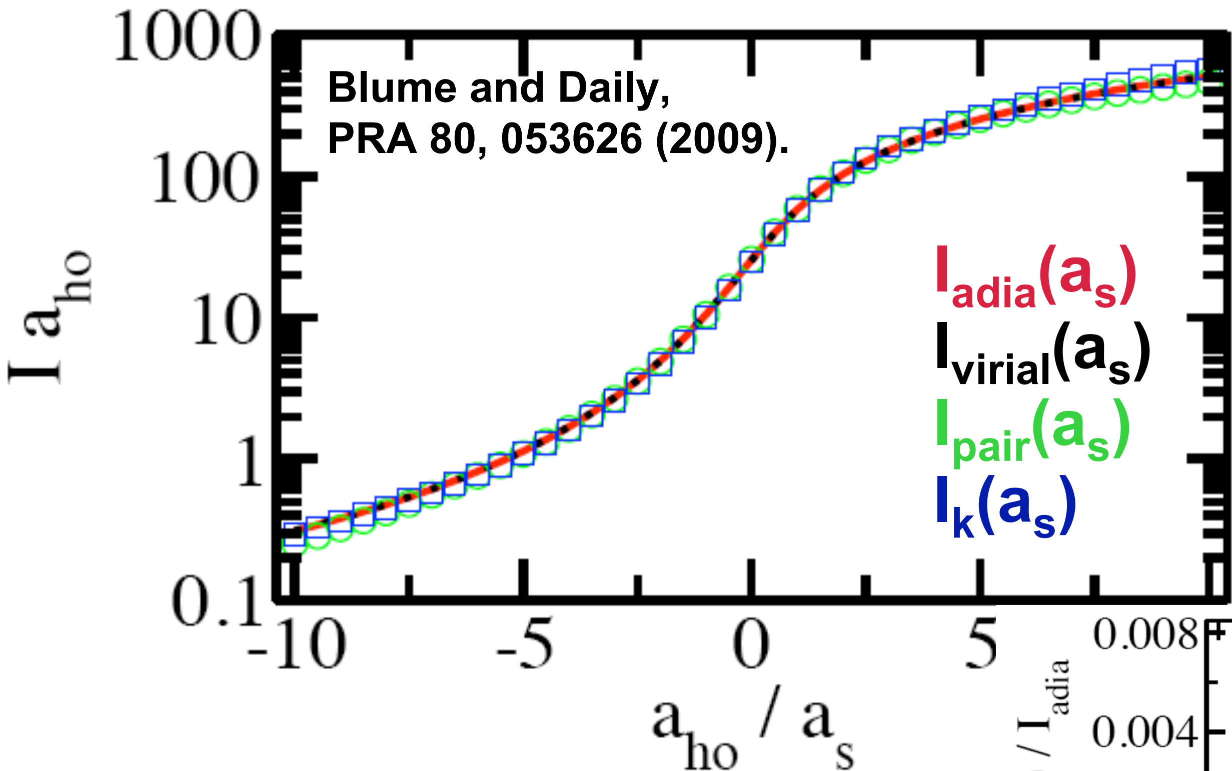
Quantitative relation between distinctly different quantities such as change of energy, trap energy, pair distribution function and momentum distribution, inelastic two-body loss rate,...

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

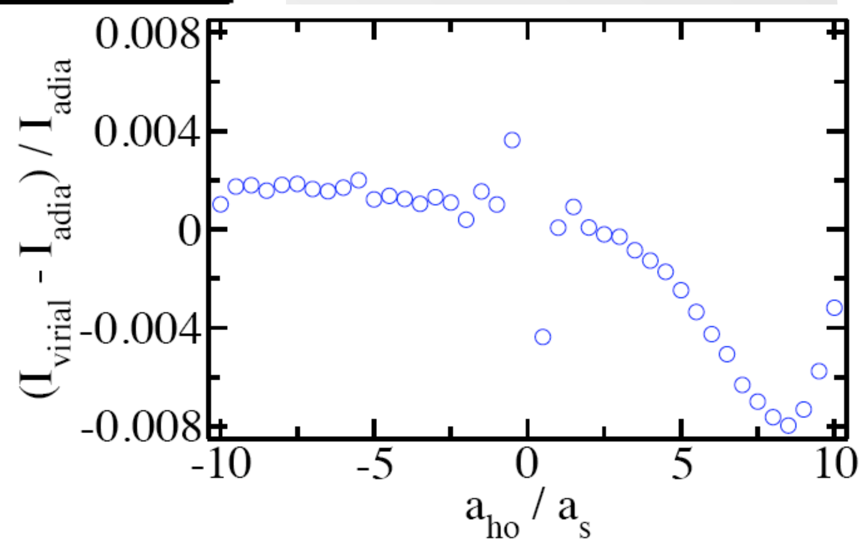
- It then follows:
  - Adiabatic relation: $\partial E(a_s,0)/\partial a_s = h^2/(16\pi^3 m a_s^2)\, I_{adia}(a_s)$.
  - Virial theorem: $E(a_s,0) = 2 \langle V_{trap}(a_s,0)\rangle - h^2/(32\pi^3 m a_s)\, I_{virial}(a_s)$.
  - Pair relation: $I_{pair}(a_s) = \lim_{s\to 0} 4\pi\, N_{pair}(r<s) / s$.

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

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

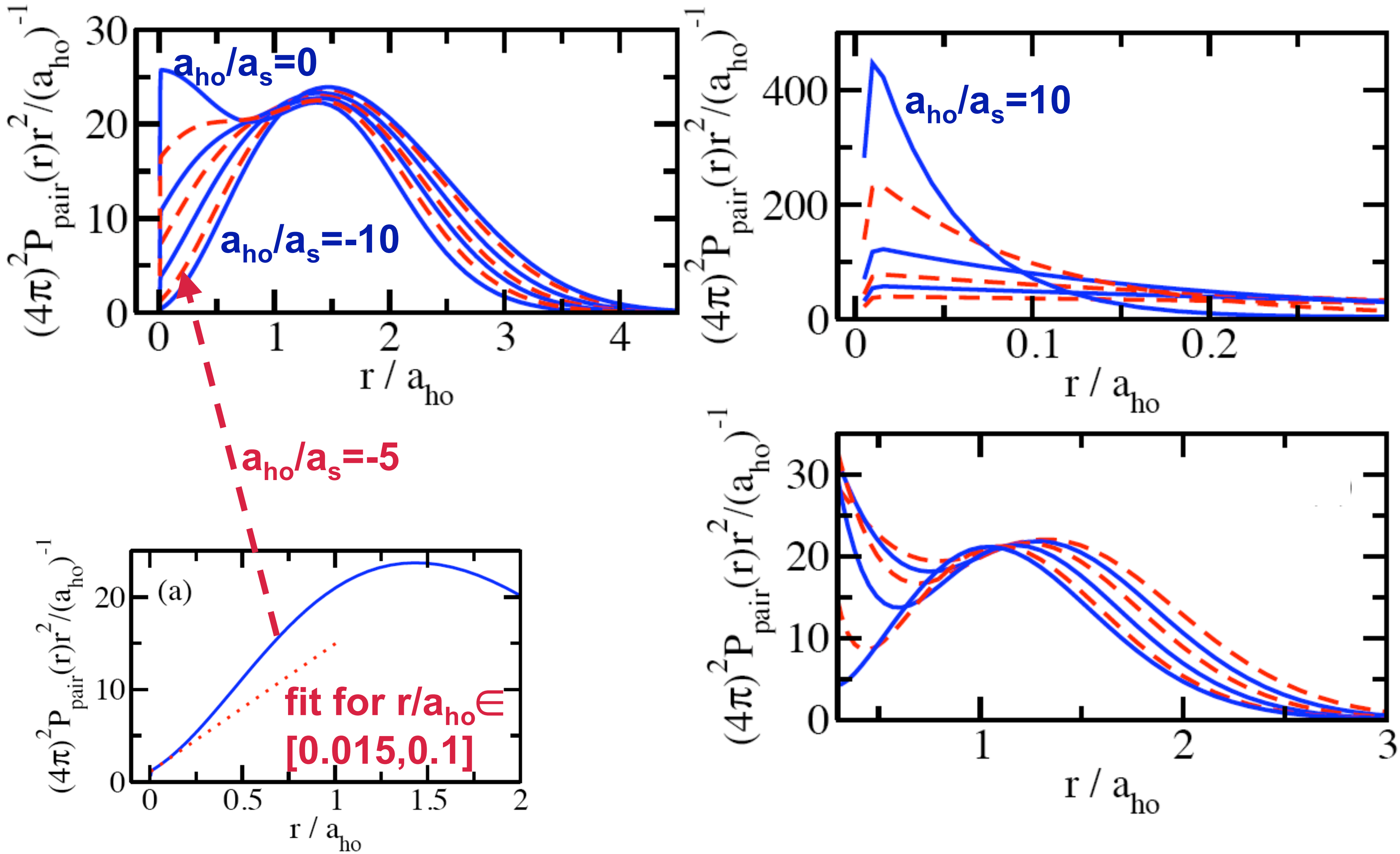


Recent experiments:
Hu et al., arXiv:1001.3200.
Stewart et al., arXiv:1002.1987.
Earlier work:
Partridge et al., PRL 95, 020404 (2005).



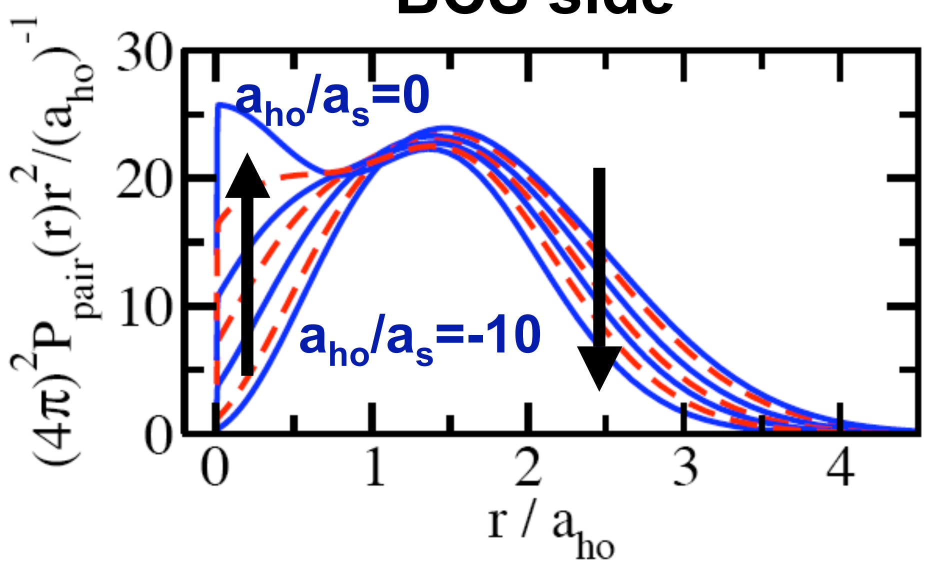
$I(a_s)$ changes by about three orders of magnitude throughout crossover.
Very good agreement among the four "different" $I(a_s)$.

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

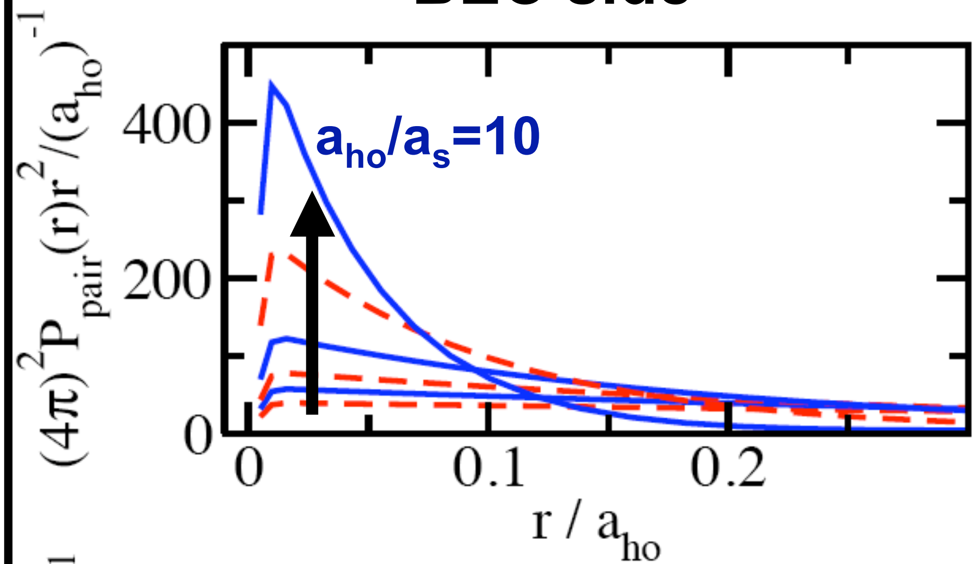


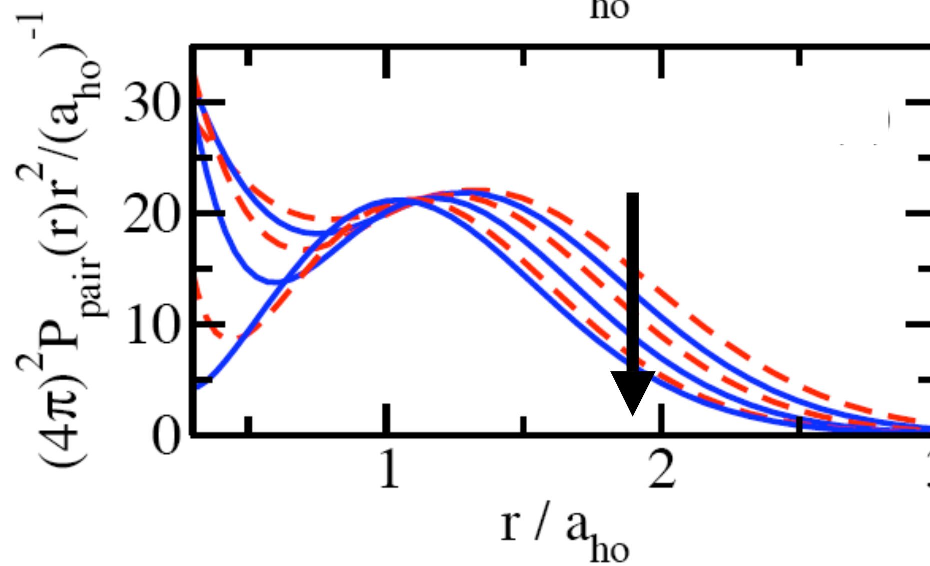
Structural Correlations (N=4): Pair Distribution Functions for $r_0=0.005a_{ho}$

"BCS side"

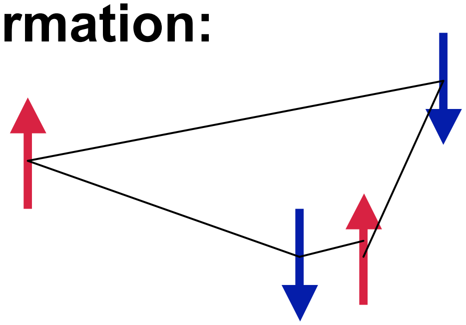


"BEC side"



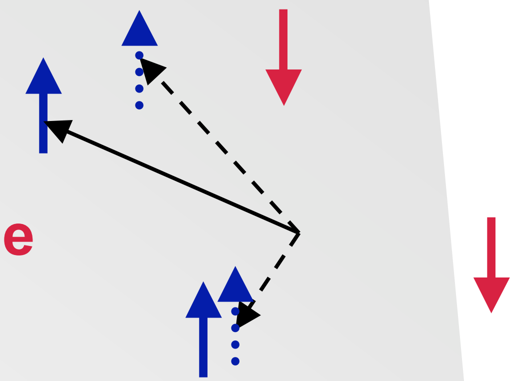


Development of two-peak structure indicates pair formation:



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 $\underline{r}'$.

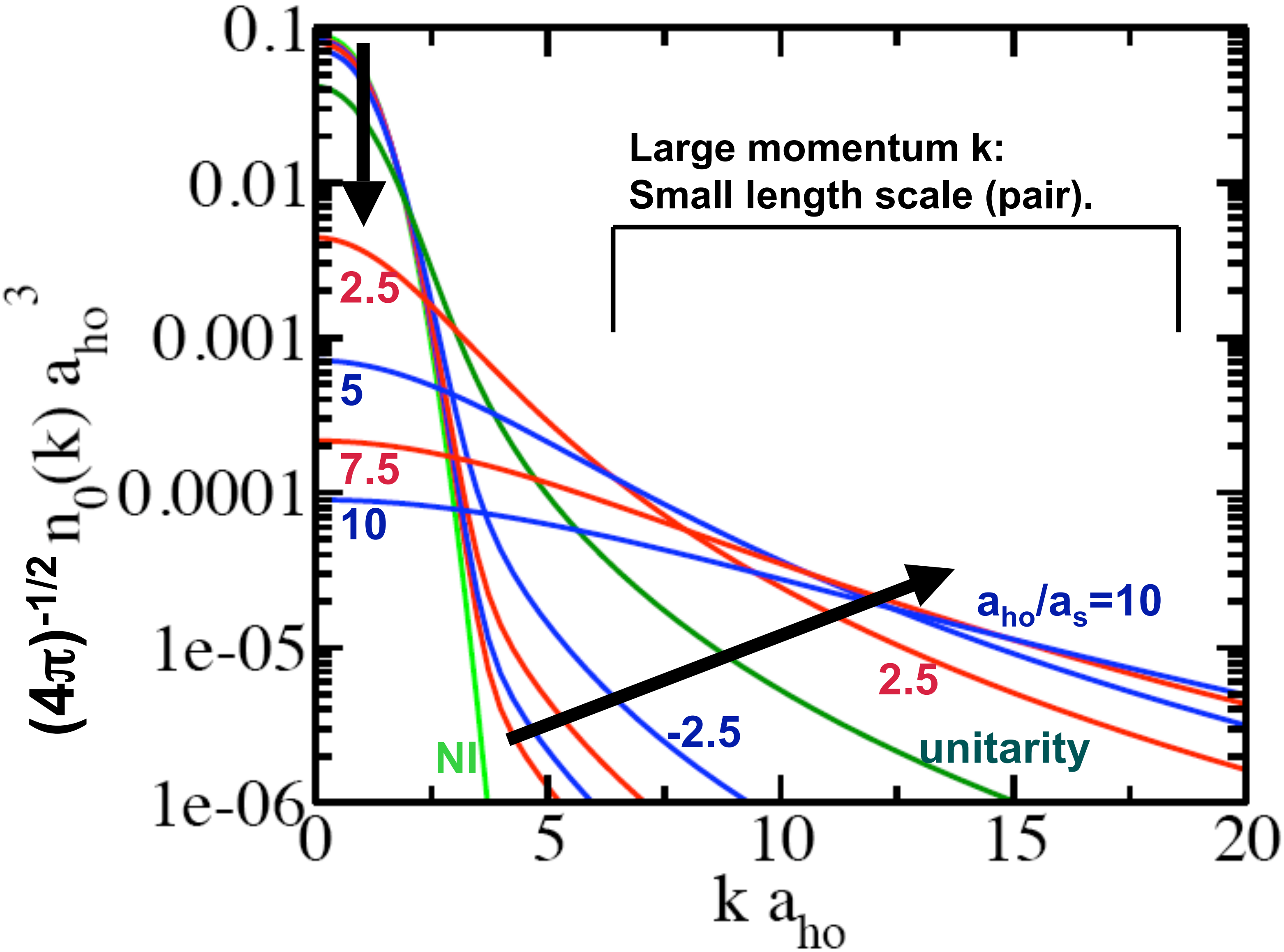
- **It follows: $n(\underline{k}) = (2\pi)^{-3} \iint \exp[i\underline{k}\cdot(\underline{r}-\underline{r}')]\rho(\underline{r}',\underline{r})\, d\underline{r}d\underline{r}'$.**

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

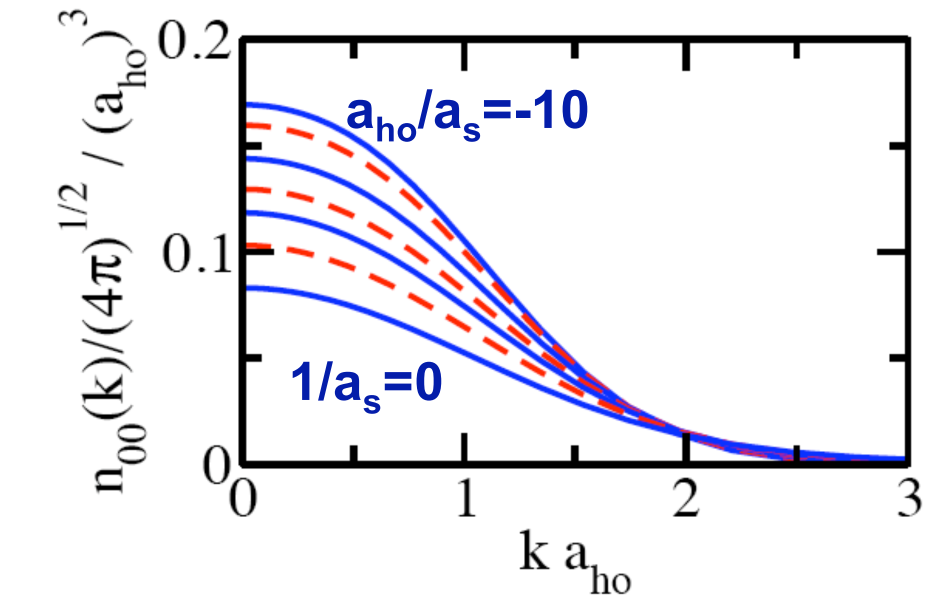
- **Then: $\int n(\underline{k})d\Omega_k = (4\pi)^{1/2}\, n_0(k)$**

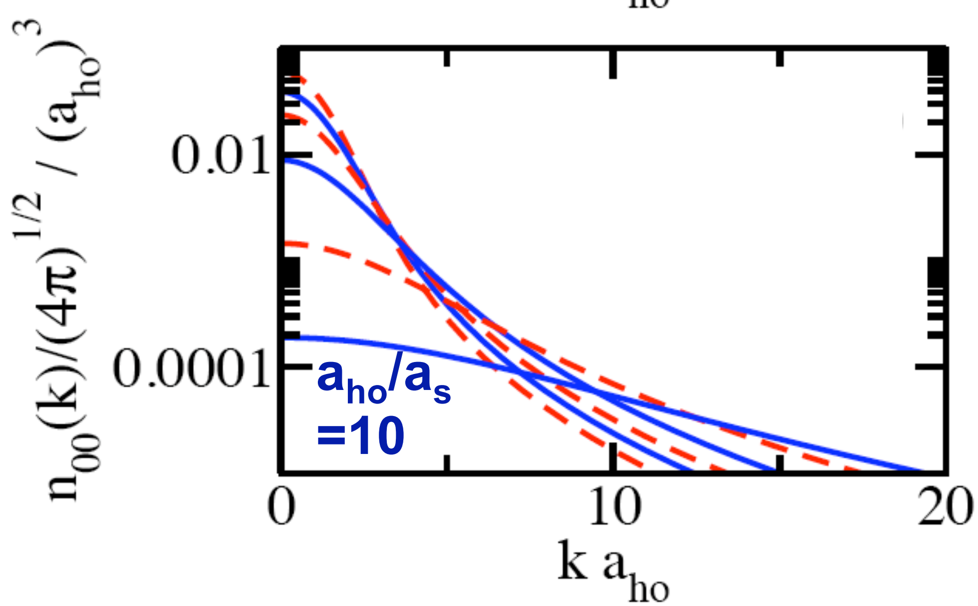
Shown on next slide for N=4

l=0 Projection of Momentum Distribution for N=4

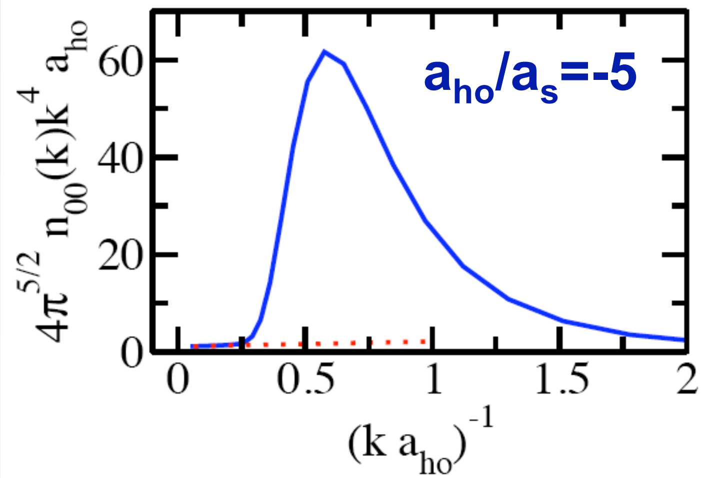


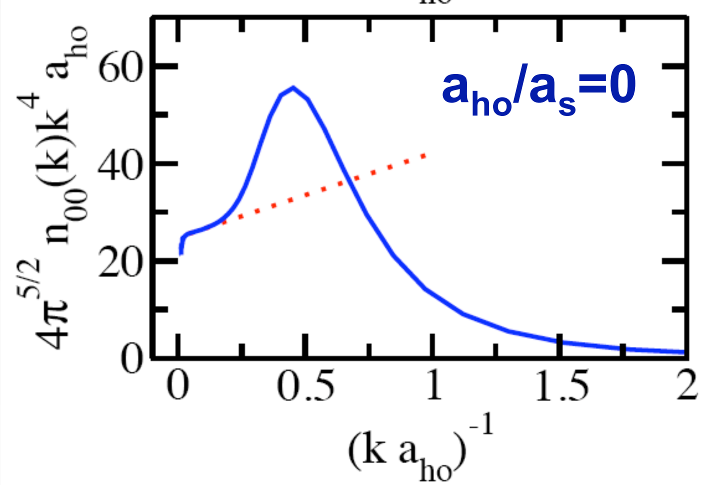
Lowest Partial Wave Projection of Momentum Distribution





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





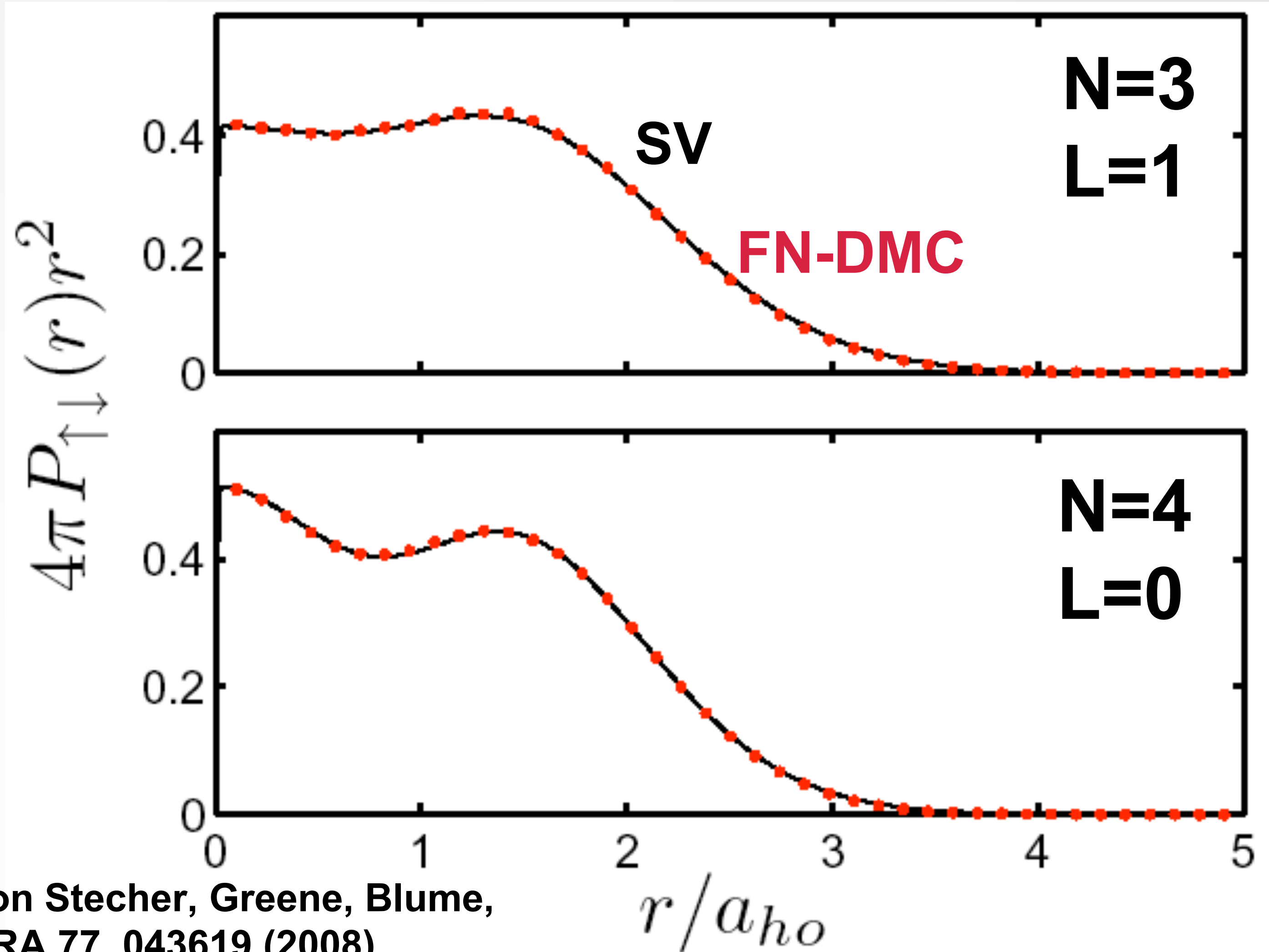
Larger Systems: Fixed Node Diffusion Monte Carlo (FN-DMC) Approach

- Stochastic approach.
- Results in upper bound for energy.
- Results are as good as input (trial wave function).

- More details in next lecture…

FN-DMC and SV: Comparison of Structural Properties at Unitarity

Pair distribution function for up-down distance:



Range $r_0 = 0.01 a_{ho}$.

Very good agreement between CG and FN-DMC results.

N=4: Enhanced probability at small r (pair formation).

von Stecher, Greene, Blume, PRA 77, 043619 (2008).

Excitation Gap and Residual Oscillations at Unitarity

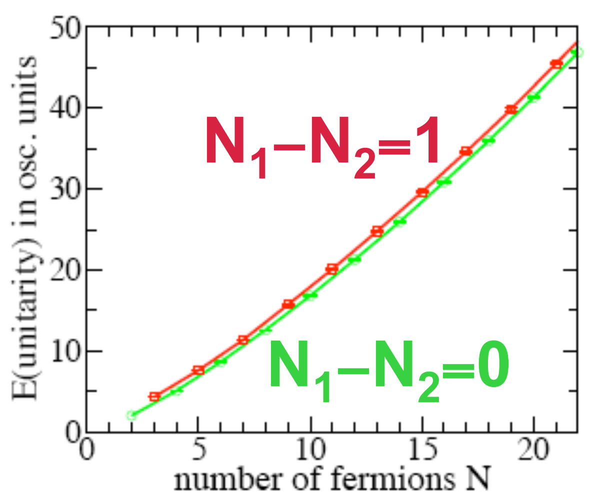
Blume/von Stecher/Greene:
PRL 99, 233201 (2007);
PRA 77, 043619 (2008).

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

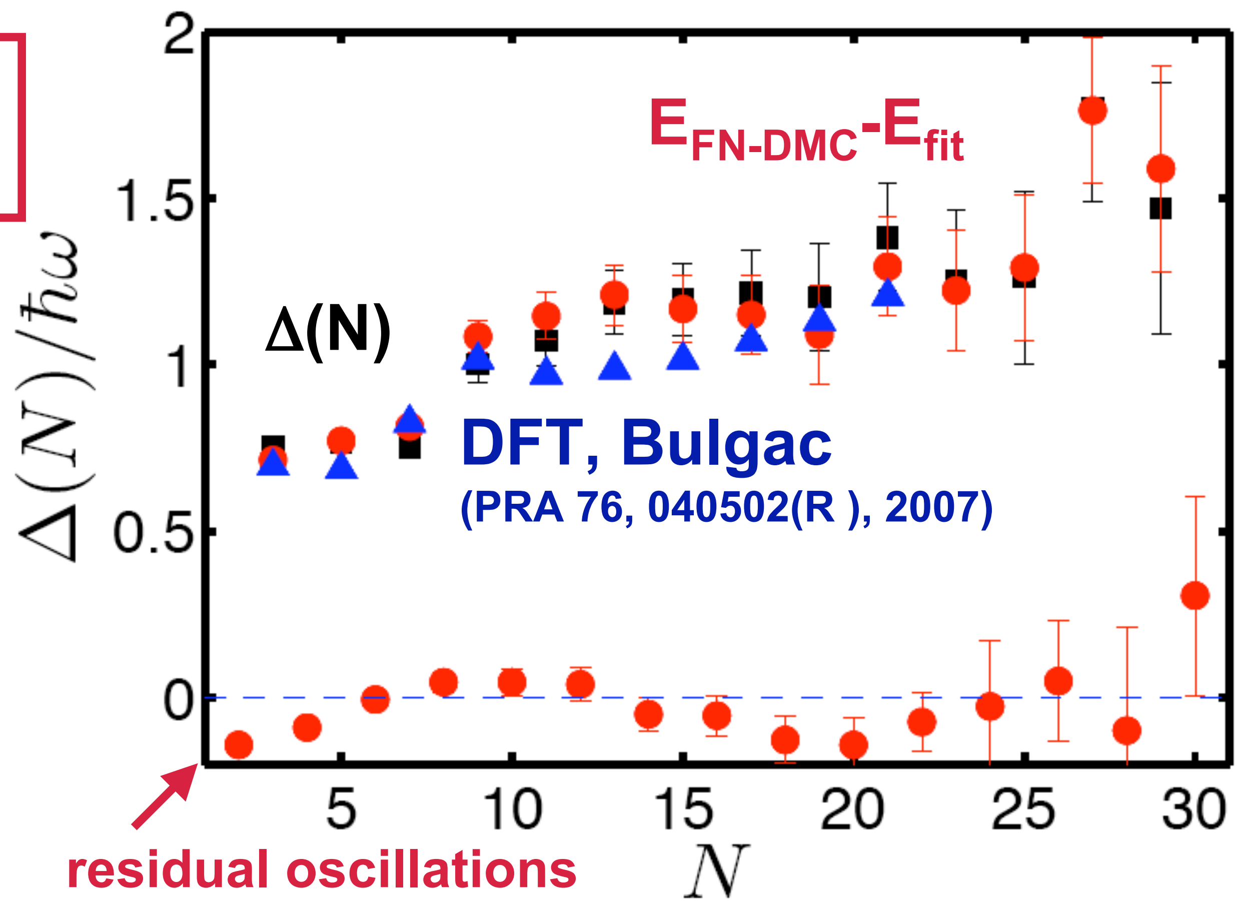
N odd, $N=N_1+N_2$ and $N_1=N_2+1$

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

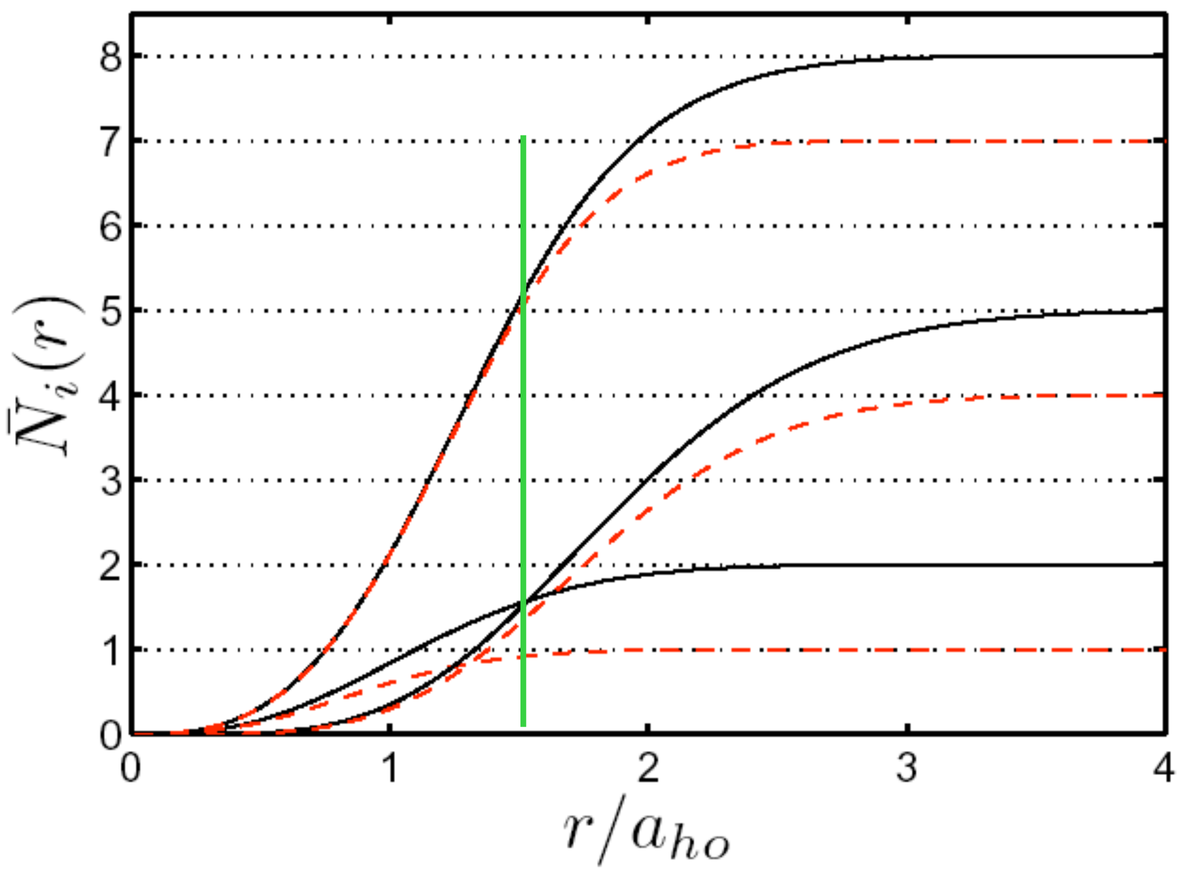
Fixed-node diffusion Monte Carlo

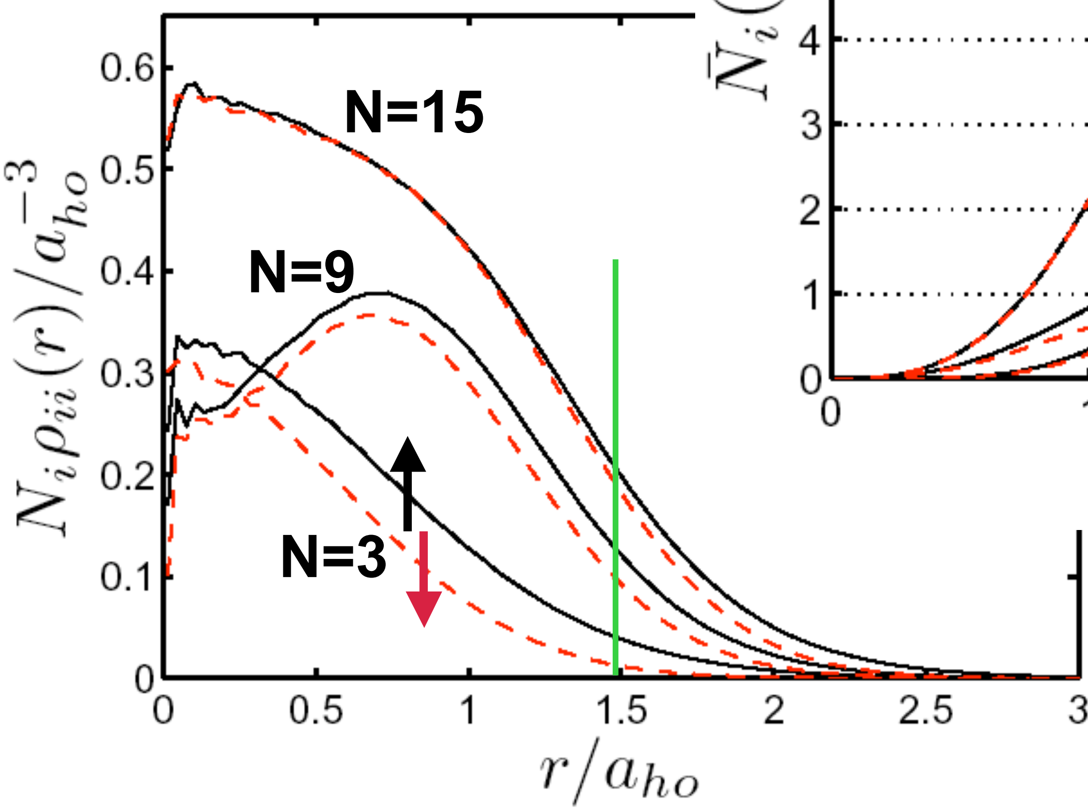


$$E_{fit}(N) = \sqrt{\xi_{tr}} E_{NI,ETF}$$



Radial Density at Unitarity: Where Is "Spare" Atom Located?





N=9: "Extra" particle more delocalized.
N=15: "Extra" particle sits near the surface.

Summary

- BCS-BEC Crossover from the few-body perspective.
- Weakly-attractive regime.
- Unitarity.

- Next lecture: BEC regime, combined with dimer-dimer scattering length for unequal masses

Related Topics and Natural Extensions

- **Two-component Fermi gases with unequal masses, unequal trapping frequencies, unequal populations:**
  - Stability of unequal-mass systems (trimer formation)?
  - Universal behavior?
  - Phase separation?

- **Multi-component s-wave interacting Fermi gas:**
  - Details of underlying two-body potential?
  - Implications of existence or absence of three-particle negative energy states?

- **Beyond s-wave:**
  - p-wave interactions?
  - p-wave induced interactions?