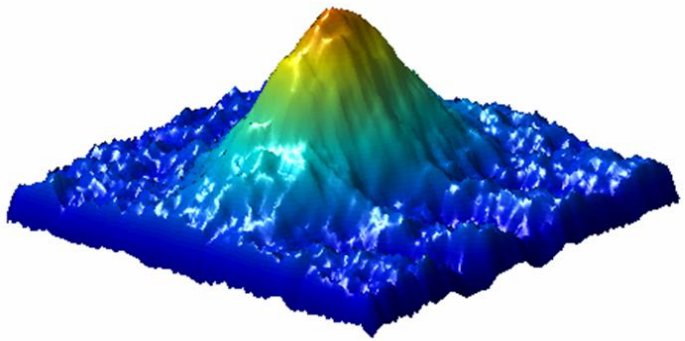
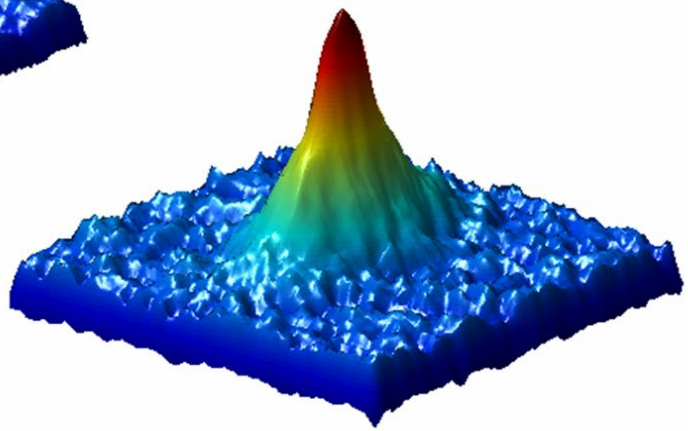
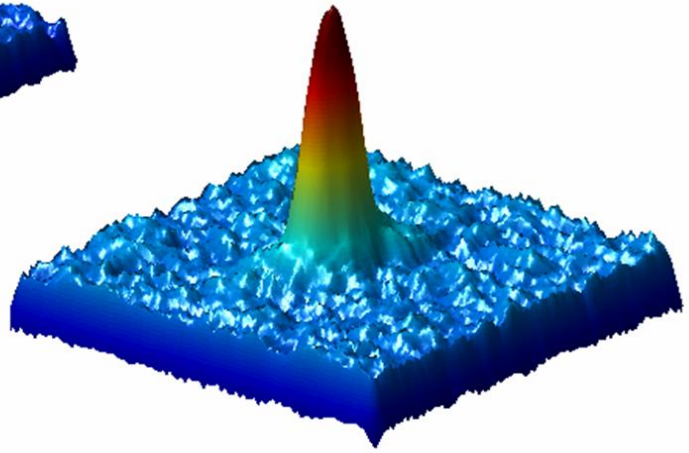


Experimental image of Rubidium condensate (Engels' group at WSU)





attractive

repulsive

Pseudopotentials for Interacting Dipoles

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Currently on sabbatical at ITAMP.

Supported by NSF PHY.

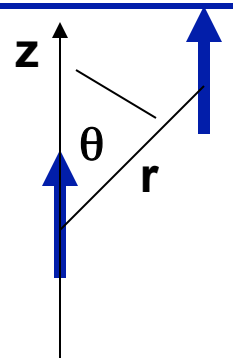
Outline

- s-wave pseudopotentials:
  - Application to two and three trapped atoms.
  - Connection to many-body system.

- Dipolar pseudopotentials:
  - Finite-range pseudopotential.
  - Zero-range pseudopotential.

Pseudopotentials

Long-range potential: $d^2 (1-3\cos^2\theta) / r^3$



- Why?
  - Mathematically convenient.
  - Some few-body calculations become tractable analytically.
  - Some many-body calculations become tractable analytically or simplify.
- Why not?
  - Details of the interactions may get lost or be difficult to put in.
  - The math can get nasty.
- Dipoles: Anisotropic and long-range interactions.
- Throughout this talk: aligned dipole = point particle.

Replace Atom-Atom Interaction by Zero-Range Pseudopotential

- Start with ab initio atom-atom potential.
- Coupled channel calculation provides phase shifts $\delta_l(k)$.
- Construct zero-range pseudo-potential with same a_s (outside solution):

$$V_{\rm ps}(\mathbf{r}_{jk}) = \frac{4\pi\hbar^2 a_s(k)}{m_a}\delta^{(3)}(\mathbf{r}_{jk})\frac{\partial}{\partial r_{jk}}r_{jk}$$

Cures 1/r divergence of radial function: $j_l \sim r^l$ and $n_l \sim r^{-l-1}$

Analytical treatments

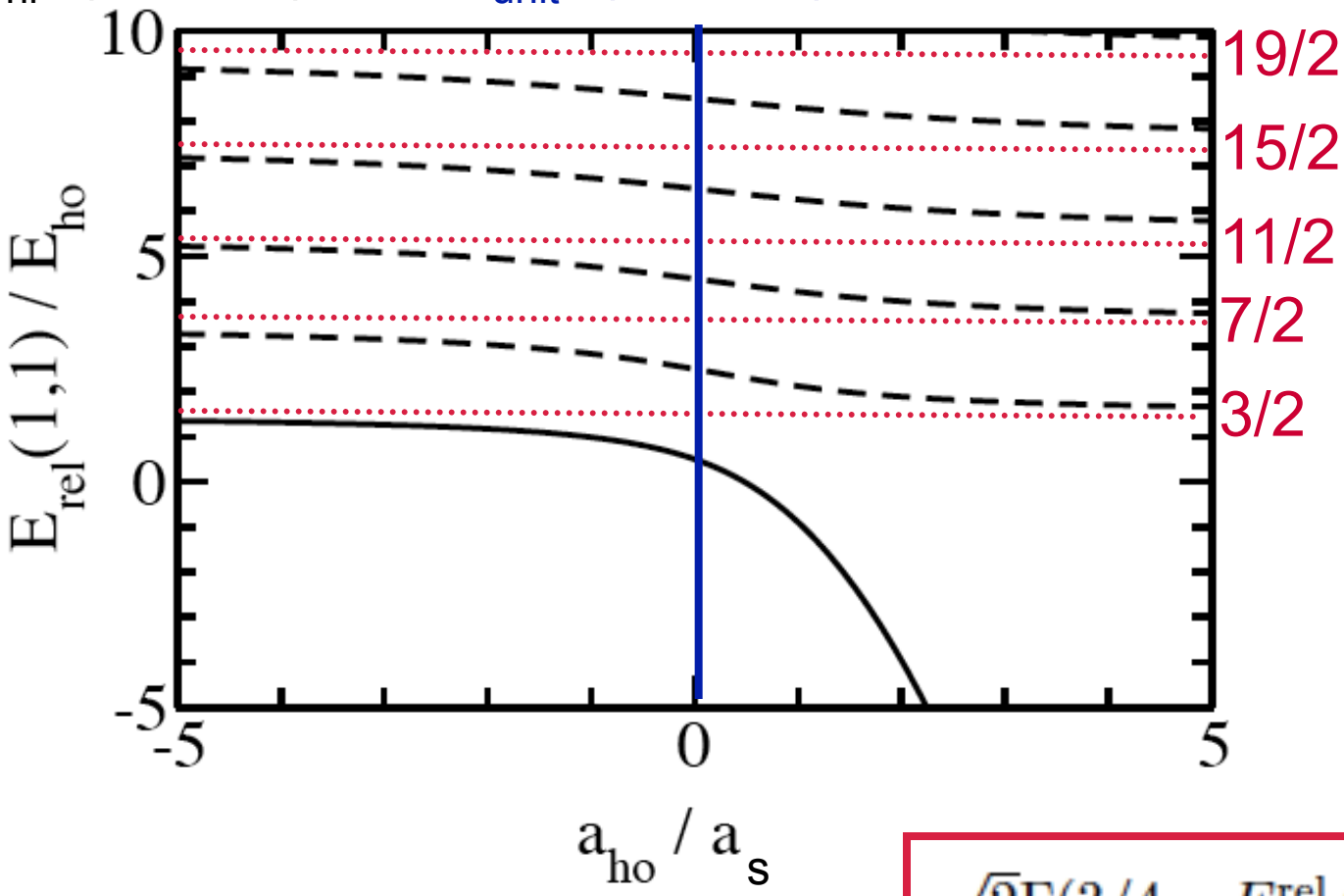
$$\left[\frac{\frac{\partial}{\partial r}\left(r\psi_{3D}(\vec{r})\right)}{r\psi_{3D}(\vec{r})}\right]_{r\to 0} = -\frac{1}{a_s}$$

- Works if λ_{dB} (and $|a_s|$) >> r_0 (for alkalis, van der Waals length).

Huang and Yang, Physical Review 105, 767 (1957).
Without regularization operator, Fermi (1934).

Two s-Wave Interacting Particles in External Spherically Harmonic Trap

$E_{ni}=(2n+3/2)h\nu$ $E_{unit}=(2n+1/2)h\nu$

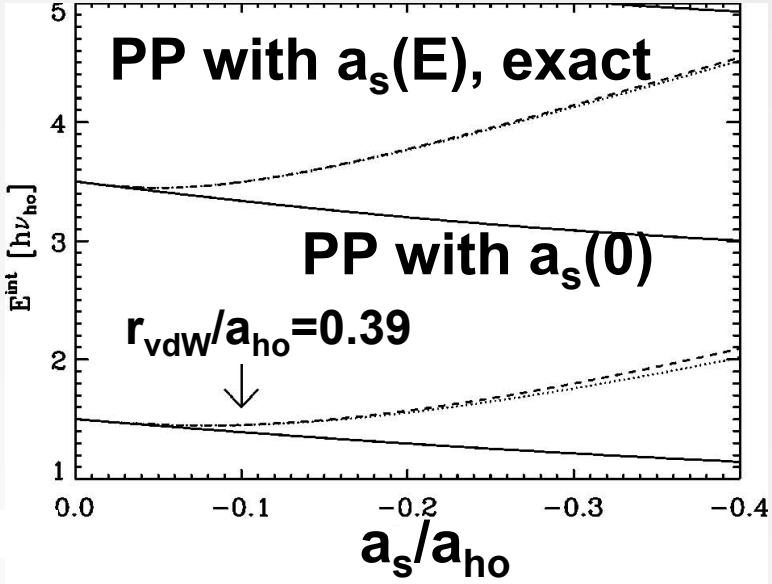


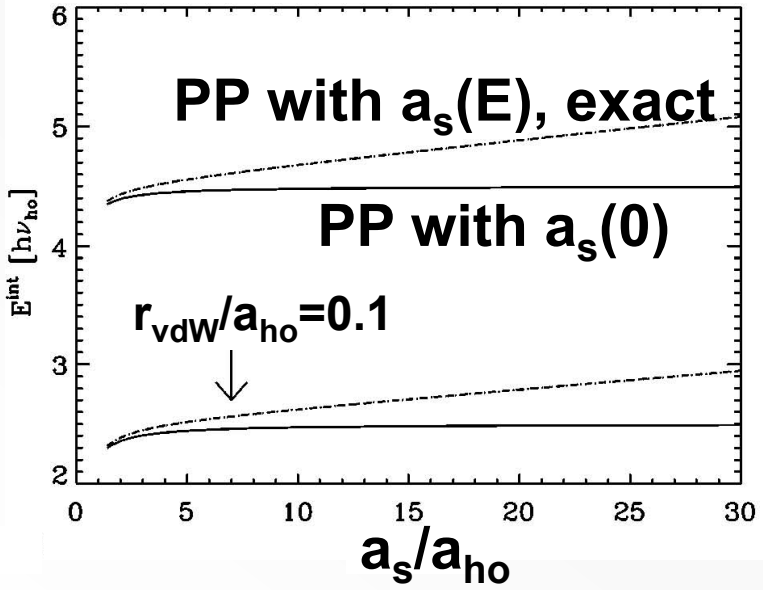
Finite angular momentum:
$E_{nl}=(2n+l+3/2)h\nu$

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

$$\frac{\sqrt{2}\Gamma(3/4 - E_2^{\mathrm{rel}}/(2\hbar\omega))}{\Gamma(1/4 - E_2^{\mathrm{rel}}/(2\hbar\omega))} = \frac{a_{\mathrm{ho}}}{a_s(E_2^{\mathrm{rel}})}$$

Comparison of Pseudopotential Solution and Full Solution





- Two-particle energy spectrum known semi-analytically: Simple transcendental equation [Busch et al., Found. of Physics (1998)].
- Self-consistent solution when $a_s=a_s(E)$ [Blume and Greene, PRA 65,043613 (2002); see also Bolda et al., PRA 66, 013403 (2002)].
- Energy-independent pseudo-potential, I.e., use of $a_s(0)$, works if $|a_s|<<a_{ho}$.
- Energy-dependent pseudo-potential, I.e., use of $a_s(E)$, works if $r_{vdW}<<a_{ho}$.

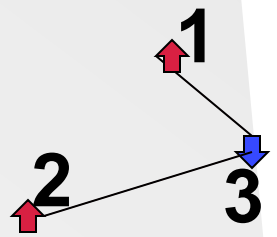
PP Treatment of Three Harmonically Trapped Fermions (s-Wave Interaction)

- **Two spin-up fermions and one impurity with interspecies zero-range s-wave interactions:**

$$H = \sum_{j=1}^{3} H_0(\mathbf{r}_j, \mathcal{M}) + V_{\rm int}$$

$$V_{\rm int} = V_{\rm ps}^{\rm 3D}(\mathbf{r}_{31}) + V_{\rm ps}^{\rm 3D}(\mathbf{r}_{32})$$

$$H_0(\mathbf{r}_j, \mathcal{M}) = \frac{-\hbar^2}{2\mathcal{M}} \boldsymbol{\nabla}_{\mathbf{r}_j}^2 + \frac{1}{2}\mathcal{M}(\omega_z^2 z_j^2 + \omega_\rho^2 \rho_j^2)$$

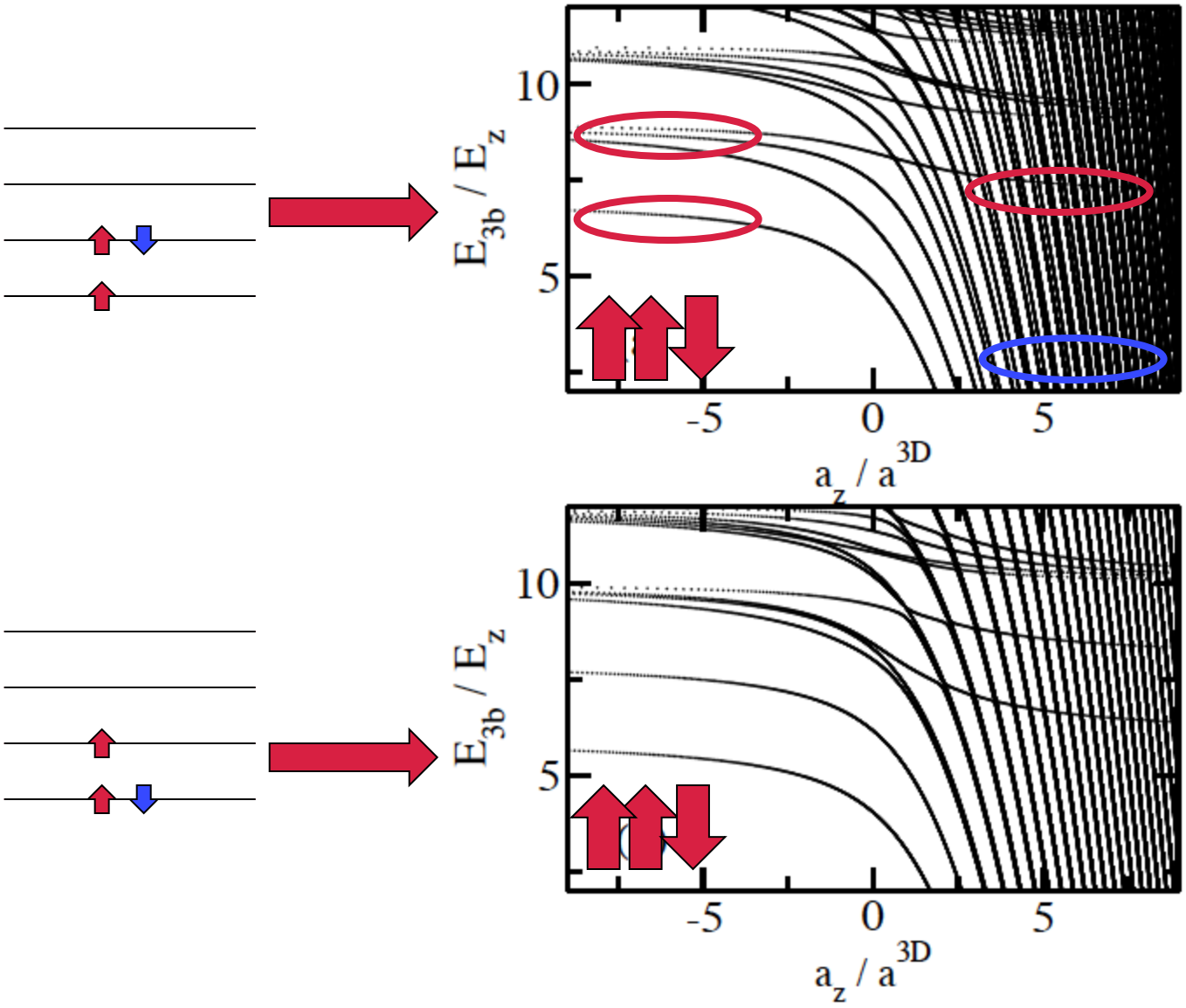


- **Determine bound state wave function in relative coordinates using Lippmann-Schwinger equation:**

$$\Psi(\mathbf{r}, \mathbf{R}) = -\int G(E_{\rm 3b}; \mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') V_{\rm int}(\mathbf{r}', \mathbf{R}') \Psi(\mathbf{r}', \mathbf{R}')\, d\mathbf{r}' d\mathbf{R}'$$

See work by Mora et al., Petrov et al., Kestner et al.,…

Elongated Trap: Aspect Ratio η=2 and "Projection" Quantum Number M=0



Π_z=+1

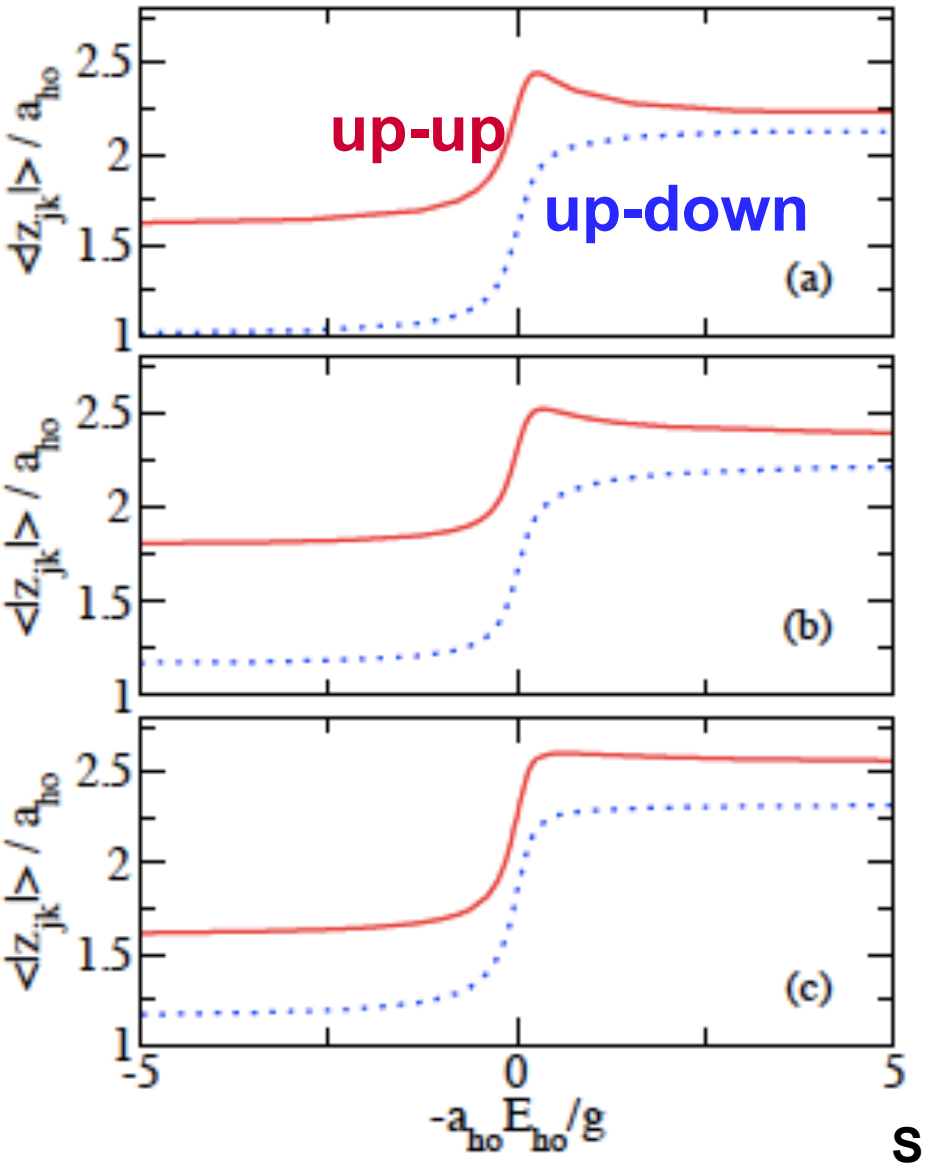
Atom-atom-atom states

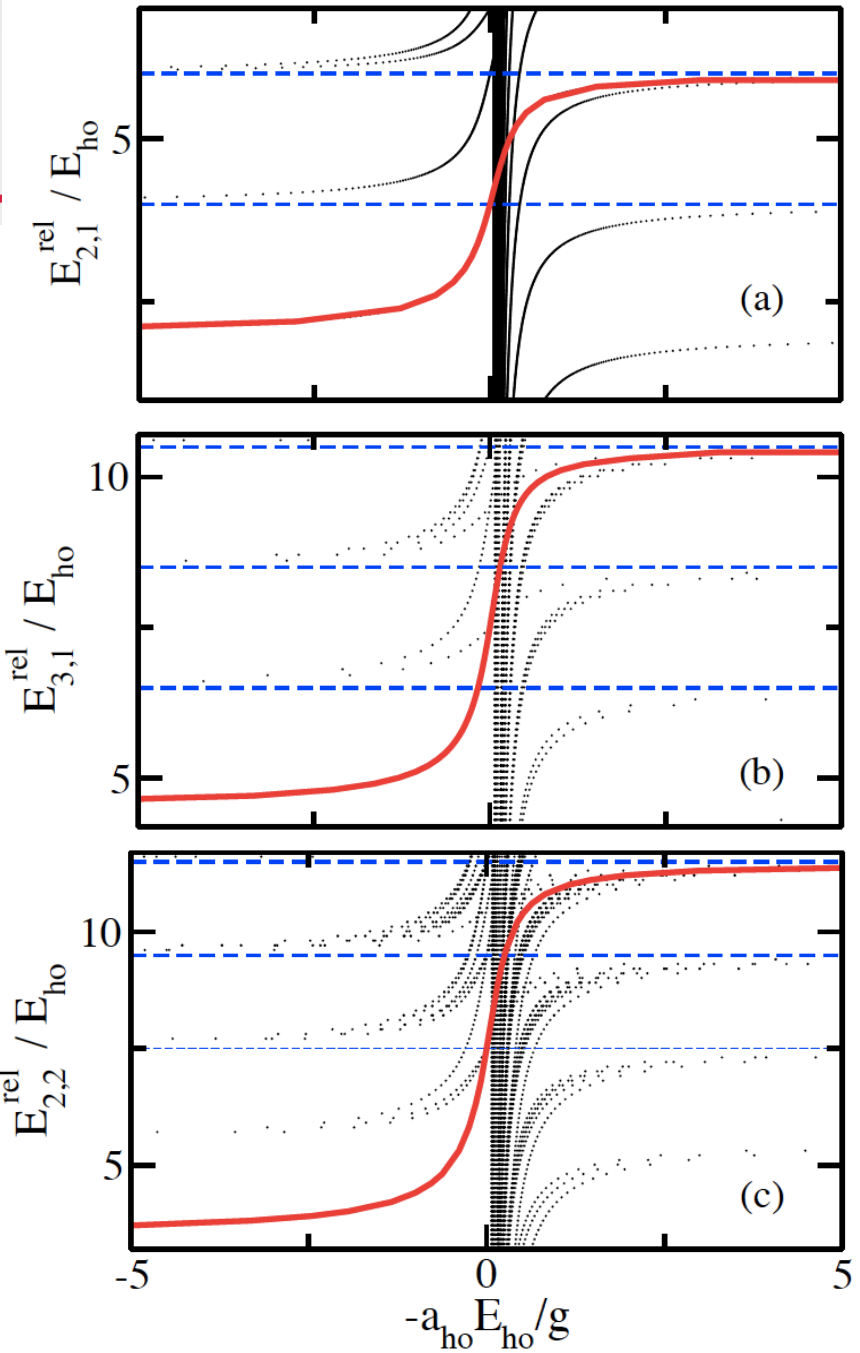
Atom-dimer states

Π_z=-1

S.E. Gharashi, K.M. Daily, D. Blume, PRA 86, 042702(2012).

Fermions in Strictly 1D: $g\delta(z_{jk})$





S.E. Gharashi and D. Blume, unpublished.

Non-regularized PP + Hartree Wave Function = GP equation

- **Many-body Hamiltonian for N bosons under confinement:**

$$H = \sum_{j=1}^{N}\left[\frac{-\hbar^2}{2m}\nabla_{\vec{r}_j}^2 + \frac{1}{2}m\omega^2\vec{r}_j^2\right] + \sum_{j<k}^{N} V_{aa}(\vec{r}_j - \vec{r}_k)$$

SW, HS,…

- **Hartree product (restricted Hilbert space):**

$$\psi(\vec{r}_1, \cdots, \vec{r}_N) = \prod_{i=1}^{N}\phi_a(\vec{r}_i)$$

- **ZR atom-atom potential:**

$$V_{aa}(\vec{r}) = \frac{4\pi\hbar^2 a_{aa}}{m}\delta^{(3)}(\vec{r}) \propto U_{aa}\delta^{(3)}(\vec{r})$$

- **Gross-Pitaevskii (GP) equation for "single atom":**

$$\left(-\frac{1}{2}\nabla_{\vec{r}}^2 + \frac{1}{2}\vec{r}^2 + U_{aa}(N-1)|\phi_a(\vec{r})|^2\right)\phi_a(\vec{r}) = \epsilon_a\phi_a(\vec{r})$$

Single atom feels effective potential/mean-field created by the other N-1 atoms.

Esry, PRA 55, 1147 (1997).

Finite-Range Pseudo-Potential For Two Interacting Dipoles

- Pseudo-potential needs to account for dipole-dependent s-wave scattering length [Yi and You, PRA 61, 041604 (2000)]:

$$V(\vec{r},\vec{r}') = \underbrace{\frac{4\pi\hbar^2 a(d)}{m}\delta(\vec{r}-\vec{r}')}_{\text{s-wave scattering (determined by interplay between SR and dipole potential)}} + \underbrace{d^2\frac{1-3\cos^2\theta}{|\vec{r}-\vec{r}'|^3}}_{\text{Mixing between different partial waves (goes all the way to zero)}}$$

- Does this pseudo-potential work if used in conjunction with Hartree wave function? Will show: Yes, if dipole length not too large.

Mean-Field Gross-Pitaevskii Description of Dipolar Bose Gas

$$i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2M}\nabla^2+\frac{M\omega_\rho^2}{2}(\rho^2+\lambda^2z^2)\right.$$
$$\left.+(N-1)\left[\frac{4\pi\hbar^2a}{M}|\psi(\boldsymbol{r},t)|^2+\int d\boldsymbol{r}'V_d(\boldsymbol{r}-\boldsymbol{r}')|\psi(\boldsymbol{r}',t)|^2\right]\right]\psi(\boldsymbol{r},t)$$

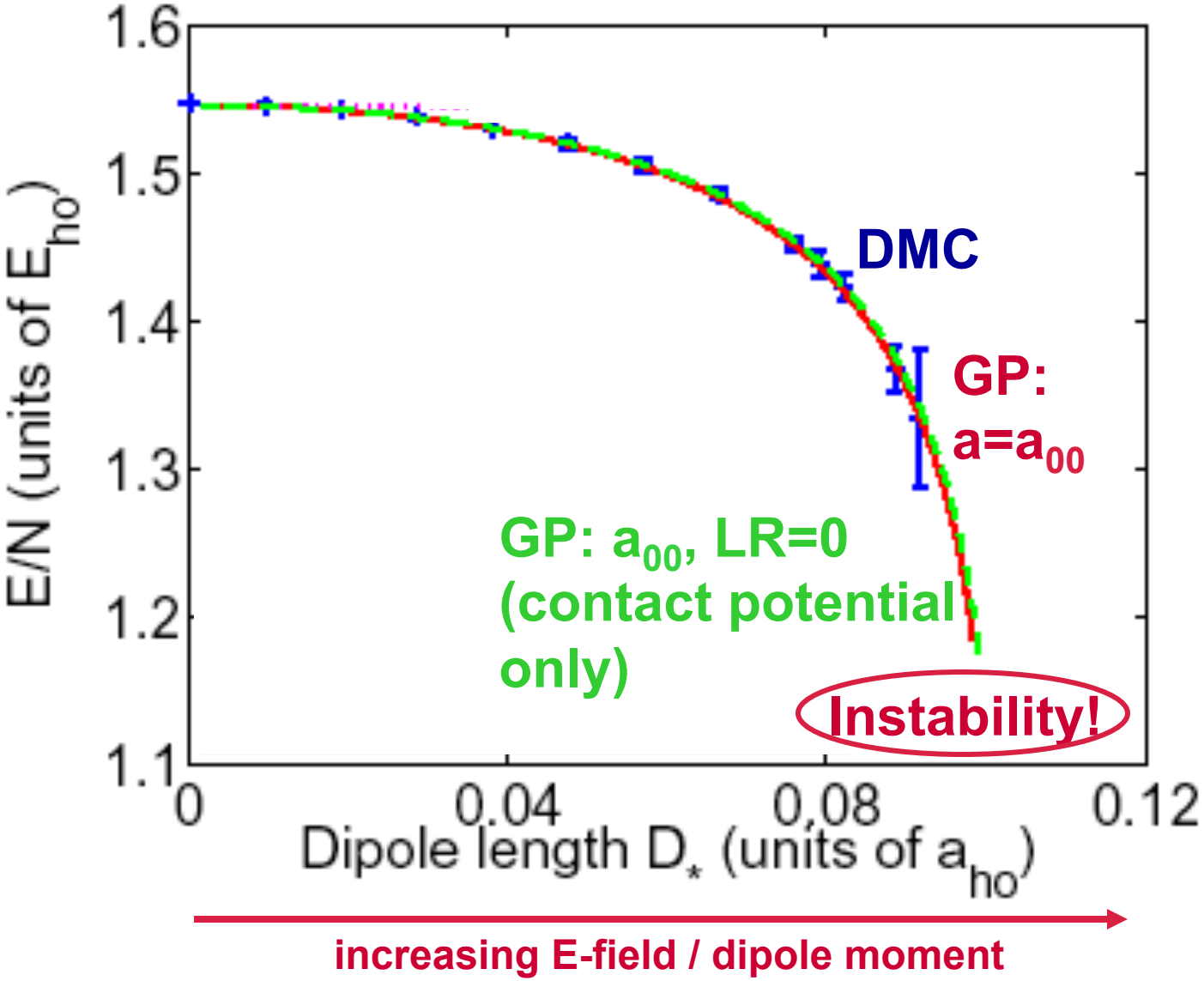
Mean-field interaction:

contact s-wave (SR) + dipole-dipole (LR)

Integro-differential equation solved following Ronen et al., PRA 74, 013623 (2006):
Take advantage of cylindrical symmetry and perform Fourier transform in z and Hankel transform in ρ.

Compare with results from many-body Schroedinger equation that uses model potential (hardwall + V_{dd}) as input.

Spherical Confinement (N=10, b=0.0137a_{ho}): GP versus Many-Body DMC Energies

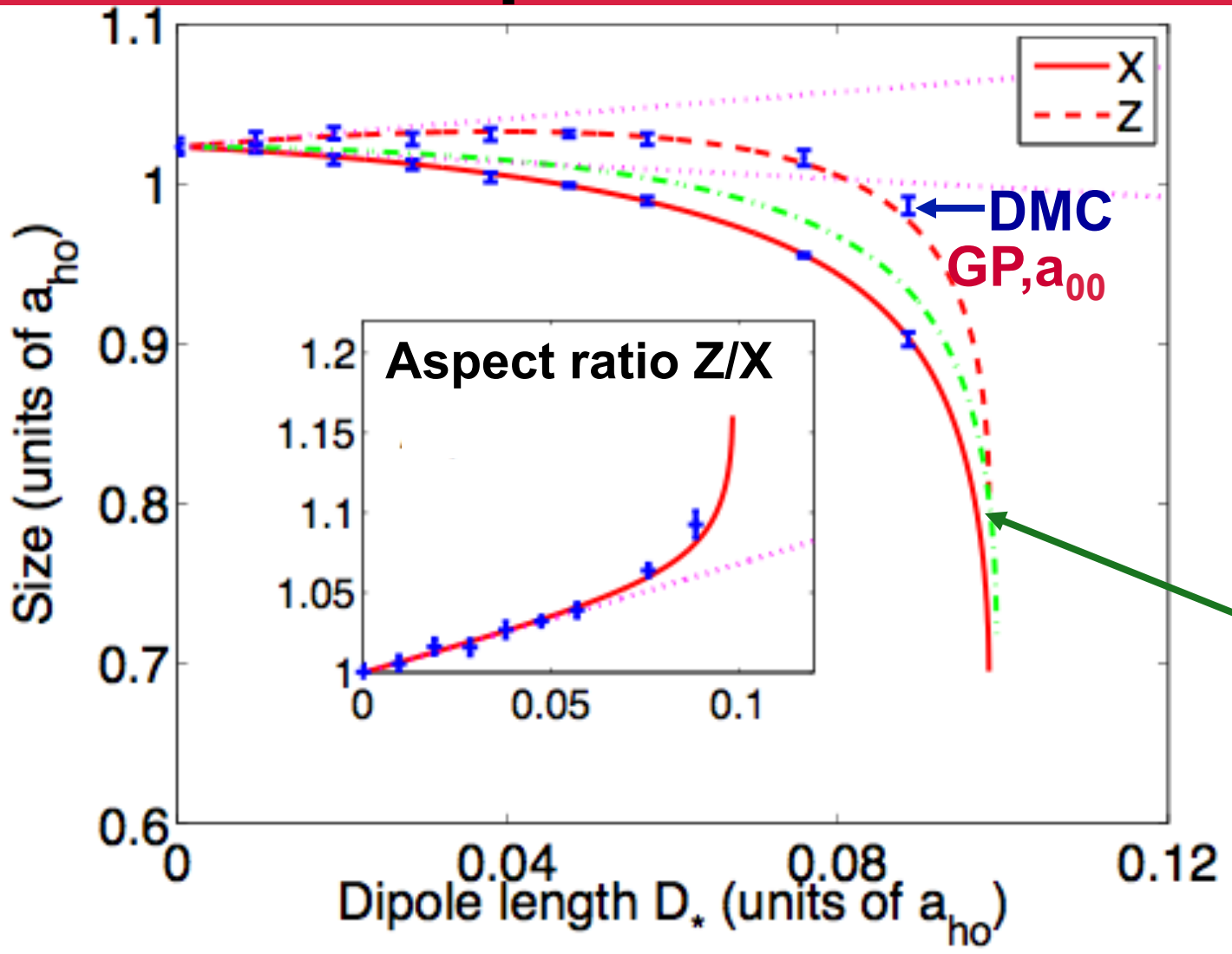


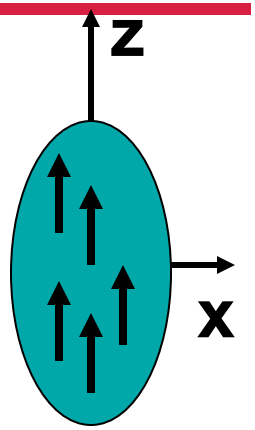
Excellent agreement between GP and DMC many-body energies! …but GP results w/ and w/o LR part are very similar!

s-wave induced instability.

Bortolotti, Ronen, Bohn, Blume, PRL 97, 160402 (2006)

Spherical Confinement (N=10, b=0.0137a_{ho}): Size and Aspect Ratio





Size X=$\sqrt{\langle x^2 \rangle}$

Size Z=$\sqrt{\langle z^2 \rangle}$

GP, a_{00}.
LR part = 0
(isotropic).

Validation of mean-field treatment!

Structural properties depend on dipole moment!

Zero-Range Pseudopotential for Dipole-Dipole Interactions

$$V_{pp,reg}(\vec{r}) = \sum_{ll'} V_{ll'}(\vec{r})$$ Here, $m_l = m_{l'} = 0$ (generalizes to any m_l).

$$V_{ll'}(\vec{r})\Phi(\vec{r}) = g_{ll'} \frac{\delta(r)}{r^{l'+2}} Y_{l'0}(\theta,\phi) \times \left[\frac{\partial^{2l+1}}{\partial r^{2l+1}} r^{l+1} \int Y_{l0}(\theta,\phi)\Phi(\vec{r})\, d\Omega \right]_{r\to 0}$$

$$g_{ll'} = \frac{\hbar^2}{2\mu} \frac{a_{ll'}}{k^{l+l'}} \frac{(2l+1)!!(2l'+1)!!}{(2l+1)!}$$

Pseudopotential proposed by Derevianko, PRA 67, 033607 (2003).

Born approximation (m_l=0):

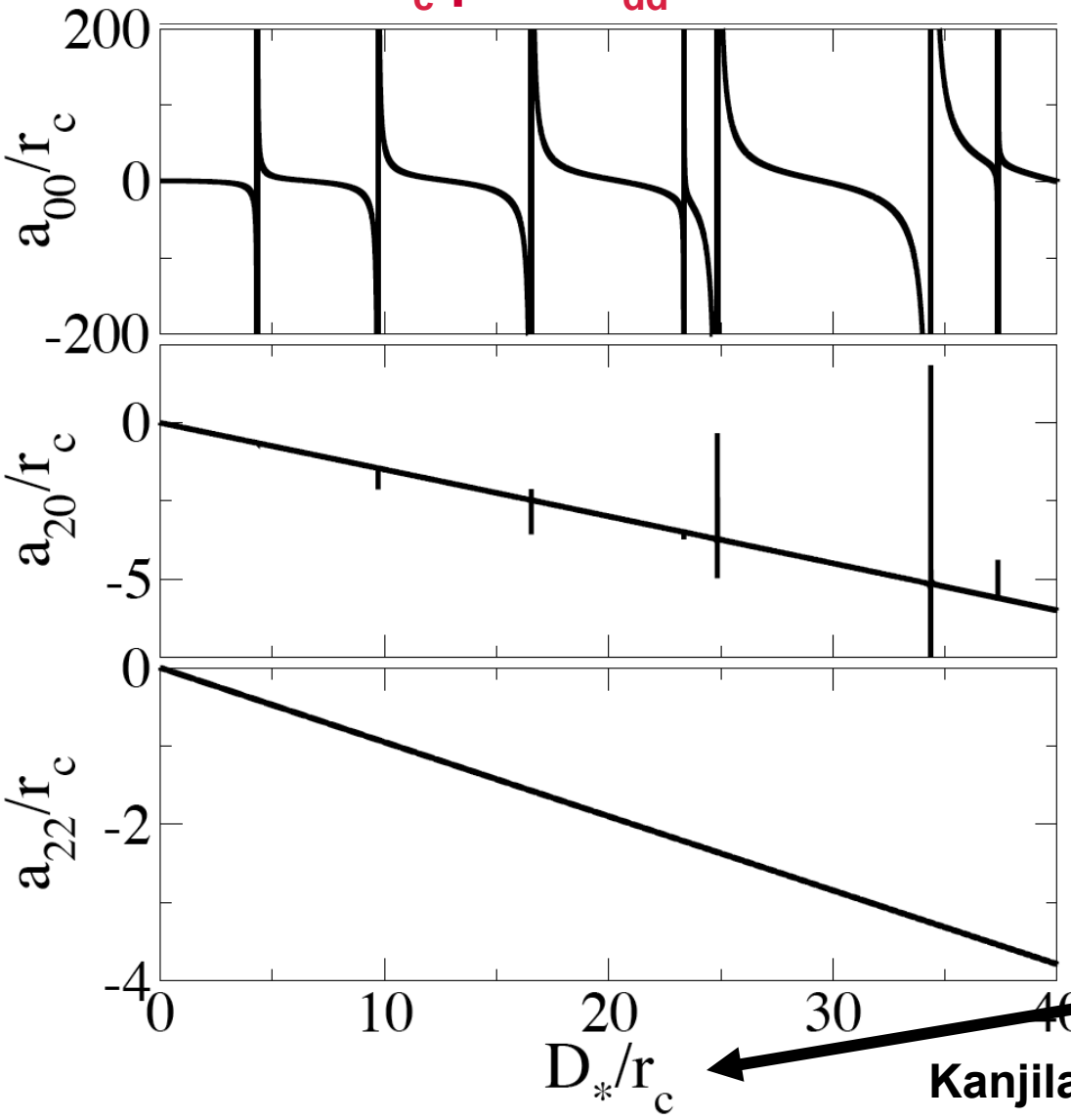
$$a_{ll} = -\frac{2D_*}{(2l-1)(2l+3)}$$

$$a_{l,l-2} = -\frac{D_*}{(2l-1)\sqrt{(2l+1)(2l-3)}}$$

System (even l):

Scattering Lengths for Two Aligned Identical Bosonic Point Dipoles

Hard wall at r_c plus V_{dd}.



Scattering length $a_{ll'}$ for each partial wave:

$a_{ll'} = \lim_{k\to 0} -\tan[\delta_{ll'}(k)]/k$

$a_{ll'}$ constant as $E \to 0$.

a_{00} depends on SR and LR part of potential.

$a_{ll'} \propto D_*$ for $l,l' > 0$ (except near resonance).

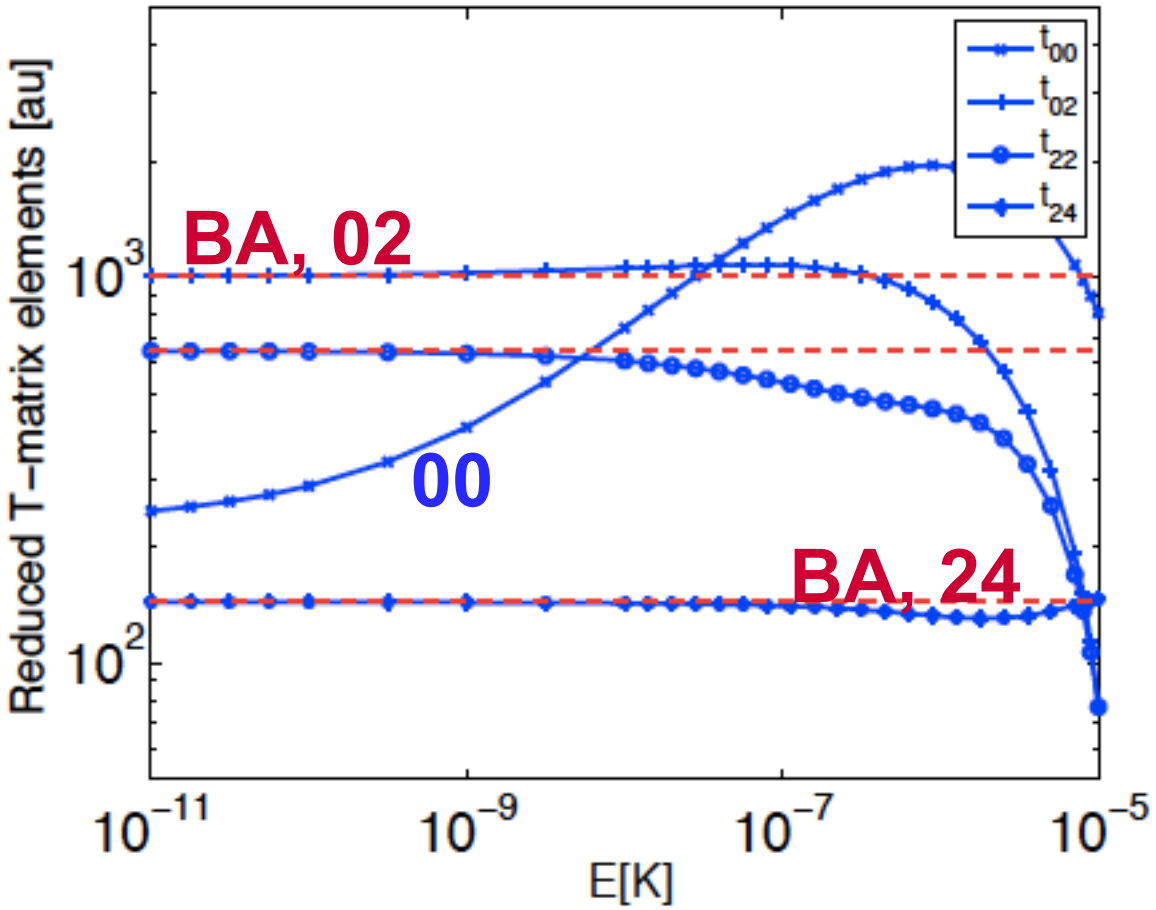
[dipole length $D_* = \mu d^2/\hbar^2$. SR cutoff r_c]

Tuning SR or LR physics.

Kanjilal and Blume, PRA 78, 040703 (2008)

Model Potential with Large Dipole Length: Energy-Dependence

Ronen, Bortolotti, Blume, and Bohn, PRA, 2007.



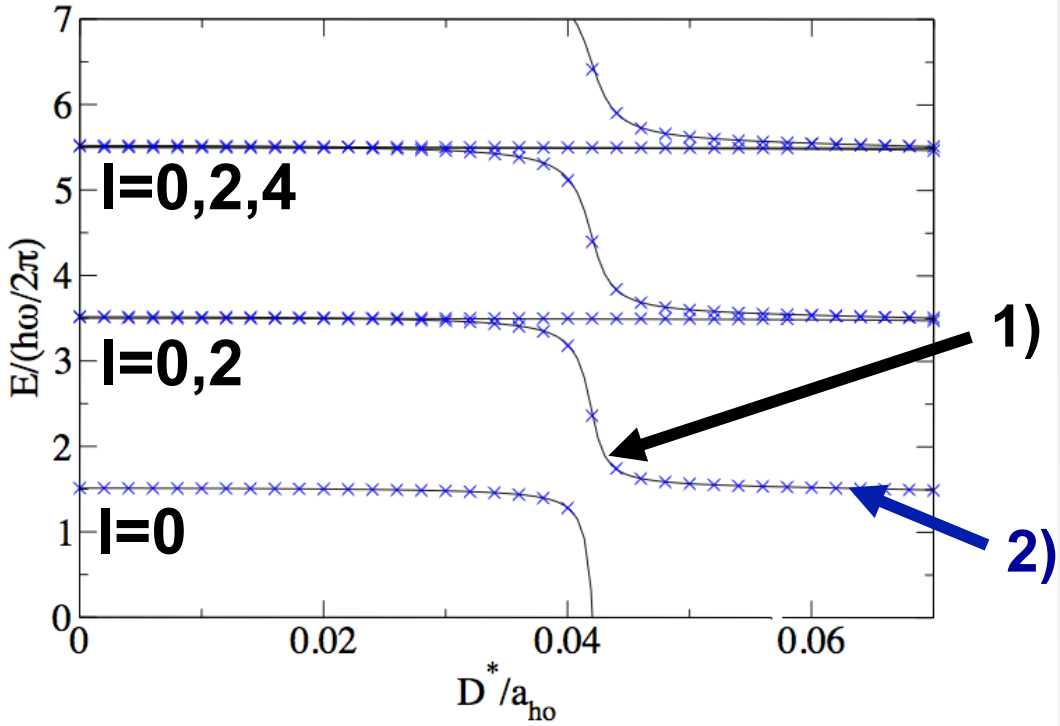
- Toy model for OH-OH:
- m=17amu
- r_c=105a.u.
- d=0.66a.u.
- D^*/r_c=128

- BA breaks down ➔ PP breaks down

Energy Spectrum of Two Dipoles Under Spherical Harmonic Confinement

Hamiltonian $H = T_1 + T_2 + V_{trap}(1) + V_{trap}(2) + V_{int}(r,\theta)$

Kanjilal, Bohn, Blume, PRA 75, 052705 (2007)



1) Finite range potential: "Brute force" numerical solution to 2d S.E..
2) Zero-range pseudo-potential that depends $a_{ll'}$: Analytical treatment.

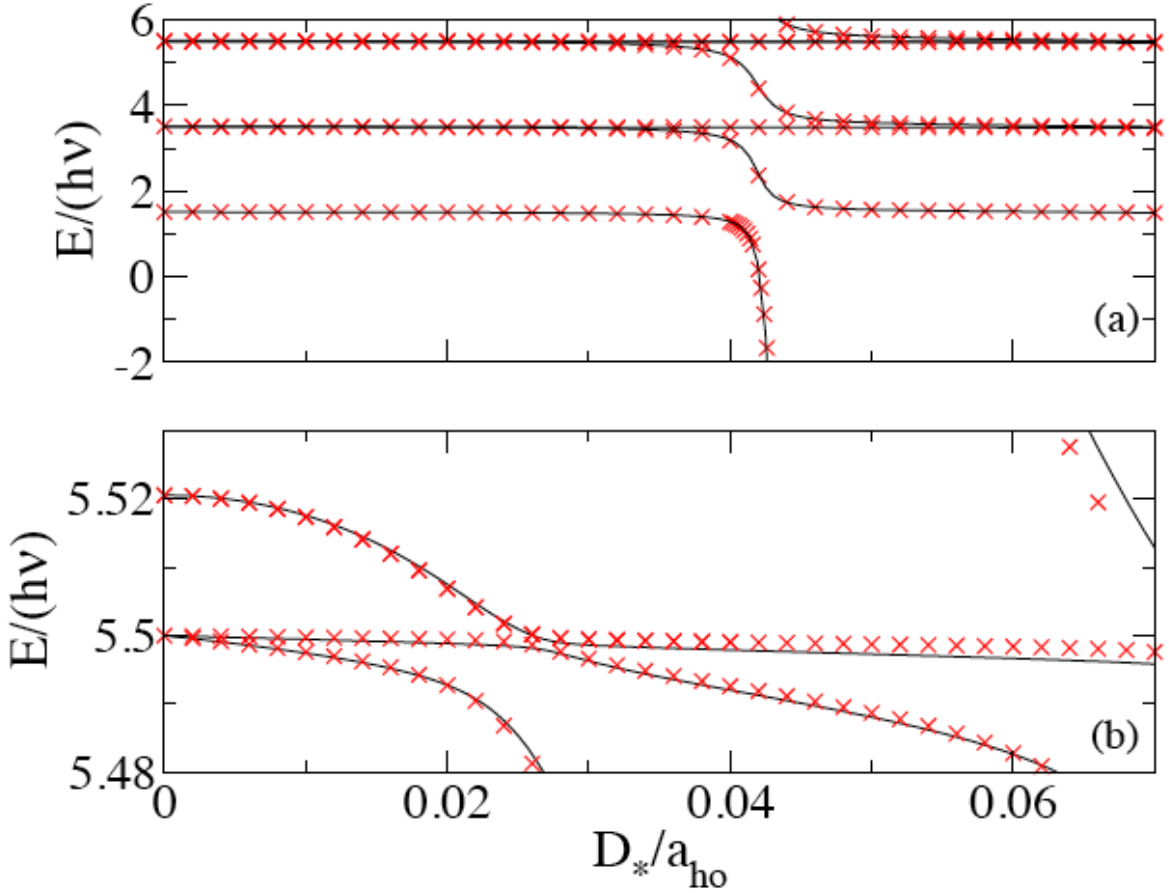
System (even l):

Good agreement indicates that scattering lengths do determine energy spectrum.

Energy Spectrum of Two Dipoles Under Spherical Harmonic Confinement

Kanjilal, Bohn, Blume, PRA 75, 052705 (2007)

Hamiltonian $H = T_1 + T_2 + V_{trap}(1) + V_{trap}(2) + V_{int}(r,\theta)$

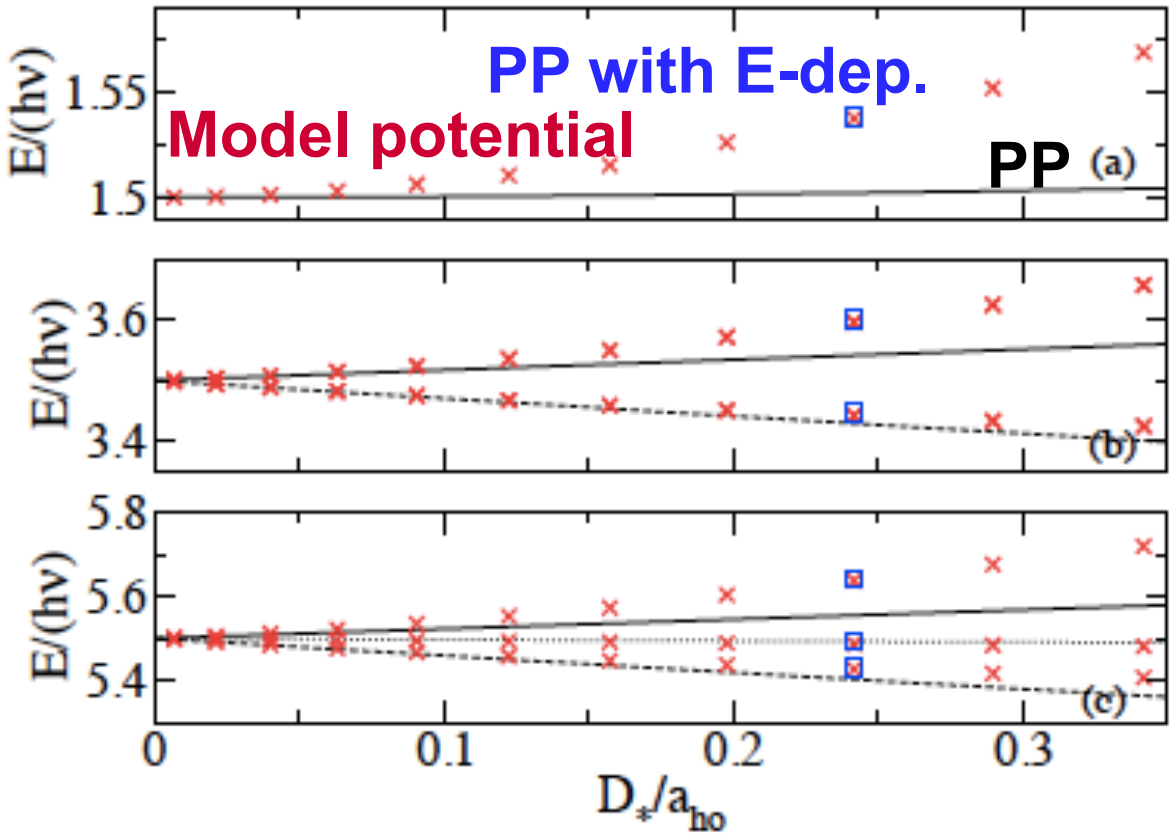


Finite range potential: "Brute force" numerical solution to 2d S.E..

Zero-range pseudo-potential that depends $a_{ll'}$.

Good agreement indicates that scattering lengths do determine energy spectrum.

Inclusion of Energy-Dependence



Here, r_c fixed and d chosen such that $a_{00}(E=0)=0$.

Accounting for energy-dependence greatly improves validity regime of pseudopotential.

Need D^*/a_{ho} somewhat smaller than 1.

What Needs Fixing?
What Doesn't Work?

- Eigenequation for spherically symmetric confinement with pseudopotential interaction possesses unphysical root in low energy regime (for even l, at around $E \sim 0.05\hbar\omega$):
  - Test: Unphysical root goes away for SR potential.
  - Fix: If we only use l=0 or l=1 part of pseudopotential, spectrum is described fairly well.

- Eigenequation for anisotropic confinement (using regularization operators proposed by Idziaszek and Calarco) shows more of these unphysical roots (unpublished work by Kanjilal and Blume).

- Modify energy-dependence of dipolar pseudopotential?