THE FEW-BODY PROBLEM WITH APPLICATION TO MANY-BODY THERMODYNAMICS

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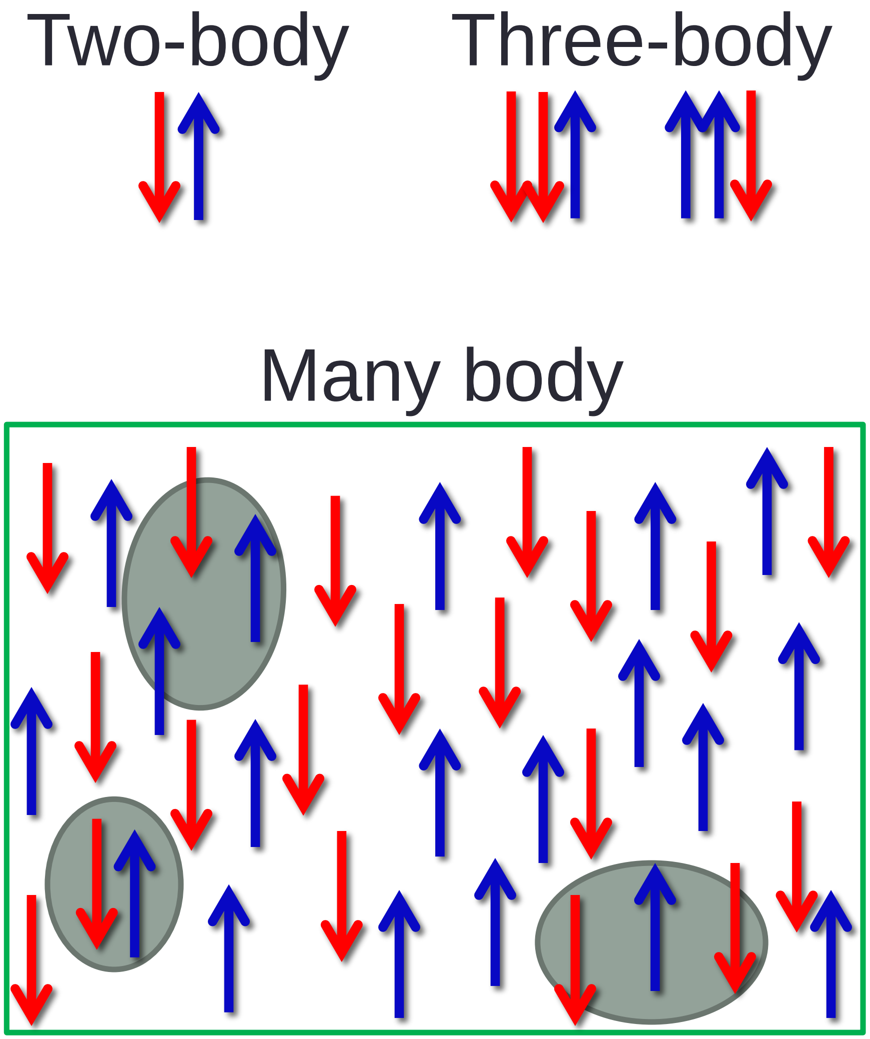
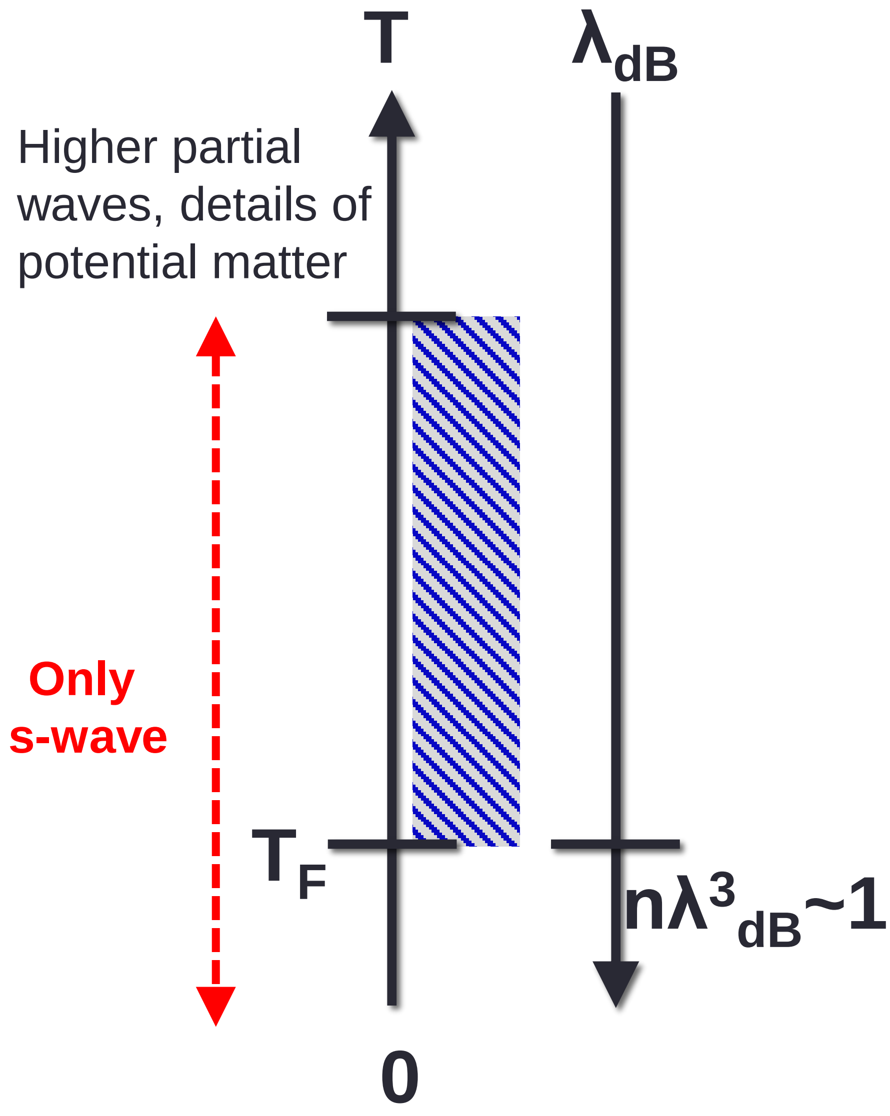
Outline

- Two-body system with zero-range interactions
  - Boundary condition
  - Condensate fraction
- FFX system
  - Entire energy spectrum, Lippmann-Schwinger approach
  - Atom-dimer approximation in a_s/a_{ho} << 1 limit
  - Green's function, Lippmann-Schwinger approach
  - Exact energies at unitarity ($s_{L,n}$ eigenvalues)
- Thermodynamics
  - High temperature thermodynamics up to third virial coefficient
  - Thermodynamics of few-body systems
- Outlook and summary

What are we concerned with?





Many-body Hamiltonian

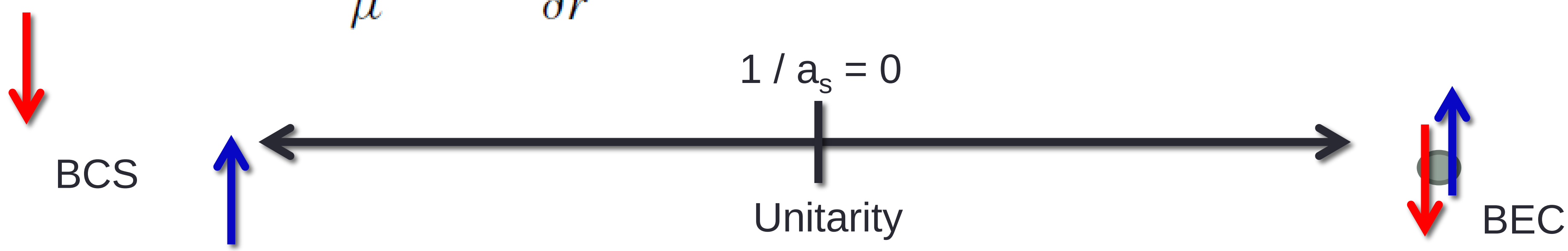
We are interested in general masses m_1 and m_2 with only two-body forces

$$H = \sum_{j=1}^{N_1} \left(\frac{-\hbar^2}{2m_1} \nabla^2_{\vec{r}_j} + \frac{1}{2} m_1 \omega^2 \vec{r}_j^{\,2} \right) + \sum_{j=N_1+1}^{N} \left(\frac{-\hbar^2}{2m_2} \nabla^2_{\vec{r}_j} + \frac{1}{2} m_2 \omega^2 \vec{r}_j^{\,2} \right) + \sum_{j=1}^{N_1} \sum_{k=N_1+1}^{N} V_{\mathrm{tb}}(r_{jk})$$

The details of the underlying potential don't matter, so I utilize a zero-range delta function potential.

$$V_{\mathrm{zr}}(r) = \frac{2\pi\hbar^2 a_s}{\mu} \delta(\vec{r}) \frac{\partial}{\partial r} r$$

Low T → large λ_{dB}, only s-wave



Two s-Wave Interacting Particles in External Spherically Harmonic Trap

Wave function is separable in relative and center of mass coordinates

r > 0 $$\Psi_{tot}(\vec{r}, \vec{R}) = \Psi_{HO}^{rel}(\vec{r})\Psi_{HO}^{CM}(\vec{R})$$

Interactions occur only in L = 0 channel in relative coordinate (a_{ho} = 1 below)
Applying boundary condition to outside solution leads to quantization condition

$$\lim_{r \to 0} \frac{\frac{\partial}{\partial r}(r\Psi_{rel})}{r\Psi_{rel}} = \frac{-1}{a_s}$$

$$\Psi_{rel}(\vec{r}) =$$

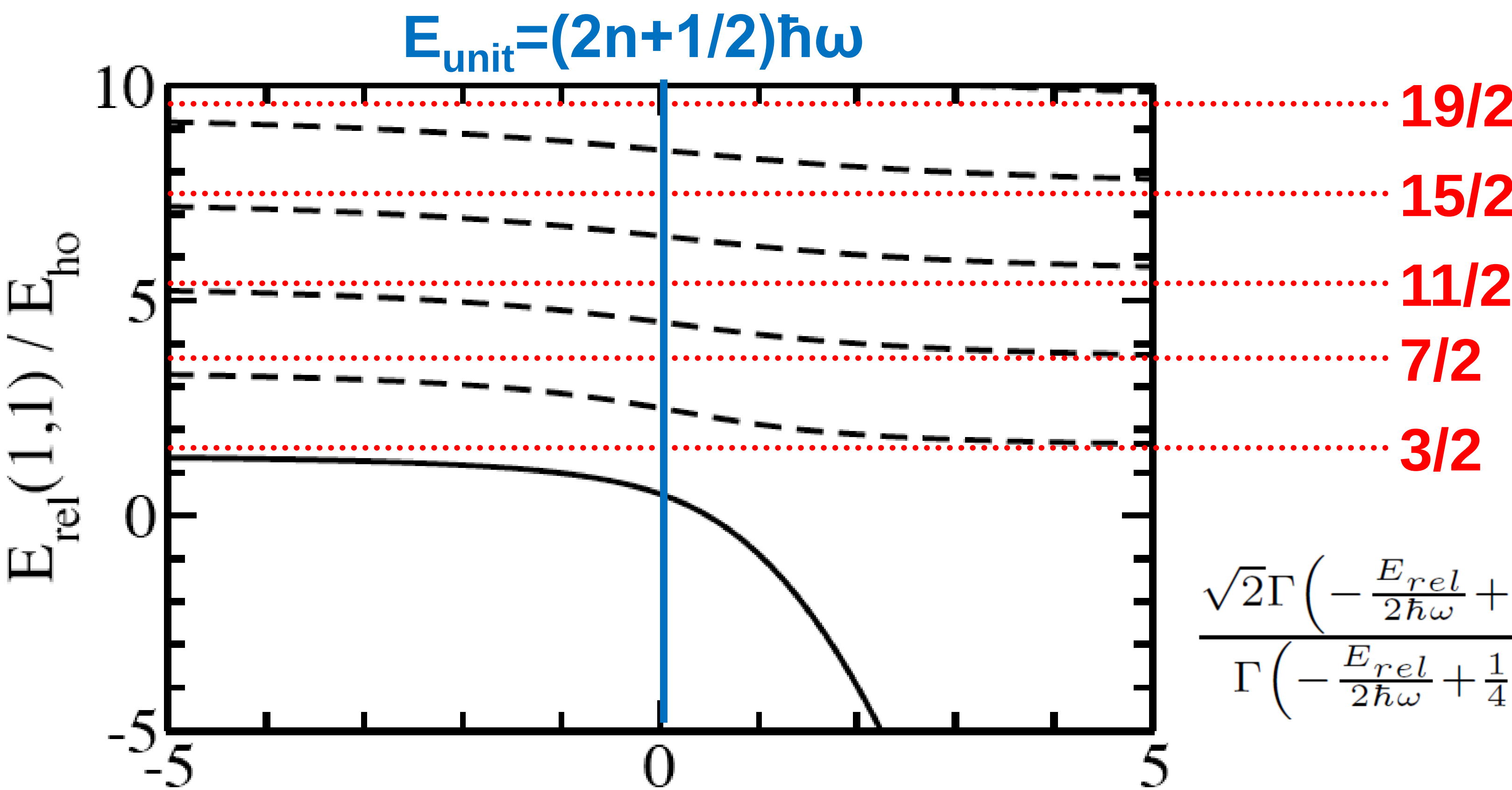
$$N(\nu)U[-\nu, 3/2, r^2/2]e^{-r^2/4}Y_{00}(\hat{r})$$

v = $E_{rel}/(2\hbar\omega) + 3/4$

$$\frac{\sqrt{2}\Gamma\left(-\frac{E_{rel}}{2\hbar\omega}+\frac{3}{4}\right)}{\Gamma\left(-\frac{E_{rel}}{2\hbar\omega}+\frac{1}{4}\right)} = \frac{1}{a_s}$$

Thomas Busch, Berthold-Georg Englert, Kazimierz Rzażewski, Martin Wilkens, Foundations of Physics, **v28** pp 549-559 (1998)

Two s-Wave Interacting Particles in External Spherically Harmonic Trap



$$\frac{\sqrt{2}\,\Gamma\left(-\frac{E_{rel}}{2\hbar\omega}+\frac{3}{4}\right)}{\Gamma\left(-\frac{E_{rel}}{2\hbar\omega}+\frac{1}{4}\right)} = \frac{1}{a_s}$$

E_{ni}=(2n+3/2)ħω a_{ho}/a_s E_{ni}=(2n+3/2)ħω

Finite-angular momentum states: E_{rel}=(2n+L+3/2)ħω.

Busch et al., Found. of Phys. (1998).

Condensate Fraction for N=2 System With Zero-Range Interactions

In general we have the one-body density matrix:

$$\rho_1(\vec{r}',\vec{r}) = \int \cdots \int \psi^*_{\mathrm{tot}}(\vec{r}',\vec{r}_2,\ldots,\vec{r}_N)\,\psi_{\mathrm{tot}}(\vec{r},\vec{r}_2,\ldots,\vec{r}_N)\,\mathrm{d}^3\vec{r}_2\cdots\mathrm{d}^3\vec{r}_N$$

$$\rho_1(\vec{r}',\vec{r}) = \sum_i n_i \chi_i^*(\vec{r}')\chi_i(\vec{r})$$

For the 2 particle system with ZR interactions, the wave function is known (here in atomic mass units, $a_{ho,m} = 1$):

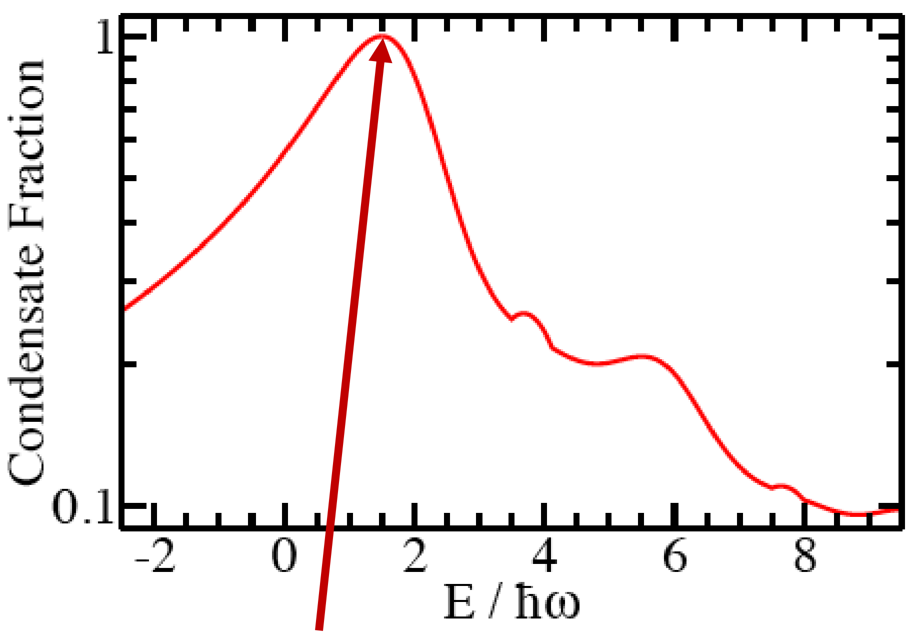
$$\Psi_{tot}(\vec{r},\vec{R}) = N(\nu)U[-\nu,3/2,r^2/2]e^{-r^2/4}e^{-R^2}Y_{00}(\hat{r})Y_{00}(\hat{R})$$

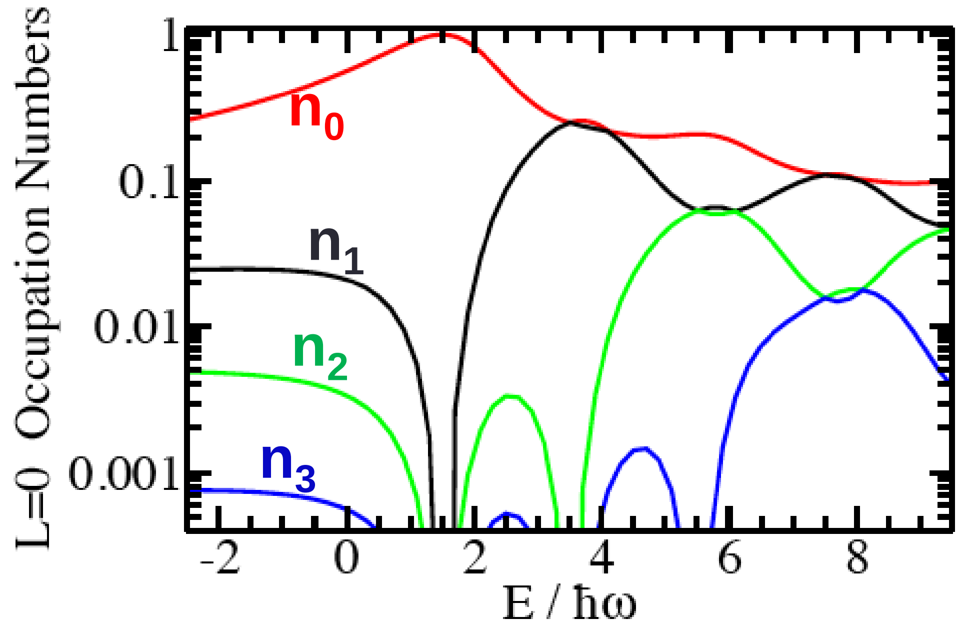
Expand the relative wave function in the non-interacting basis:

$$\Psi_{rel}(\vec{r}) = \sum_i c_i \Psi_i^{NI}(\vec{r})$$

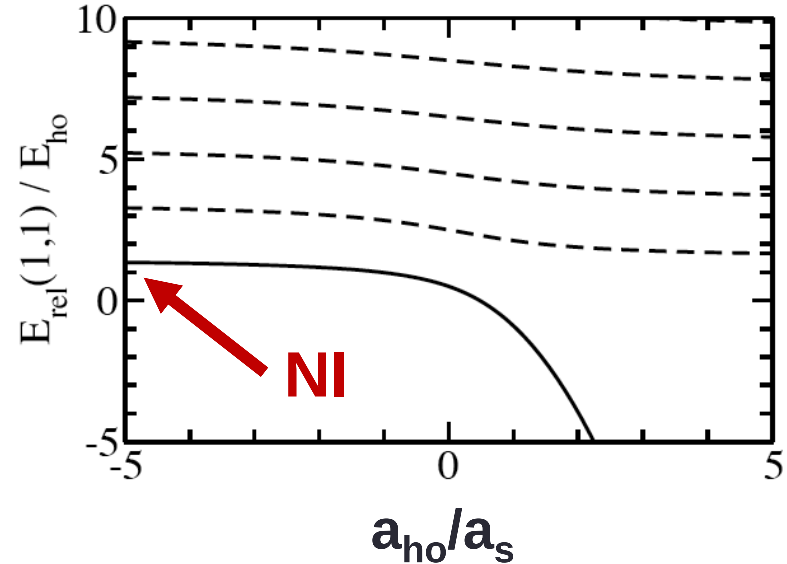
C_i are known

Condensate Fraction for N=2 System With Zero-Range Interactions





NI (expansion in $x=a_s/a_{ho}$):
$n_0=1-0.42000429\ldots x^2 - 0.373241\ldots x^3+\ldots$

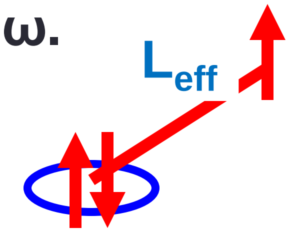


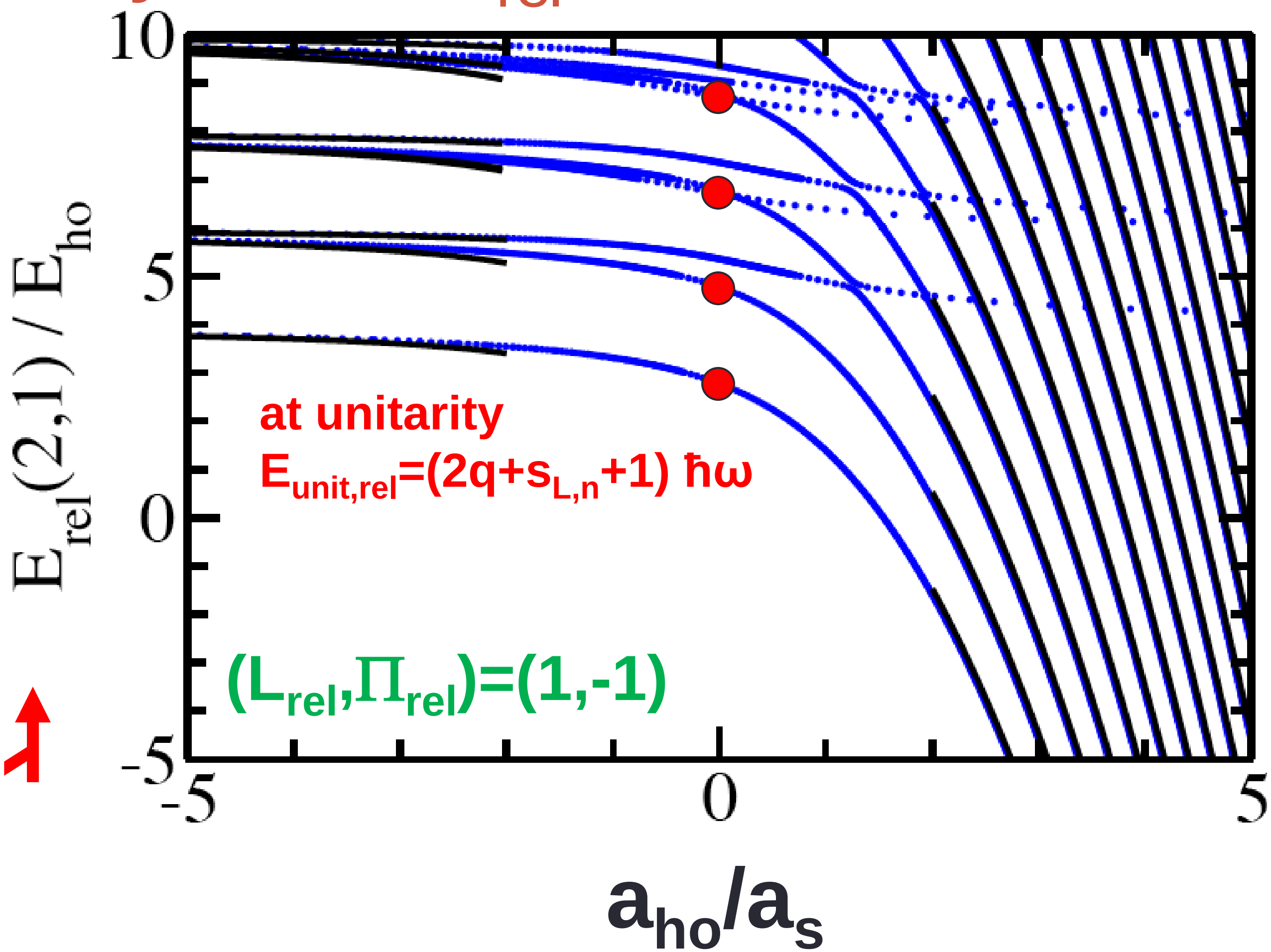
Calculate (projected) one-body density matrix (semi-analytically). Diagonalize to obtain occupation numbers and natural orbitals. Results are very accurate.

How to Understand Energy Spectrum of Three-Fermion System? $L_{rel}>0$.

$E_{ni,rel} = (2q+s^{NI}_{L,n}+1)\hbar\omega$, $q=0,1,\ldots$
(1 more state for each higher q).

1 state of each $E_{ni,rel}$ manifold goes to "atom plus dimer state" with energy $E_{ni,rel} = E_{dimer} + (2n_{eff}+L_{eff}+3/2)\hbar\omega$.





In blue, energies calculated according to Kestner and Duan PRA 76, 033611 (2007)
In red, energies calculated according to Werner and Castin PRL (2006)
In black, perturbative treatment

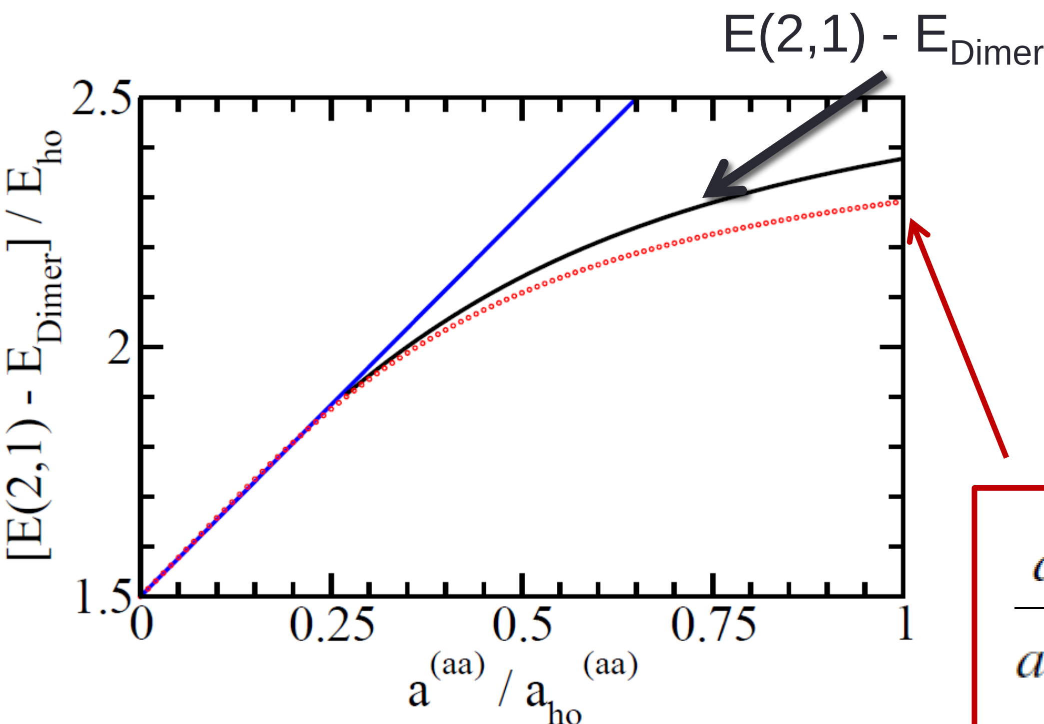
Aside: Estimation of $a^{(ad)}$ scattering length

$$\frac{E}{\hbar\omega} \approx \frac{3}{2} + \frac{2}{\sqrt{\pi}} \frac{a^{(ad)}}{a_{ho}^{(ad)}} + O\left(a^{(ad)^2}\right)$$

Prediction:

$a^{(ad)} \sim 1.179\ a^{(aa)}$

See G. V. Skorniakov and K. A. Ter-Martirosian, Zh. Eksp. Teor. Fiz. **31**, 775 (1956) [Sov. Phys. JETP **4**, 648 (1957)]; D.S. Petrov, PRA **67**, 010703(R) (2003); Shina Tan (2008)



Fit gives $a^{(ad)} \sim 1.18 a^{(aa)}$

See J. von Stecher *et. al.*, PRA **77**, 043619 (2008)

$$\frac{a^{(k)}}{a_{\mathrm{ho},\mu}^{(k)}} = \frac{\Gamma\left(-\frac{E_{\mathrm{eff}}}{2\hbar\omega} + \frac{1}{4}\right)}{2\Gamma\left(-\frac{E_{\mathrm{eff}}}{2\hbar\omega} + \frac{3}{4}\right)}$$

k = ad

A brief reminder of hyperspherical coordinates…

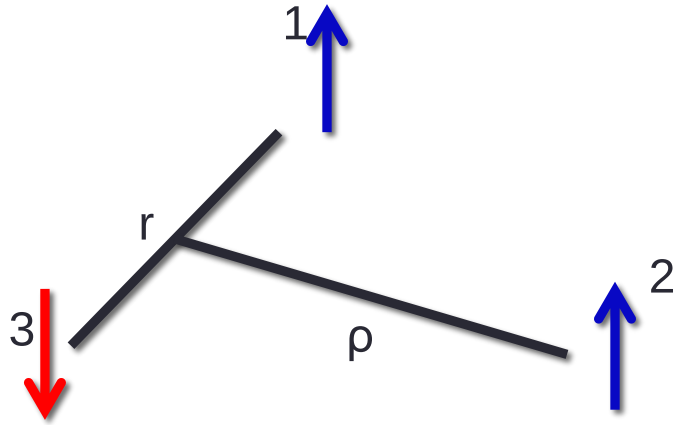
We define one length, the hyperradius R, and 3N-4 angles

$$R, \alpha, \vec{\Omega}_r, \vec{\Omega}_\rho$$

Hyperradius describes overall size of the system, α defines geometry

$$R^2 = r^2 + \rho^2$$

$$\tan(\alpha) = \frac{|\vec{r}|}{|\vec{\rho}|}$$



Green's function + Lippmann-Schwinger

In hyperspherical coordinates, full relative wave function leads to a set of coupled 1-D equations

$$\Psi_{rel}(R;\vec{\Omega}) = \sum_{s,q} F_{sq}(R)\Phi_s(R;\vec{\Omega})$$

For fixed hyper radius, psi solves the adiabatic hyper angular Schrödinger equation

$$\left[\Lambda^2 + \frac{2\mu R^2}{\hbar^2}\sum_{i<j} V(r_{ij}) - s^2 + 4\right]\Phi_s(R;\vec{\Omega}) = 0$$

The Lippmann-Schwinger equation is one method to solve for the channel functions

$$\Phi_s(R;\vec{\Omega}) = -\frac{2\mu R^2}{\hbar^2}\int_5 d\vec{\Omega}' G(\vec{\Omega},\vec{\Omega}')\left[\sum_{i<j} V(r_{ij}')\right]\Phi_s(R;\vec{\Omega}')$$

Green's function + Lippmann-Schwinger

1. smart choice of the Green's function

$$G(\vec{\Omega},\vec{\Omega}') = \sum_{\lambda_1,\mu_1}\sum_{\lambda_2,\mu_2} g(\alpha,\alpha')Y^*_{\lambda_1,\mu_1}(\vec{\Omega}_1')Y_{\lambda_1,\mu_1}(\vec{\Omega}_1)Y^*_{\lambda_2,\mu_2}(\vec{\Omega}_2')Y_{\lambda_2,\mu_2}(\vec{\Omega}_2)$$

2. Limiting behavior of the wave function at small interparticle distance

$$\lim_{r\to 0}\Phi_\nu(R;\vec{\Omega}) = \left(1-\frac{a}{r}\right)Y_{LM}(\hat{\rho})C_{LM}$$

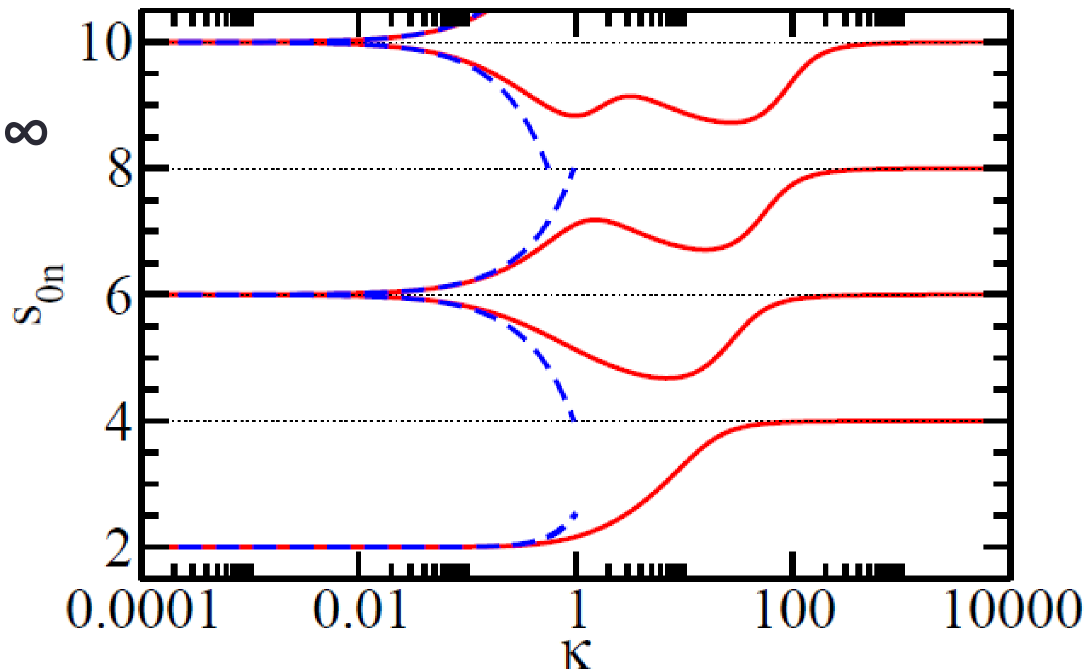
Works for <u>any</u> combination of two-body scattering lengths, mass ratio κ, angular momentum L, and particle exchange symmetry!

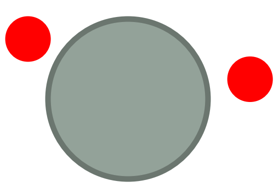
See details in Seth Rittenhouse, PhD. thesis, on JILA website, and Rittenhouse, Mehta and Greene, PRA **82**, 022706 (2010)

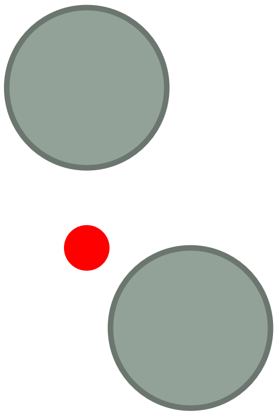
FFX transcendental equation

$$\frac{(1+2\kappa)^{1/4}}{(1+\kappa)^{1/2}}\Gamma\left[\frac{2+L-s_{L,n}}{2}\right]\Gamma\left[\frac{2+L+s_{L,n}}{2}\right] \times \left(\frac{2}{\Gamma[(1+L-s_{L,n})/2]\Gamma[(1+L+s_{L,n})/2]} + \left(\frac{-\kappa}{1+\kappa}\right)^{L} \frac{1}{\sqrt{\pi}\,\Gamma[L+3/2]}\,{}_2F_1\left[\frac{2+L-s_{L,n}}{2}, \frac{2+L+s_{L,n}}{2}, L+\frac{3}{2}, \frac{\kappa^2}{(1+\kappa)^2}\right]\right) = \frac{R}{a_s}$$

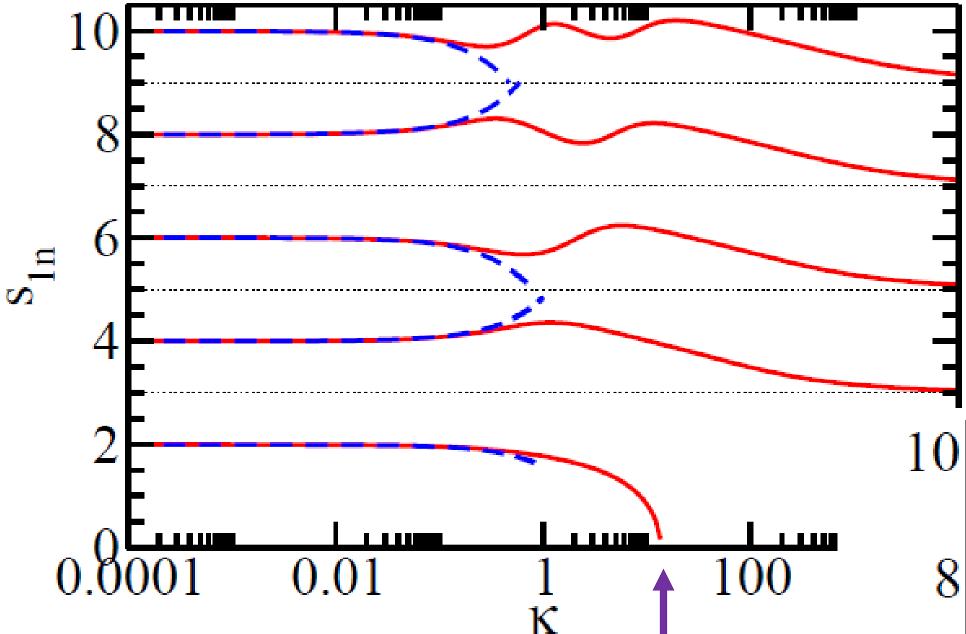
$L = 0$, $a_s \to \infty$







FFX unitarity $s_{L,n}$ eigenvalues vs κ

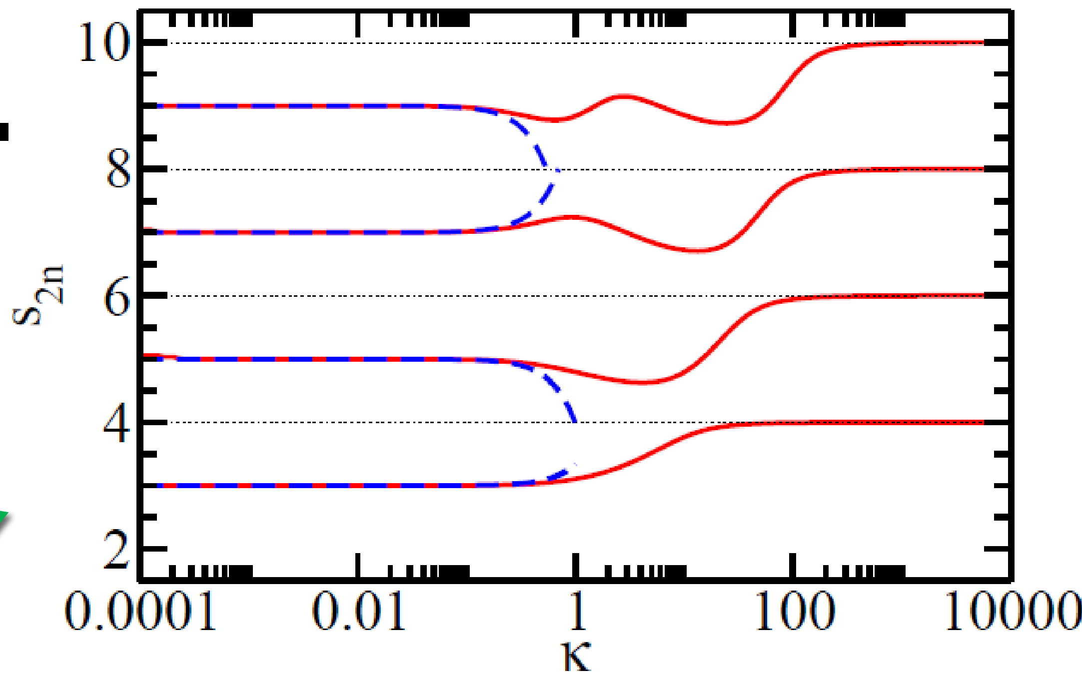


Odd L behavior

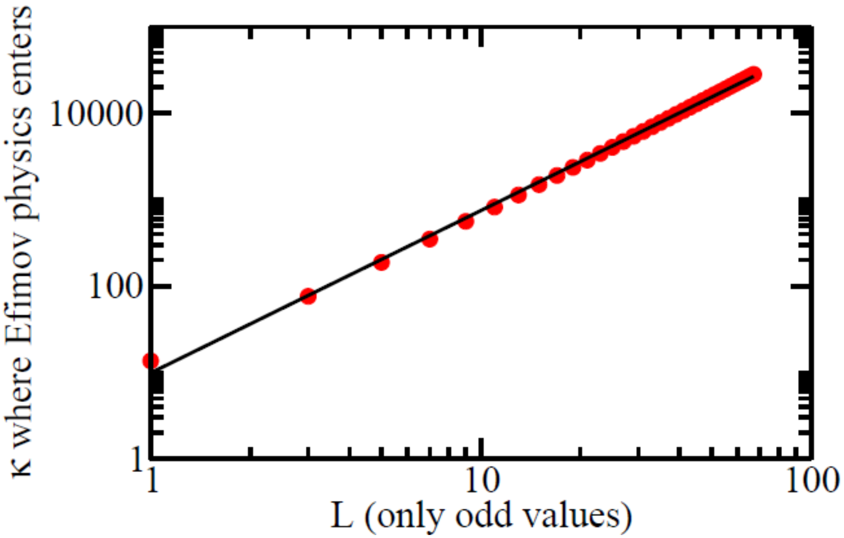
Even though resonances can appear, for this work we assume universal physics

κ=13.607 Efimov physics enters

Even L behavior



More from transcendental equation…



For each odd L, lowest $s_{L,0}$ will become imaginary at some mass ratio κ

Roughly power law behavior,
$\kappa \sim 9.864\, L^{1.88}$

What do we have now?

- **2-body energy spectrum (independent of mass ratio)**
- **3-body energy spectrum, at unitarity any mass ratio**

What can we do with these?

Thermodynamics of a two-component Fermi gas

Properties like pressure, entropy, energy calculated from derivatives of the grand canonical potential

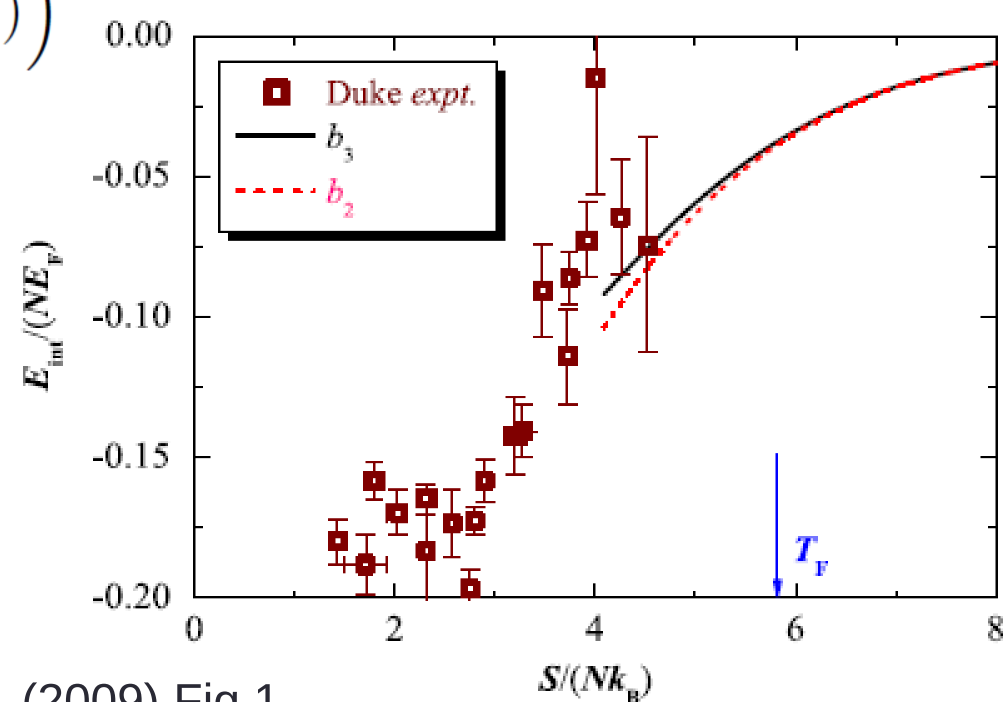
$\Delta b_{1,1}$ $\Delta b_{1,2}$

$$\Omega - \Omega^{NI} = -k_B T Q_1 \left(\frac{\Delta Q_{1,1}}{Q_1} z_1 z_2 + \left[\frac{\Delta Q_{1,2}}{Q_1} - \Delta Q_{1,1} \right] z_1 z_2^2 + \left[\frac{\Delta Q_{2,1}}{Q_1} - \Delta Q_{1,1} \right] z_1^2 z_2 + O(z^4) \right)$$

$\Delta b_{2,1}$

$$Q_{N_\uparrow, N_\downarrow} = \sum_j e^{-E_j^{N_\uparrow, N_\downarrow}/k_B T}$$

$$Q_N = \sum_j e^{-E_j^N / k_B T}$$

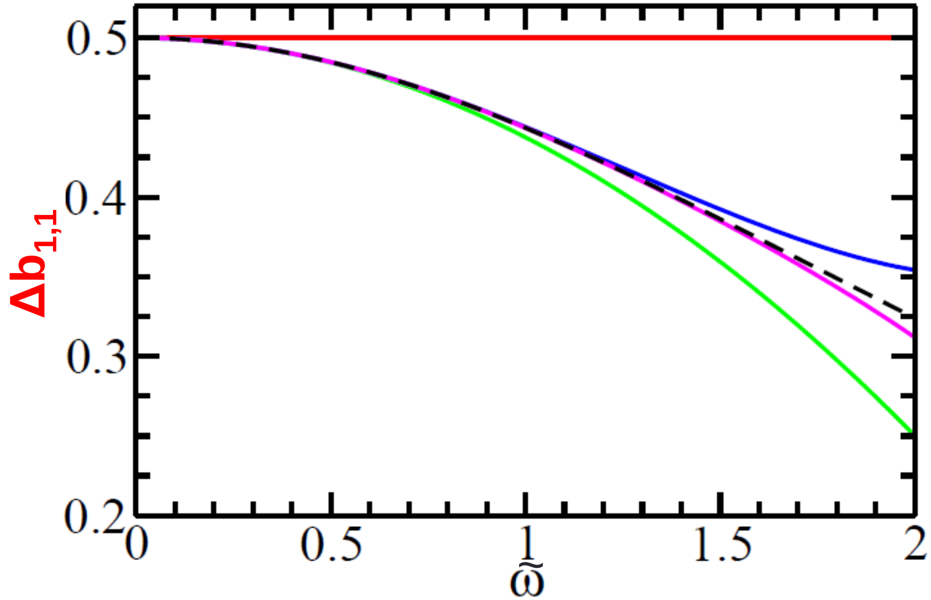


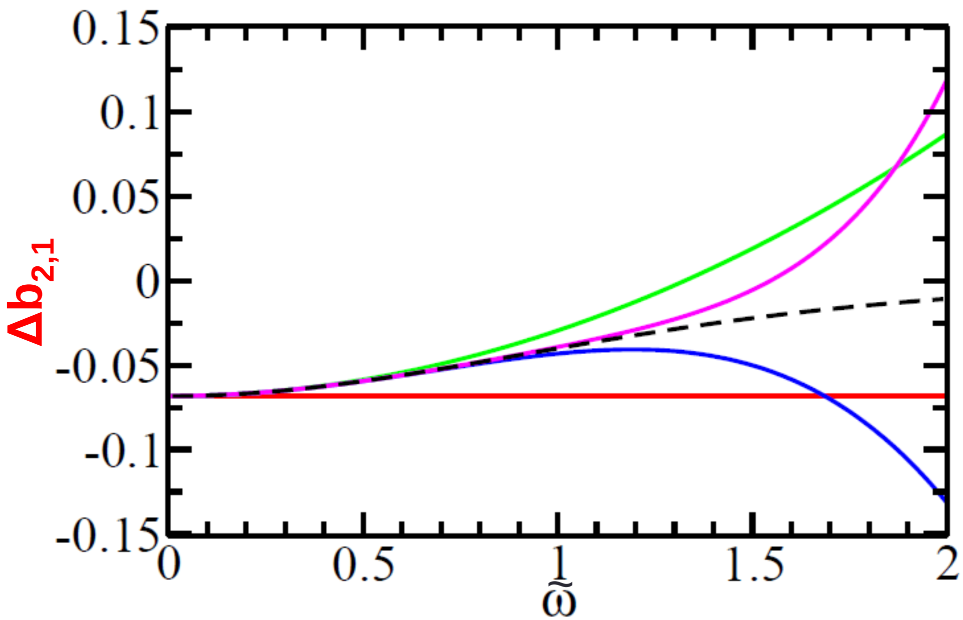
Liu and Hu, PRA **82**, 043626 (2010)
Liu, Hu and Drummond PRL **102**, 160401 (2009) Fig 1

$\kappa = 1$ virial coefficients versus $\tilde{\omega} = \hbar\omega/k_B T$

Red: universal piece (0th order)
Green: up to 2nd order
Blue: up to 4th order
Purple: up to 6th order

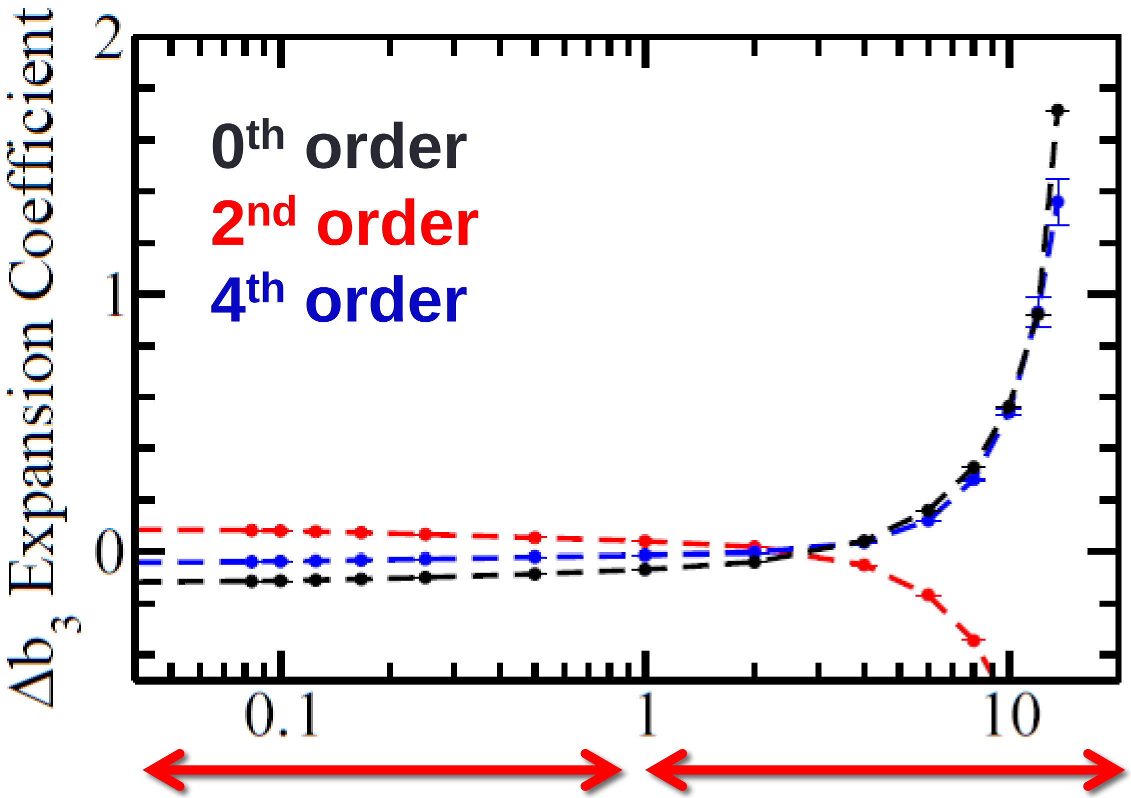
Odd orders vanish





Δb_3 values
Drummond = -0.06833960
My result = -0.06833960931128 6(3)

$\Delta b_{3=2,1 \text{ or } 1,2}$ as a function of mass ratio κ at unitarity



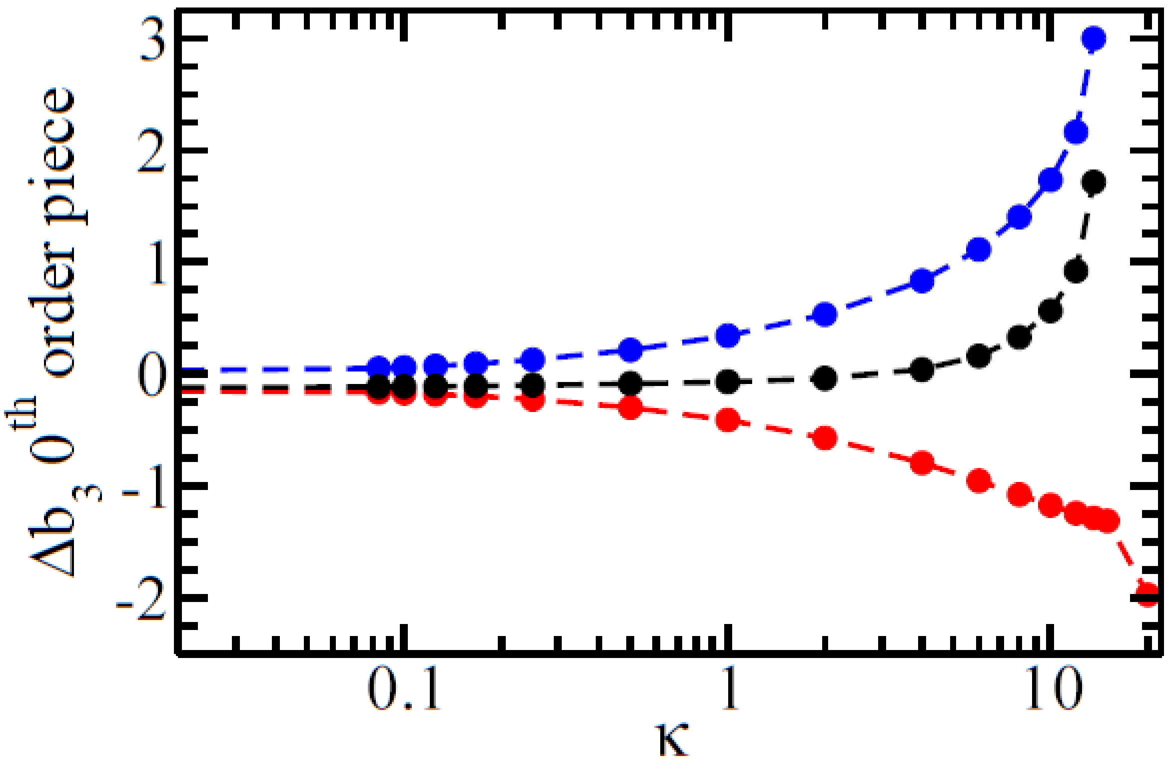
1 heavy, 2 light

2 heavy, 1 light

$$\frac{\Delta Q_{1,2}}{Q_1} - \Delta Q_{1,1} \qquad \frac{\Delta Q_{2,1}}{Q_1} - \Delta Q_{1,1}$$

Interesting behavior at κ~3 where 2 heavy + 1 light are no different from the non-interacting system
On the other hand, 1 heavy + 2 light is weakly different from NI system

Origin of “diverging” behavior…



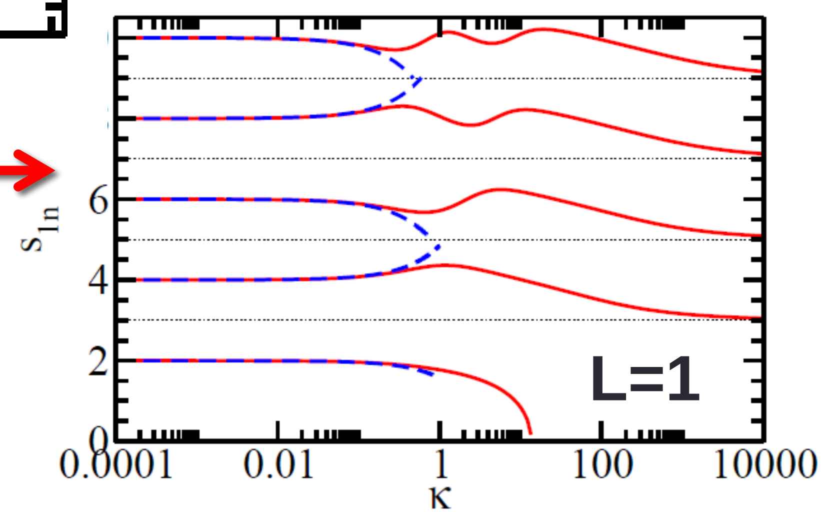
$S_{L=1,n=0}$ contibution

Full coefficient

All but $S_{L=1,n=0}$

1 heavy, 2 light

2 heavy, 1 light



Recall Δb_3 involves sum over all energy states

Next steps

- Understand high T thermodynamics in trap for unequal mass systems
  - So far ignored questions related to stability
- “undo” trap via LDA to get high T thermodynamics of homogeneous system
- Few-body thermodynamics (Canonical ensemble)
  - From optical lattices with few particles per lattice site, deep lattice
  - Jochim’s group at Heidelberg, single microtrap with few particles

Conclusion

- Determined condensate fraction of trapped two-body system
- Characterized energy spectrum of three-body system with unequal masses
- Determined two- and three-body virial coefficients at unitarity with high accuracy