Nuclear Physics within Finite Volumes

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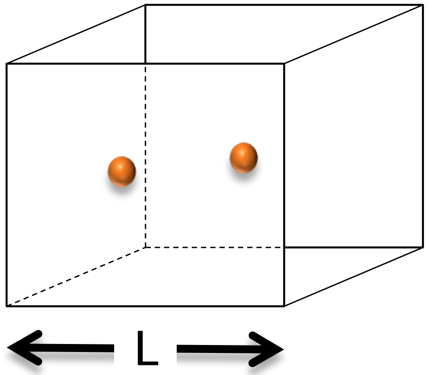
Simulations and Symmetries: Cold Atoms, QCD, and Few-hadron Systems

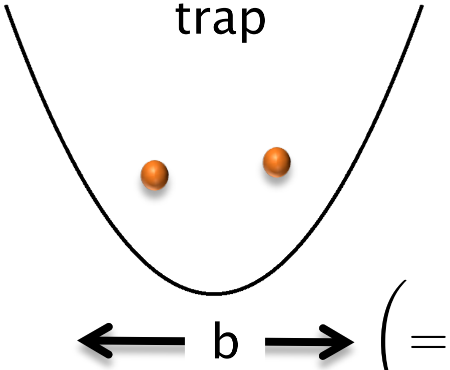
What do I mean by finite volumes?

For this talk, I really mean two scenarios

Cubic volume



External oscillator trap

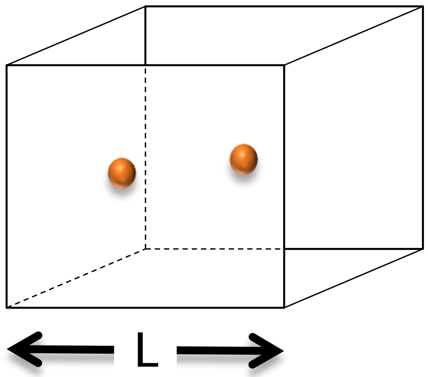


$$\left(= \frac{\hbar^2}{\sqrt{\mu\omega}} \right)$$

What’s so special about these scenarios?

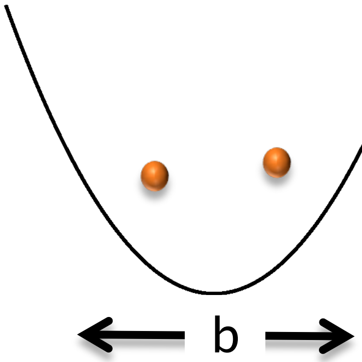
<u>Non-perturbative methods utilize the box:</u>

- LQCD
- LEFT



<u>Experiments utilize the oscillator trap :</u>

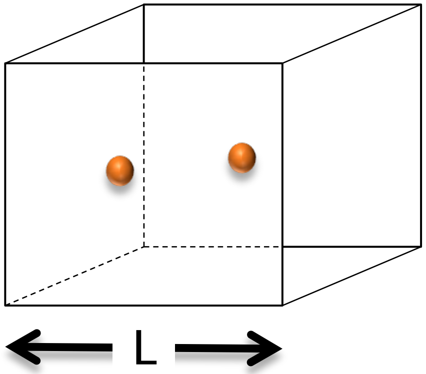
- Cold atoms



How can these finite-volume systems advance our understanding of fundamental interactions and few-body physics?

Have you heard of Luscher's formula?

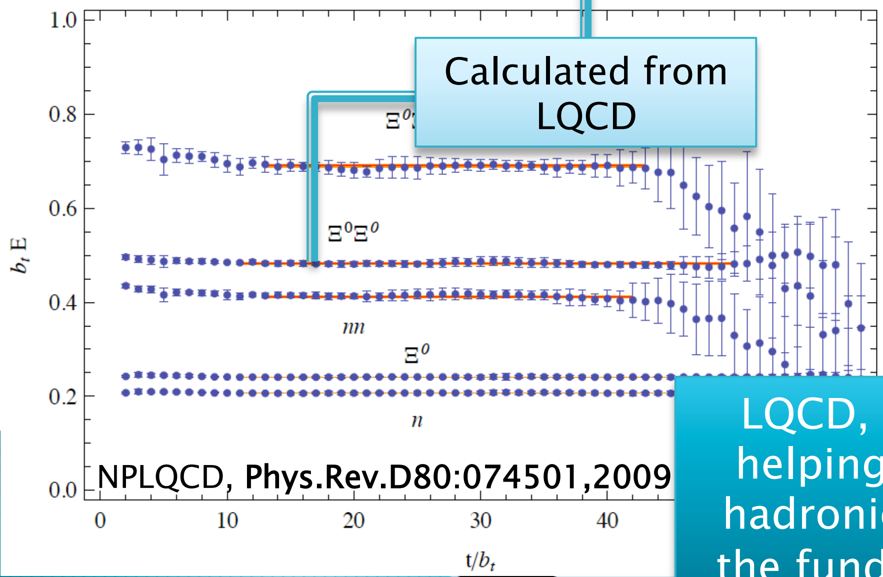
Luscher, Commun. Math. Phys. 105, 153 (1986)
Beane *et al.*, hep-lat/0312004



For interaction range $r_0 \ll L$

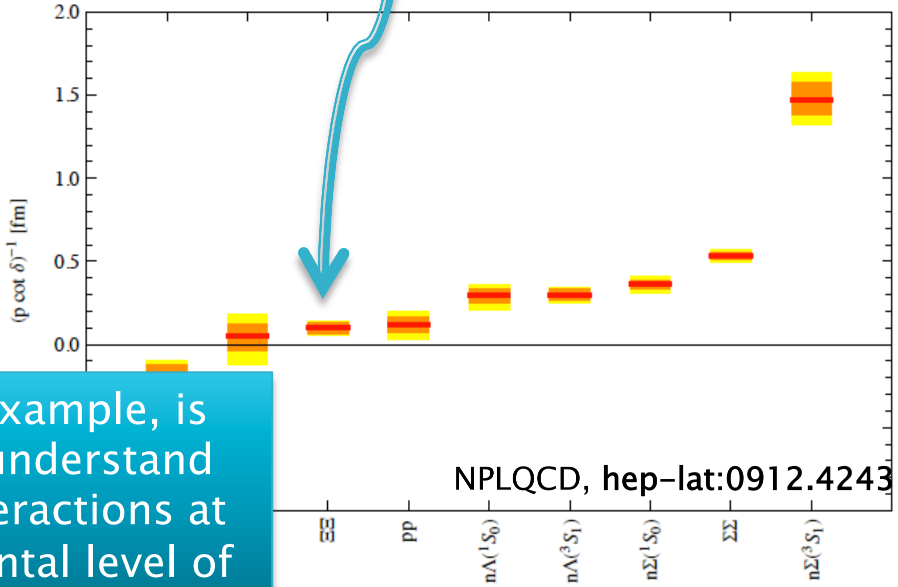
$$\frac{4}{L}\left(\pi \sum_{\vec{n}}^{|\vec{n}|<\Lambda} \frac{1}{4\pi^2\vec{n}^2-\epsilon} - \Lambda\right) = p\ \cot\delta_0(p)$$

$$\epsilon = EmL^2$$



Calculated from LQCD

NPLQCD, Phys.Rev.D80:074501,2009

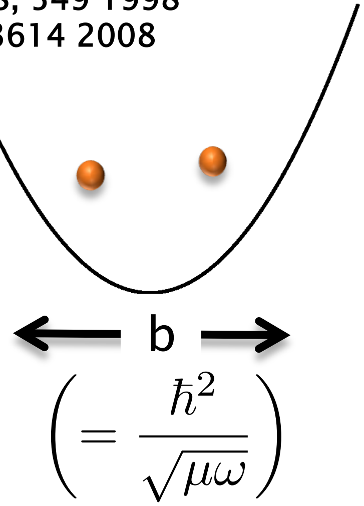


NPLQCD, hep-lat:0912.4243

LQCD, for example, is helping us understand hadronic interactions at the fundamental level of quarks and gluons

There is an analogous formula for the oscillator trap

T. Busch *et al.*, Found. Phys. 28, 549 1998
T. Mehen, Phys. Rev. A 78, 013614 2008



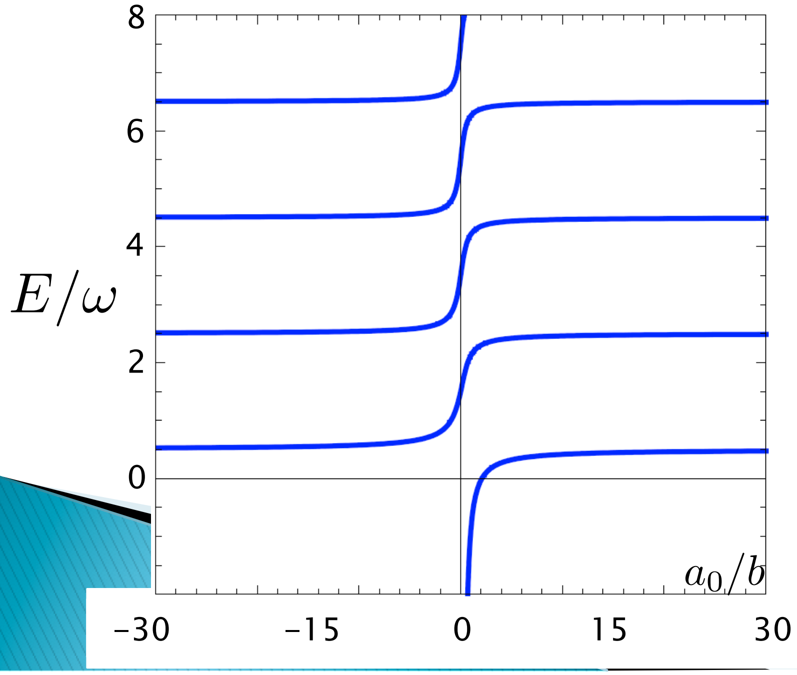
$$\left(= \frac{\hbar^2}{\sqrt{\mu\omega}} \right)$$

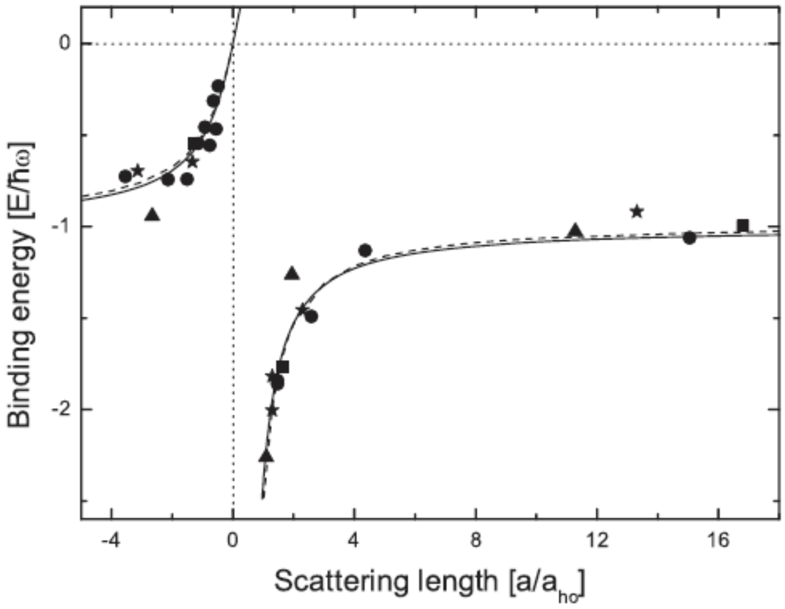
Cold atom traps are helping us understand the universal properties of finely tuned systems

For interaction range $r_0 \ll b$

$$-\frac{2}{b}\frac{\Gamma(\frac{3}{4}-\frac{\epsilon}{2})}{\Gamma(\frac{1}{4}-\frac{\epsilon}{2})} = p\ \cot\delta_0(p)$$

$$\epsilon = \frac{E}{\omega}$$





Stöferle *et al.*, Phys. Rev. Lett. 96, 030401 2006

But we've just started to utilize finite-volume techniques. . .

Cubic volume

- Cubic volume calculations of hadronic interactions (via LQCD) have not utilized
    - Asymmetric spatial volumes
    - Non-zero CM motion
    - Excited states
- These calculations are statistically daunting
    - Requires big computers
    - Advances in algorithms
    - New breed of physicists

No show-stoppers! Will be done—just a matter of time.

Oscillator well

- Recently Stetcu, van Kolck *et al.* have proposed a novel way for calculating nuclear physics observables within an oscillator well
    - Stetcu, Barrett, van Kolck, Vary, Phys. Rev. A 76, 063613 (2007)
    - Stetcu, Barrett, van Kolck, Phys. Lett. B 653 (2007) 358
    - Stetcu, Rotureau, Barrett, van Kolck, nucl-th:0912.3015, nucl-th:1001.5071

The upshot: a lot can be gained by putting particles in a trap!

But's let's take a closer look at those finite-volume formulas

van Kolck, DOE Nuclear Physics
Extreme Scale Workshop, 2009

$$\frac{4}{L}\left(\pi\sum_{\vec{n}}^{|\vec{n}|<\Lambda}\frac{1}{4\pi^2\vec{n}^2-\epsilon}-\Lambda\right)=p\,\cot\delta_0(p)=-\frac{2}{b}\frac{\Gamma\left(\frac{3}{4}-\frac{\epsilon}{2}\right)}{\Gamma\left(\frac{1}{4}-\frac{\epsilon}{2}\right)}$$

$$\epsilon=EmL^2 \qquad E=\frac{p^2}{2\mu} \qquad \epsilon=\frac{E}{\omega}$$

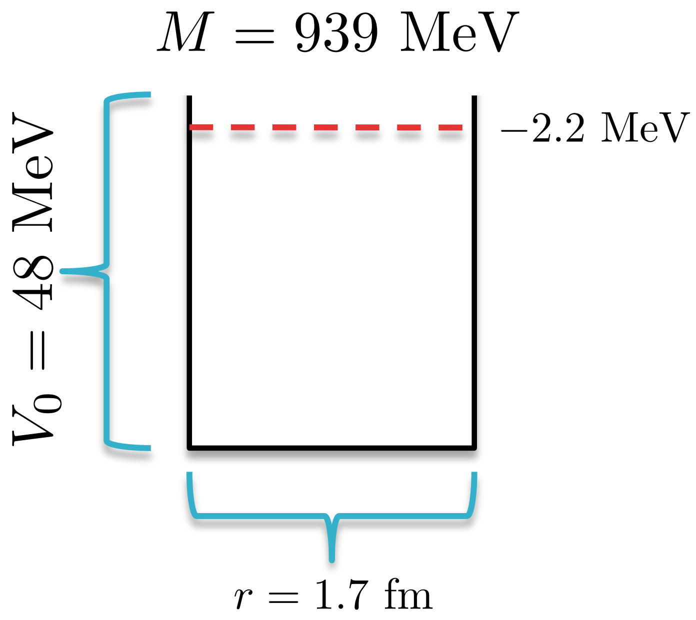
- Both equations relate *bound state* energies to *continuum* phase shifts
  - Extracting scattering parameters from bound states!
- Independent of the form of the interaction
- Valid not just for ground state, but for excited states, but. . .
- . . . the energy must be below inelastic thresholds
  - No pion production, etc. . .

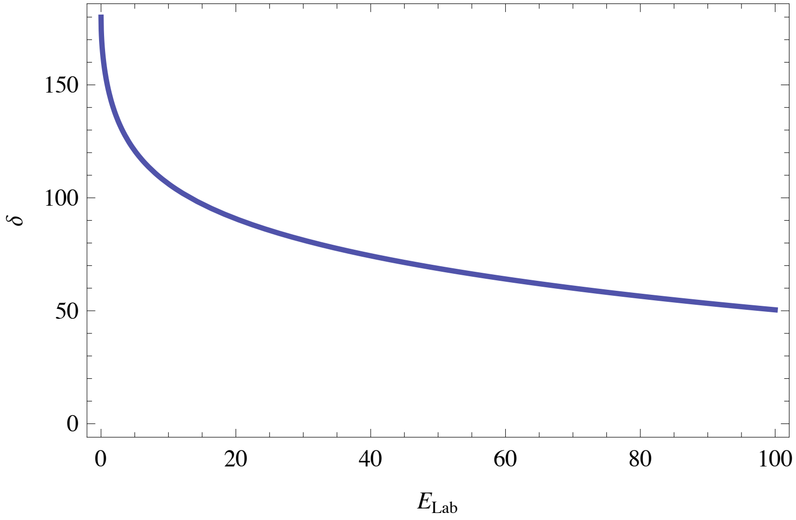
Let’s see some action: spherical well primer

- We can tune the parameters of the well to make a ‘deuteron’

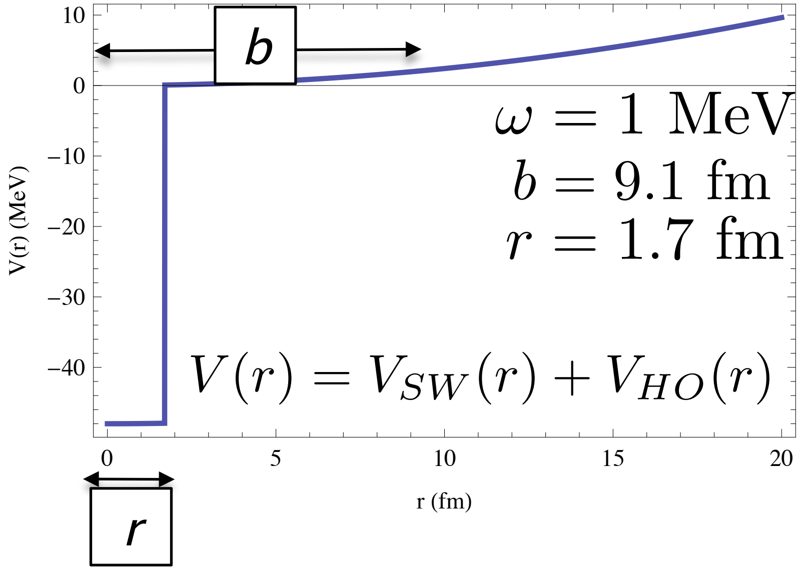
- The phase shift is known analytically

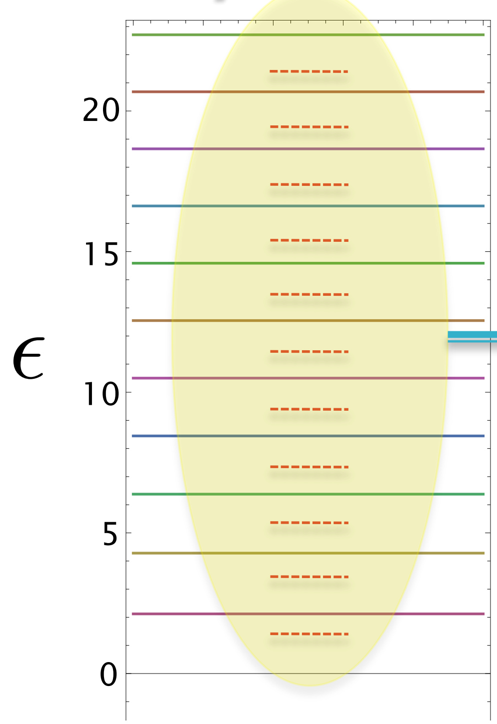
$$\delta = \tan^{-1}\left(\sqrt{\frac{E_{\mathrm{lab}}}{E_{\mathrm{lab}}+2V_0}}\tan\left(\sqrt{r^2\mu\left(E_{\mathrm{lab}}+2V_0\right)}\right)\right)-\sqrt{E_{\mathrm{lab}}r^2V_0\mu}$$





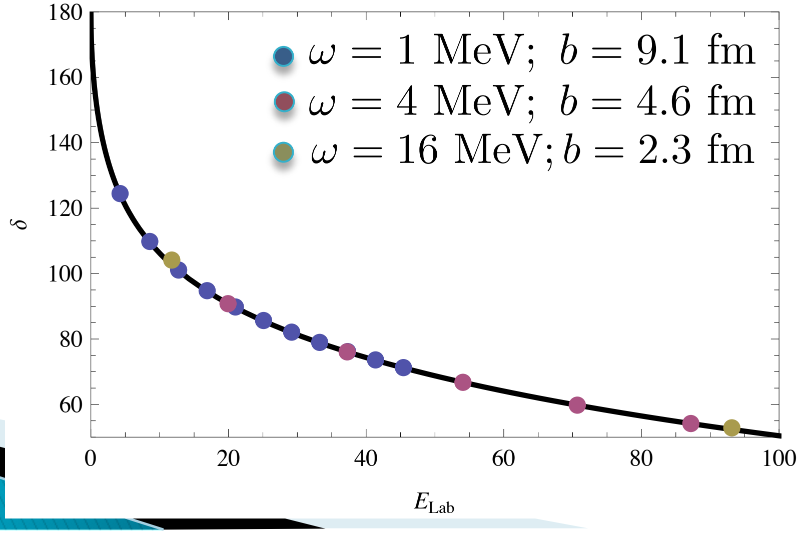
Now let's put the system in an oscillator well





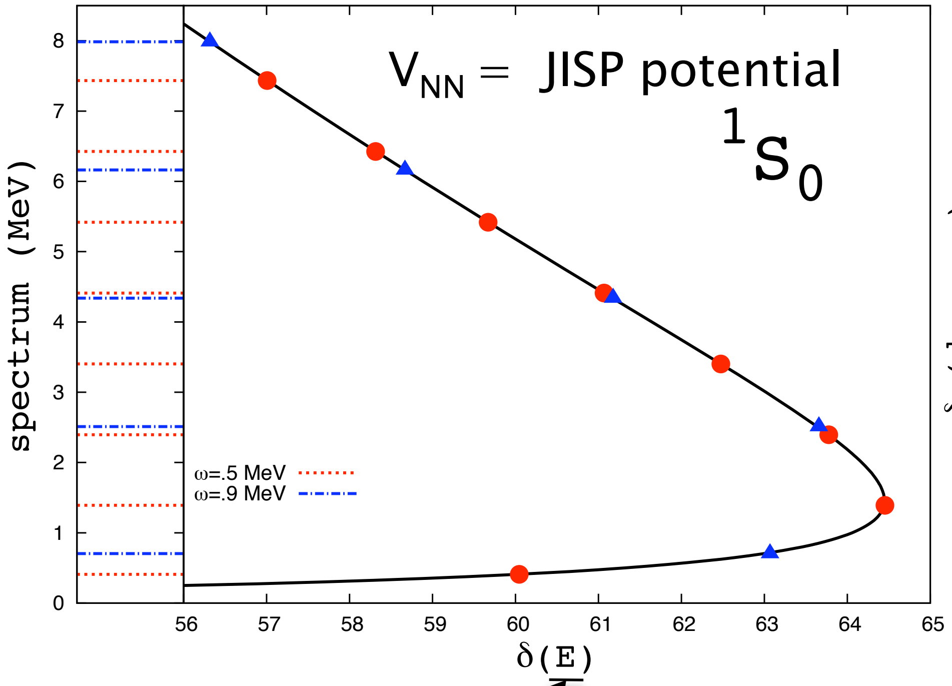
$$-\frac{2}{b}\frac{\Gamma(\frac{3}{4}-\frac{\epsilon}{2})}{\Gamma(\frac{1}{4}-\frac{\epsilon}{2})} = p\ \cot\delta_0(p)$$

$$\epsilon = \frac{E}{\omega}$$

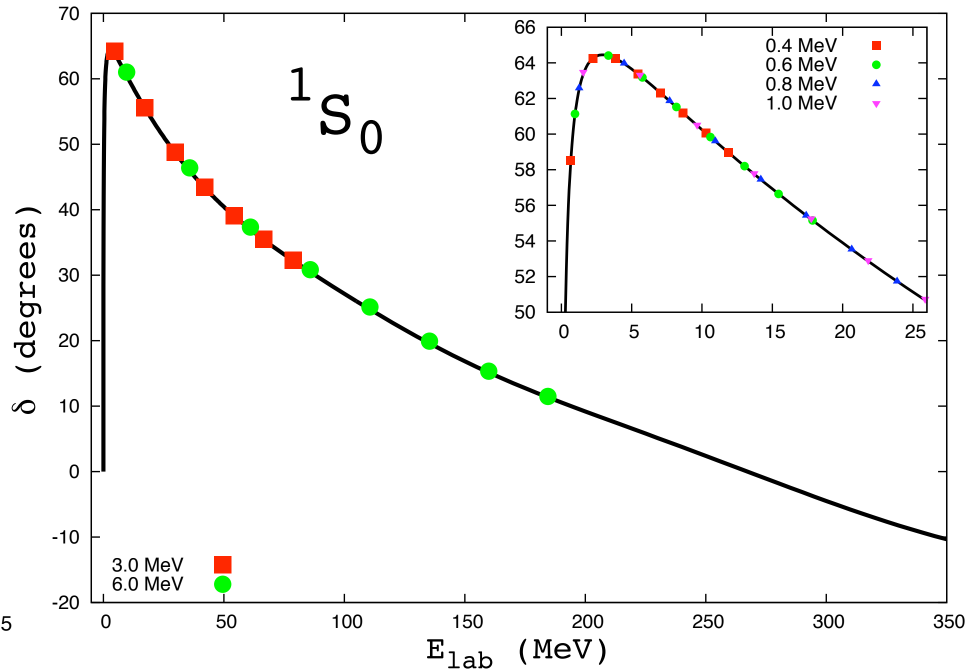


Luu, Savage, Schwenk, Vary, *in preparation*

What about ‘realistic’ potentials?



Relative energy



For low ω can extract effective range parameters from spectrum:

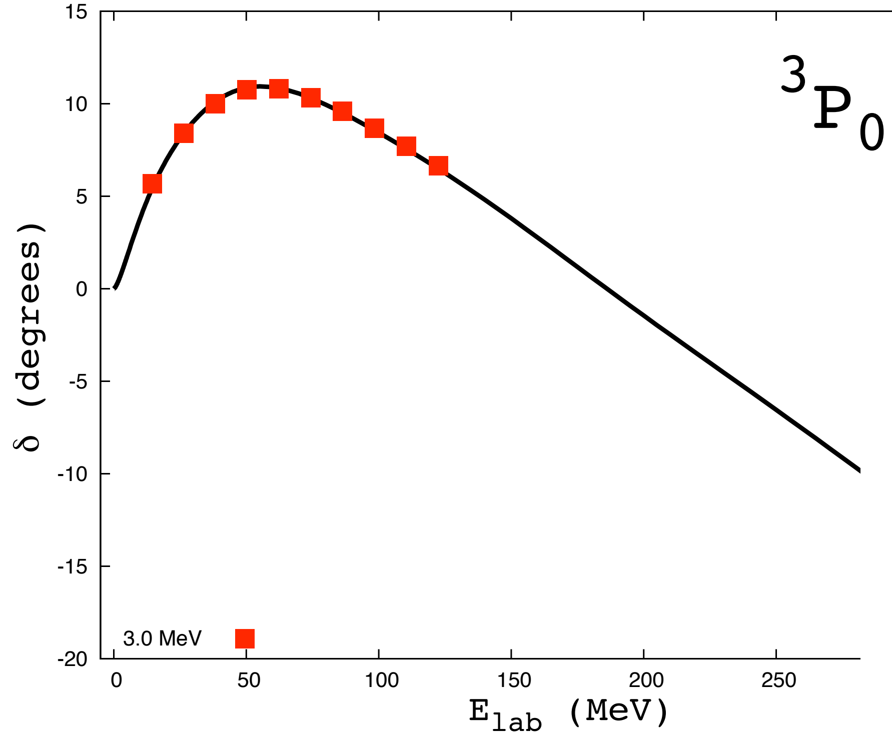
$$-\frac{2}{b}\frac{\Gamma(3/4-\epsilon/2)}{\Gamma(1/4-\epsilon/2)} = -\frac{1}{a_0} + \frac{r_0 m\omega}{2}\epsilon + \ldots$$

$$\omega = 1 \text{ MeV} \qquad \begin{aligned} a_0 &= -22.47 \text{ fm} \\ r_0 &= 2.55 \text{ fm} \end{aligned}$$

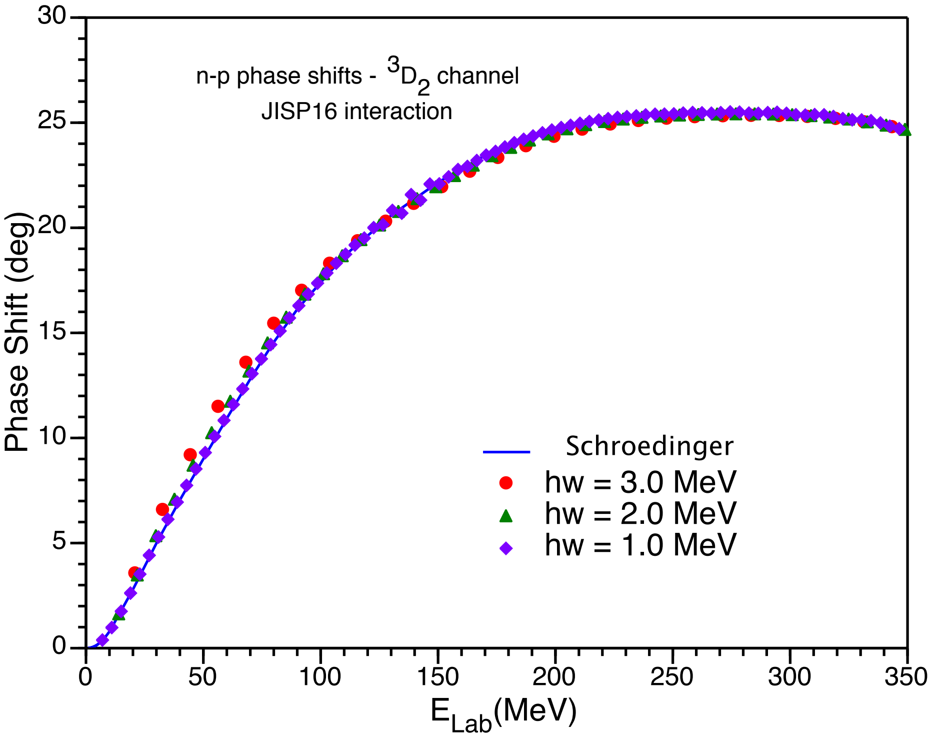
Calculations done by J. Vary

Luu, Savage, Schwenk, Vary, *in preparation*

And we can do higher partial waves. . .

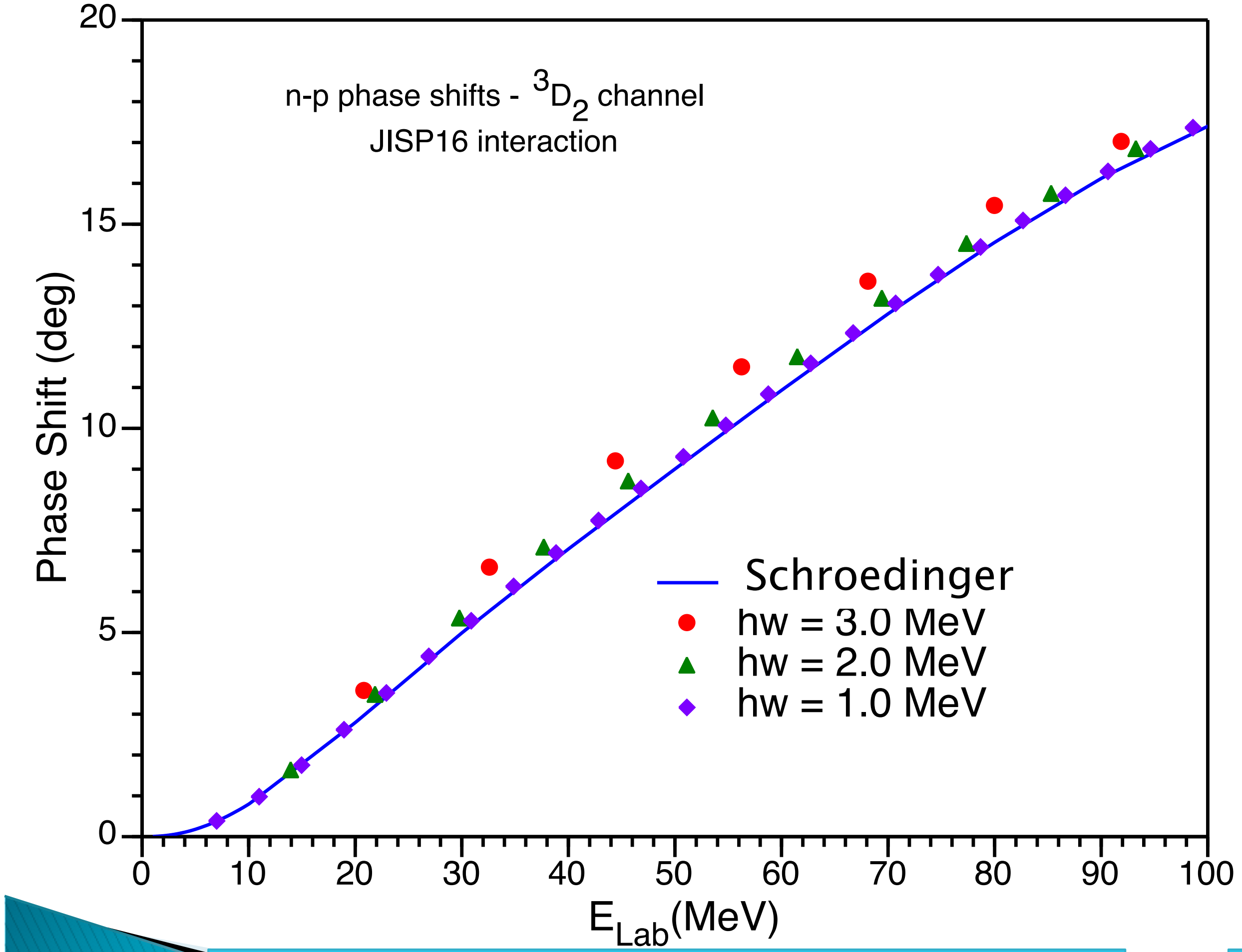


The finite-volume formula generalizes for higher partial waves



Calculations done by J. Vary

Let's take a closer look at the D-wave result



- For higher partial waves, the centripetal force causes the particles to see more of the HO well

- The competition between the range of V_{NN} and the HO well becomes more dramatic

- This gives finite volume corrections that depend on the asymptotic part of the V_{NN}

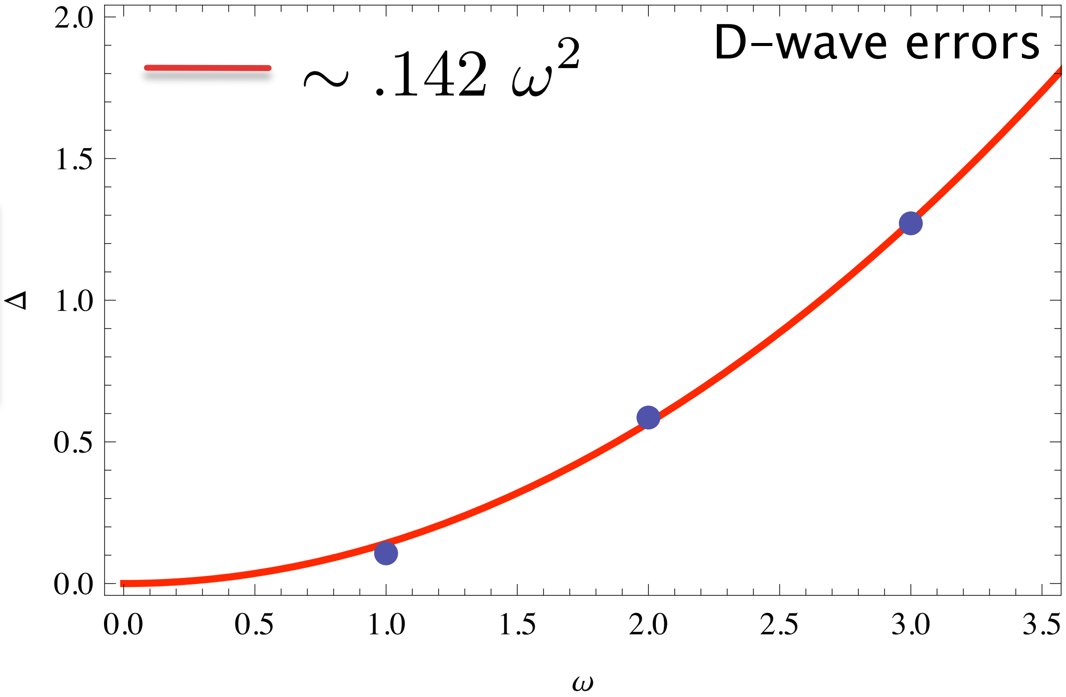
For a given accuracy, the higher the partial wave *l* means one must use a smaller trapping frequency ω . . .

. . . or we could try to correct these finite-volume effects

Do we understand the nature of these finite volume corrections?

yes . . . and . . . no

Average finite-volume errors between 40-50 MeV lab energy



Trapping frequency

Our numerical analysis suggests that LO power law corrections that scale as:

$$\sim \frac{1}{b^4}$$

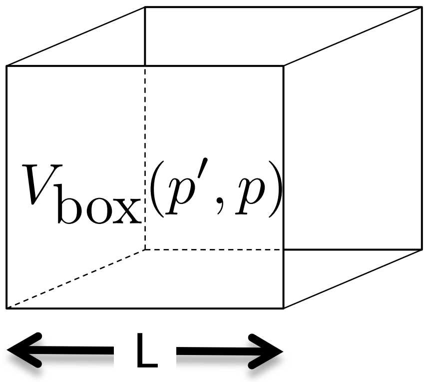
These HO finite-volume corrections are fundamentally different from the cubic volume corrections!

"Hey Tom, have you thought about doing this in cubic volumes?"—M.Savage

- First off, cubic volumes break rotational symmetry
  - Respect O_d symmetry
  - Spatial irreps $A_1,\ A_2,\ E,\ T_1,\ T_2$
  - Spin irreps $G_1,\ G_2,\ H$

Group theory tells us how to construct these states and their relation to SO(3)

- Momentum representation of your interaction is a little bit off



$$V_{\text{free}}(p',p) \neq V_{\text{box}}(p',p)$$

But for L>>r, the difference is exponentially small

The boundary conditions mess with your mind as well. . .

- The CM and relative coordinates don't exactly decouple Christ *et al.*, Phys. Rev. D 72 114506 (2005)

$$T|\vec{N}_{cm} > \otimes|\vec{n}_{rel} >= |\vec{N}_{cm} > \otimes|\vec{n}_{rel} > \frac{4\pi^2}{L}\left(\frac{N_{cm}^2}{4m}+\frac{n_{rel}^2}{2\mu}\right)$$

Completeness relation:

$$1 = \sum_{\vec{N}_{cm}} |\vec{N}_{cm} >< \vec{N}_{cm}| \otimes \sum_{\vec{n}\ integer} \underbrace{|\vec{n} - \frac{\mathrm{mod}(\vec{N}_{cm},2)}{2} >}_{|\vec{n}_{rel} >} < \vec{n} - \frac{\mathrm{mod}(\vec{N}_{cm},2)}{2}|$$

Examples:

$$|\vec{N}_{cm} >= |0,0,0 > \rightarrow |\vec{n}_{rel} >= |integer, integer, integer >$$

$$|\vec{N}_{cm} >= |0,1,0 > \rightarrow |\vec{n}_{rel} >= |integer, \frac{odd}{2}, integer >$$

Nonzero CM reduces states to subgroups of O_d

Luu, SciDAC 2009 proceedings

So far, I've only done perturbation theory in (1/L). . . (sorry Martin—Can I still graduate?)

$$
\begin{aligned}
V_0(\vec{p}\,',\vec{p}) &= \frac{4\pi a_0}{m}\left[1+\frac{a_0 r_0}{2}\left(\frac{p'^2+p^2}{2}\right)+\ldots\right] && \text{(s-wave)}\\
V_1(\vec{p}\,',\vec{p}) &= \frac{12\pi a_1}{m}\vec{p}\,'\cdot\vec{p}\left[1+\frac{a_1 r_1}{2}\left(\frac{p'^2+p^2}{2}\right)+\ldots\right] && \text{(p-wave)}\\
V_2(\vec{p}\,',\vec{p}) &= \frac{10\pi a_2}{m}\left(3(\vec{p}\,'\cdot\vec{p})^2-p'^2\,p^2\right)\left[1+\frac{a_2 r_2}{2}\left(\frac{p'^2+p^2}{2}\right)+\ldots\right] && \text{(d-wave)}\ ,
\end{aligned}
$$

$$
V_\pi(\vec{q}) = -\left(\frac{g_A}{\sqrt{2}f_\pi}\right)^2(\tau_1\cdot\tau_2)\frac{(\vec{\sigma}_1\cdot\vec{q})\ (\vec{\sigma}_2\cdot\vec{q})}{q^2+m_\pi^2}
$$

Assumption: short-ranged repulsive interactions of 'natural size'

$$
\begin{aligned}
a_0/L \ll 1 \quad &; \quad r_0/L \ll 1\\
a_1/L^3 \ll 1 \quad &; \quad r_1 L \ll 1
\end{aligned}
$$

Let's look at some 'P-wave' cases:

$$
E_{(T_{1u}A_1)T_{1u}} = \frac{4\pi^2}{mL^2}+\frac{96\pi^3 a_1}{mL^5}+\frac{24\pi^2 g_A^2}{f_\pi^2 m_\pi^2 L^5}+O(L^{-7}) \qquad \sim |{}^1P_1>
$$

$$
E_{(T_{1u}T_1)A_{1u}} = \frac{4\pi^2}{mL^2}+\frac{96\pi^3 a_1}{mL^5}+\frac{8\pi^2 g_A^2}{3f_\pi^2 m_\pi^2 L^5}-\frac{80\pi^2 g_A^2}{3f_\pi^2 m_\pi^2 L^5}+O\left(L^{-7}\right) \qquad \sim |{}^3P_0>
$$

$$
E_{(T_{1u}T_1)T_{1u}} = \frac{4\pi^2}{mL^2}+\frac{96\pi^3 a_1}{mL^5}+\frac{8\pi^2 g_A^2}{3f_\pi^2 m_\pi^2 L^5}+\frac{40\pi^2 g_A^2}{3f_\pi^2 m_\pi^2 L^5}+O\left(L^{-7}\right) \qquad \sim |{}^3P_1>
$$

$$
\left.
\begin{aligned}
E_{(T_{1u}T_1)T_{2u}} &= \frac{4\pi^2}{mL^2}+\frac{96\pi^3 a_1}{mL^5}+\frac{8\pi^2 g_A^2}{3f_\pi^2 m_\pi^2 L^5}+O\left(L^{-7}\right)\\
E_{(T_{1u}T_1)E_u} &= \frac{4\pi^2}{mL^2}+\frac{96\pi^3 a_1}{mL^5}+\frac{8\pi^2 g_A^2}{3f_\pi^2 m_\pi^2 L^5}+O\left(L^{-7}\right)\ ,
\end{aligned}
\right\} \sim |{}^3P_2>
$$

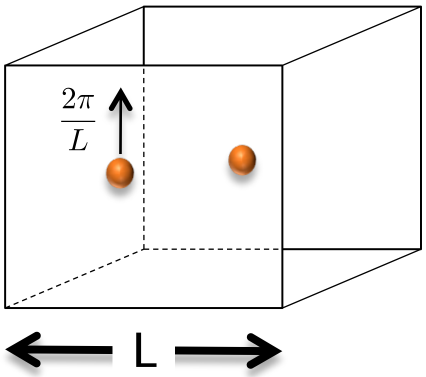
Luu, SciDAC 2009 proceedings

Turning *vices* into *virtues*. . .

- Obviously working in cubic volumes presents its own challenges
- But we can take advantage of peculiarities of the cubic volume!

Example: non-zero CM

$$|\vec{N}_{cm} >= |0,0,1>$$



Group structure is reduced to cubic rotations that leave the CM vector

$$O_d \rightarrow C_{4v}$$

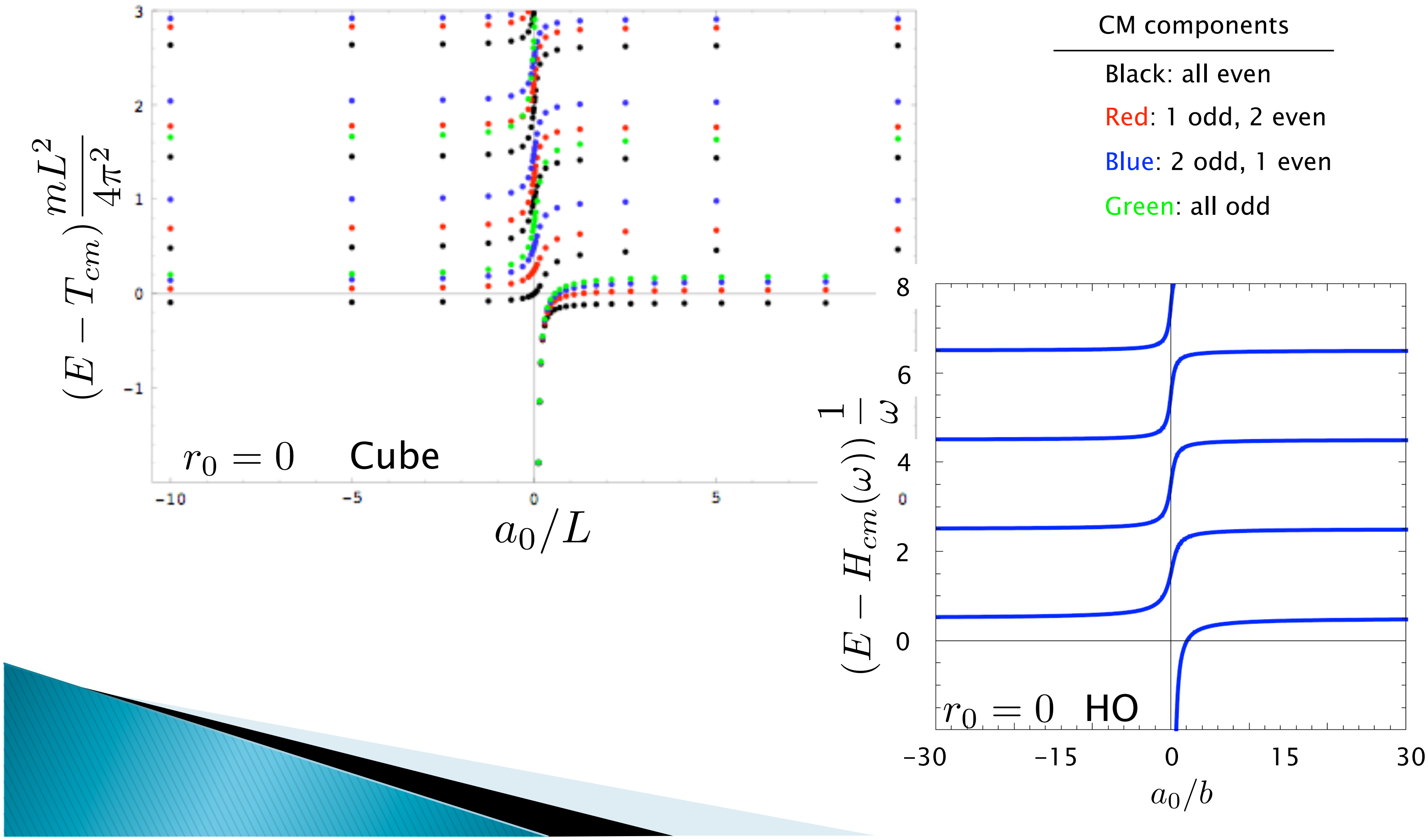
$$E_{A_1} = \frac{2\pi^2}{mL^2} + \frac{8\pi a_0}{mL^3} - \frac{8a_0^2}{mL^4}\mathcal{L} + \frac{8a_0^3}{\pi m L^5}\left[\mathcal{L}^2 - \mathcal{M}\right] + \frac{4\pi^3 a_0^2 r_0}{mL^5} + O(L^{-6})$$

Opposite spins

$$E_{A_1} = \frac{2\pi^2}{mL^2} + \frac{24\pi^3 a_1}{mL^5} + O(L^{-6})$$

Aligned spins

Example: zero-range s-wave with arbitrary CM motion

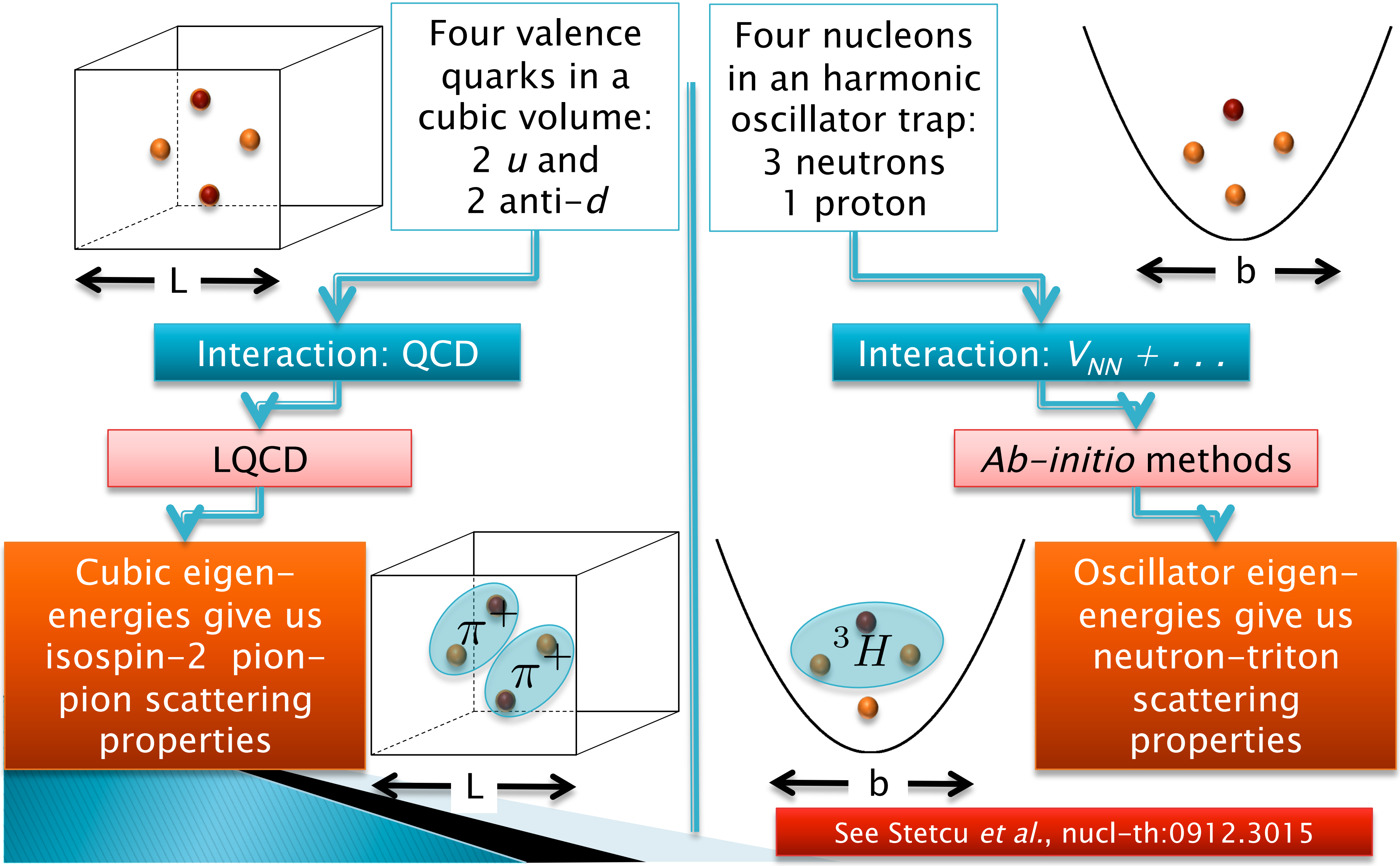


LQCD offers an ideal place for performing nuclear physics "experiments"

- Through LQCD we can probe various aspects of hadronic interactions
  - Project onto different 'partial waves'
  - Excited state spectrum
- We can change the nature of the boundary conditions themselves
- By taking advantage of certain aspects of the cubic volume, we can isolate different aspects of the interaction
  - Non-zero CM motion
  - Asymmetric spatial volumes

But what about the oscillator well? It's just a two-body problem. How does it advance many-body nuclear physics???

Let's look at LQCD as a guide



Four valence quarks in a cubic volume: 2 *u* and 2 anti-*d*

Interaction: QCD

LQCD

Cubic eigen-energies give us isospin-2 pion-pion scattering properties

Four nucleons in an harmonic oscillator trap: 3 neutrons 1 proton

Interaction: $V_{NN} + \ldots$

Ab-initio methods

Oscillator eigen-energies give us neutron-triton scattering properties

See Stetcu *et al.*, nucl-th:0912.3015

Finite-volume oscillator perks:

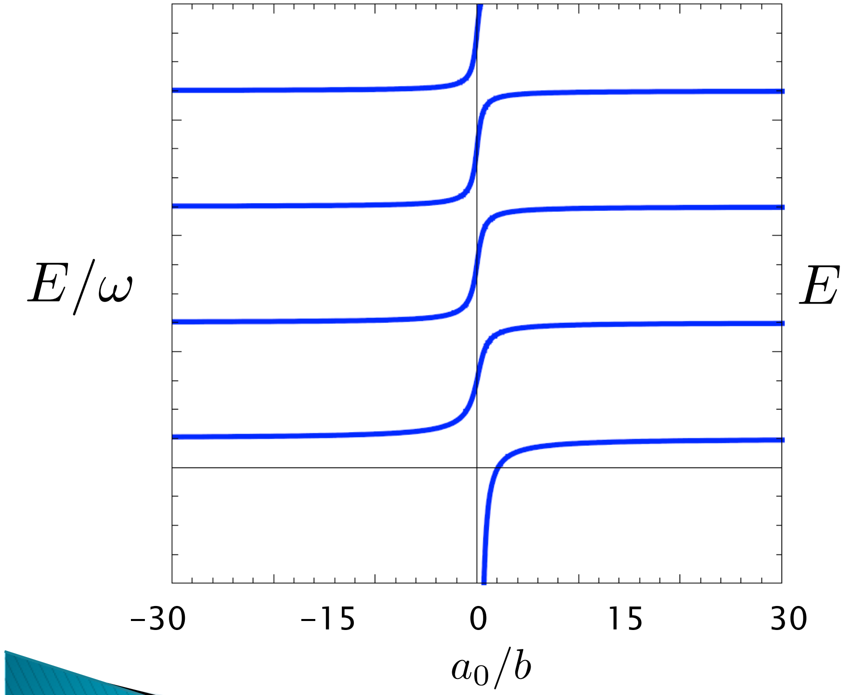
- We've made great progress in bound-state nuclear many-body algorithms
  - Different algorithms
  - Strongly coupled with HPC
- We are now using a basis that has the correct asymptotic behavior!
  - The HO basis is no longer "convenient" to use, but is mandatory
- The system is confined
  - Can external well increase convergence of calculations?

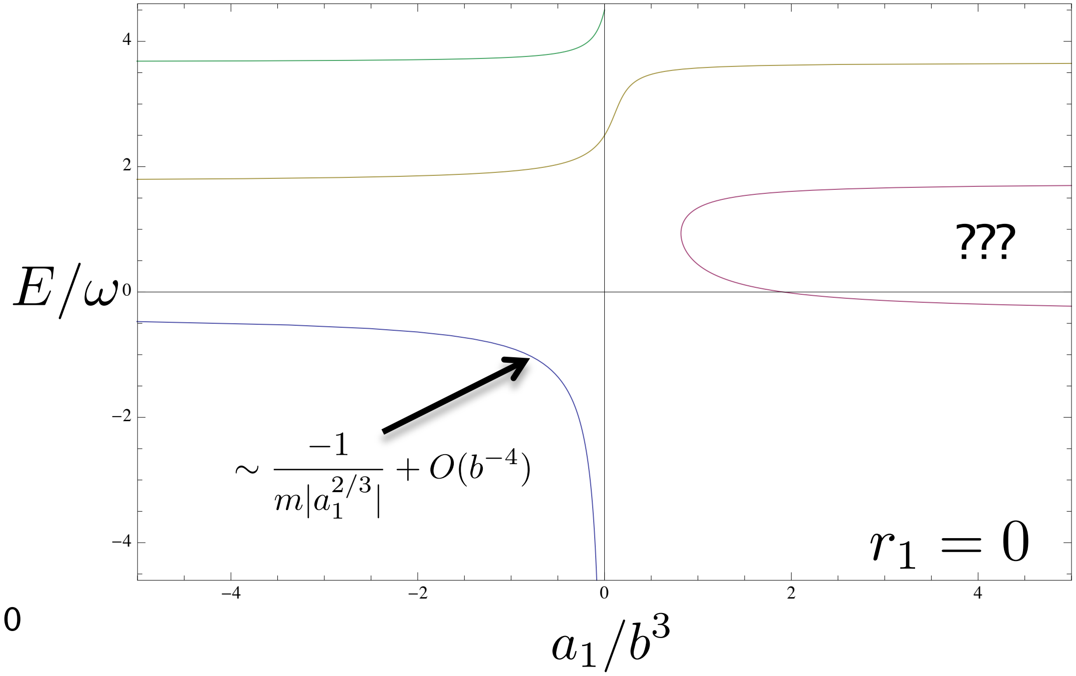
Let me end with a question(s)

Yip, Phys. Rev. A **78, 013612 2008**

$$\frac{b}{a_0} = 2\frac{\Gamma(3/4-\epsilon/2)}{\Gamma(1/4-\epsilon/2)}$$

$$-\frac{b^3}{a_1} + (r_1 b)\epsilon = 8\frac{\Gamma(5/4-\epsilon/2)}{\Gamma(-1/4-\epsilon/2)}$$





- Can I set r_1 to zero as $|a_1|$→ infinity?
- Can AMR guys tune *a* and *r* independently?
- How does the spectrum behave as ω→ zero?