Bound states in a box

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in collaboration with D. Lee, H.-W. Hammer; S. Bour, U.-G. Meißner

Light nuclei from first principles @ INT, University of Washington

Seattle, WA

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Bonn-Cologne Graduate School
of Physics and Astronomy

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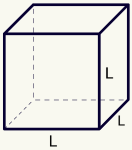
Overview

The box

- periodic finite volume
- cube of size L^3



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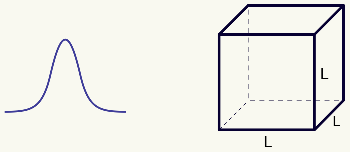
The bound states

- 2-body bound states
- wavefunction ψ



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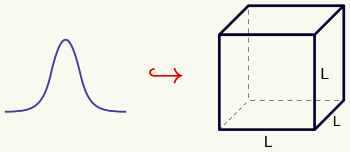

The finite volume changes the properties of the system!

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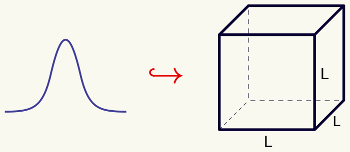


The finite volume changes the properties of the system!

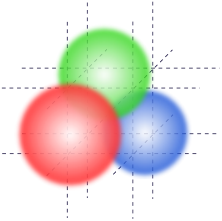
Important for numerical calculations $\rightarrow$ **Lattice**

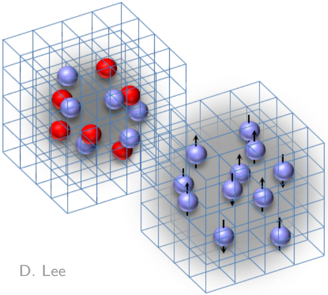
Lattice calculations

Solve a physical theory by putting it on a spacetime-lattice!

Lattice QCD

- QCD observables from first principles
- quarks and gluons as degrees of freedom





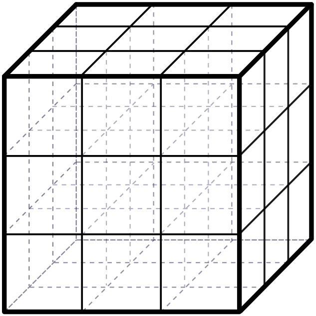
D. Lee

Nuclear Lattice Calculations

- nuclei from first principles
- nucleons and pions as d.o.f.
- based on chiral effective theory

Lattice artifacts

lattice spacing a



lattice size L

- $a \to 0$: continuum limit
- $L \to \infty$: infinite-volume limit

Lüscher's famous formula

Lüscher's idea

Use the volume dependence as a tool!

$$p\cot\delta_0(p) = \frac{1}{\pi L} S(\eta) \quad , \quad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

$$p = p(E(L))$$

- measure energy levels in finite volume
- extract physical scattering phase shift

Outline

- **Overview**
- **Part I –**
  Mass shift of bound states with angular momentum
  arXiv:1103.4468, 1109.4577
- **Part II –**
  Topological factors in scattering systems
  arXiv:1107.1272
- **Summary**

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Part I

Mass shift of bound states with angular momentum

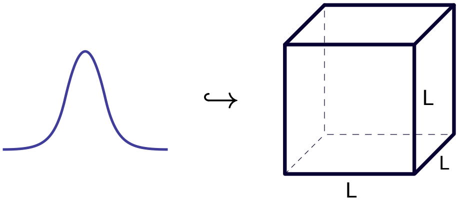
- **Lüscher's result for S-waves**
- **Bound states in a finite volume**
- **General result for arbitrary partial waves**
- **Sign of the mass shift**
- **Numerical tests**

Starting point

S-wave bound state

Lüscher (1986)

$$\Delta m_B = -24\pi |A|^2 \frac{e^{-\kappa L}}{mL} + \mathcal{O}(e^{-\sqrt{2}\kappa L})$$



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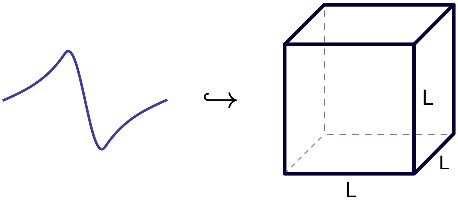
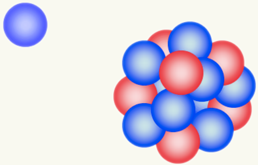


What's the the result for states with angular momentum?

Why care about higher partial waves?

Halo nuclei

- single nucleon weakly bound to a tight core



nucleus by Cam-Ann, Wikimedia Commons

Halo nuclei

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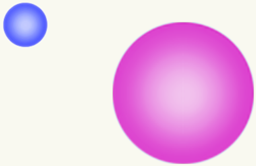
- can be described as an effective 2-body state



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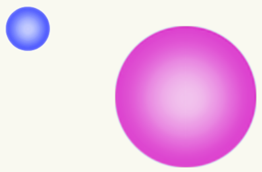

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Halo-EFT

expansion in $R_{\mathrm{core}}/R_{\mathrm{halo}} \to$ effective field theory

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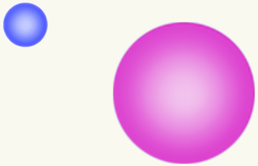

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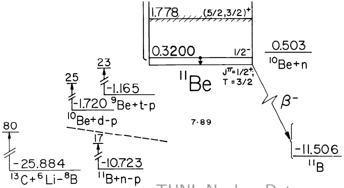


TUNL Nuclear Data

Example

P-wave state just below $^{10}\mathrm{Be} + \mathrm{n}$ threshold in $^{11}\mathrm{Be}$

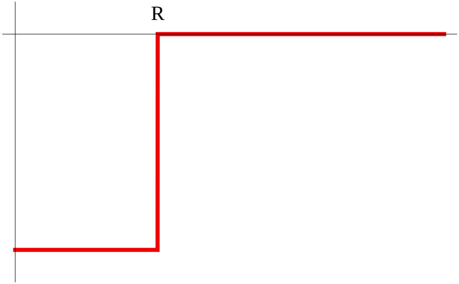
Schrödinger equation

$$\hat{H} = -\frac{1}{2\mu}\Delta_r + V(r)$$

$$\hat{H}\,|\psi_B\rangle = -\frac{\kappa^2}{2\mu}\,|\psi_B\rangle$$

finite-range interaction:

$V(r) = 0$ for $r > R$



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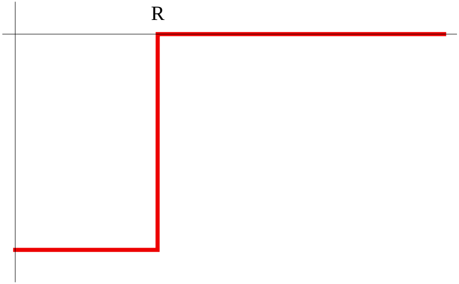

Radial Schrödinger equation

$$\psi_B(\mathbf{r}) = \frac{u_\ell(r)}{r}Y_\ell^m(\theta,\phi) \rightsquigarrow \left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell(\ell+1)}{r^2} - 2\mu V(r) - \kappa^2\right)u_\ell(r) = 0$$

Asymptotic wavefunction

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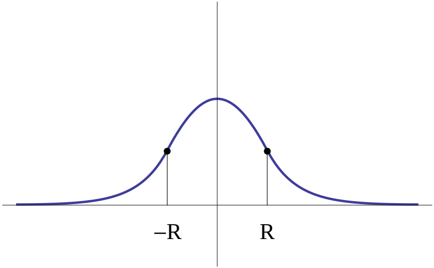

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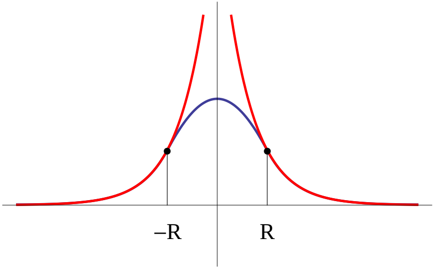
$$\rightsquigarrow u_\ell(r) = \mathrm{i}^\ell \gamma\, \hat{h}_\ell^+(i\kappa r)$$

Riccati–Hankel functions

$$\hat{h}_0^+(z) = \mathrm{e}^{\mathrm{i}z}$$

$$\hat{h}_1^+(z) = \left(1 + \frac{\mathrm{i}}{z}\right) \mathrm{e}^{\mathrm{i}(z - \pi/2)}$$

$$\hat{h}_2^+(z) = \cdots$$



Finite volume

Periodic boundary conditions

$\rightarrow$ infinitely many copies of the potential

$$V_L(\mathbf{r}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(\mathbf{r} + \mathbf{n}L) \quad , \quad L \gg R$$

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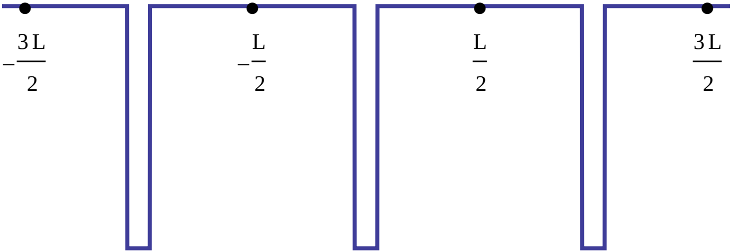

$$V(r) = V_0\,\theta(R-r)$$

Finite volume

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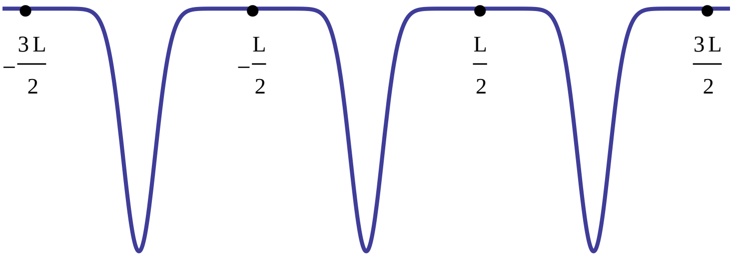

$$V(r) = V_0 \, \exp(-r^2/R^2)$$

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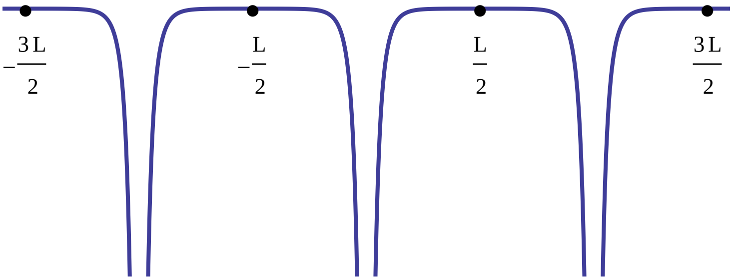

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Finite volume

$$\hat{H}_L \left|\psi\right\rangle = -E_B(L) \left|\psi\right\rangle$$
$$\hat{H} \left|\psi_B\right\rangle = -E_B(\infty) \left|\psi_B\right\rangle$$

Mass shift

$$\Delta m_B \equiv E_B(\infty) - E_B(L)$$
$$m_B = M - E_B$$

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Ansatz: $\psi_0(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \psi_B(\mathbf{r}+\mathbf{n}L)$

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$$\eta(\mathbf{r}) = \sum_{\mathbf{n}\neq\mathbf{n}'} V(\mathbf{r} + \mathbf{n}L)\, \psi_B(\mathbf{r} + \mathbf{n}'L)$$

$$\left\langle\psi\right| \hat{H}_L \left|\psi_0\right\rangle = -E_B(L) \left\langle\psi|\psi_0\right\rangle = -E_B(\infty) \left\langle\psi|\psi_0\right\rangle + \left\langle\psi|\eta\right\rangle$$

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Result

$$\Delta m_B = \frac{\langle\psi|\eta\rangle}{\langle\psi_0|\psi_0\rangle} = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3r\,\psi_B^*(\mathbf{r})\,V(\mathbf{r})\,\psi_B(\mathbf{r}+\mathbf{n}L) + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

Finite volume

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \, \psi_B^*(\mathbf{r}) \, V(\mathbf{r}) \, \psi_B(\mathbf{r} + \mathbf{n}L) + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right)$$

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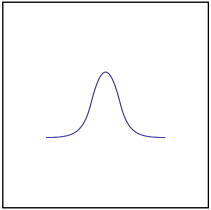

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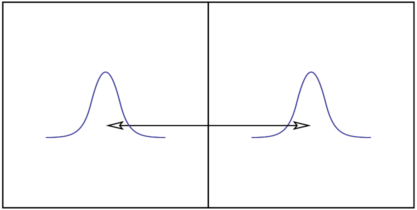

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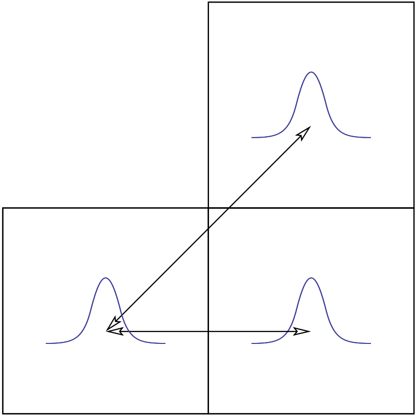

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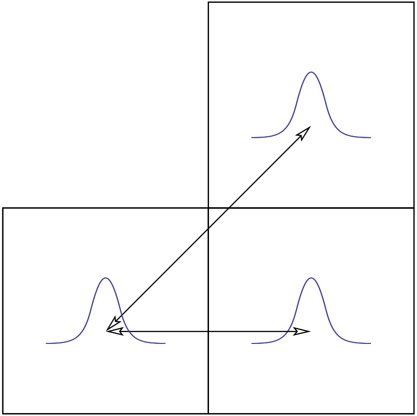

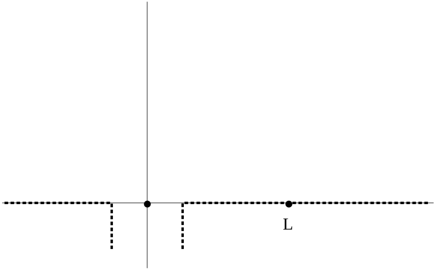

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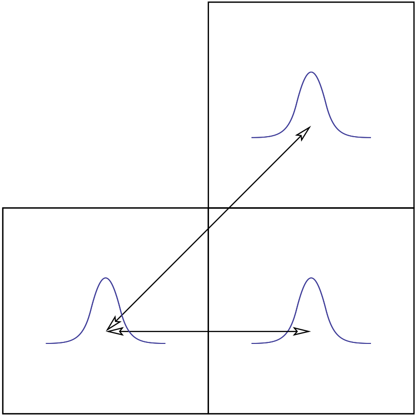

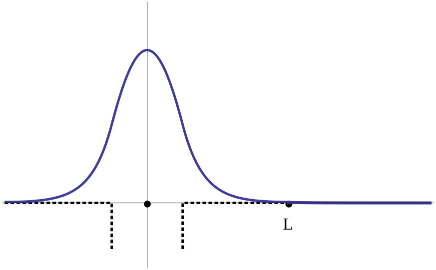

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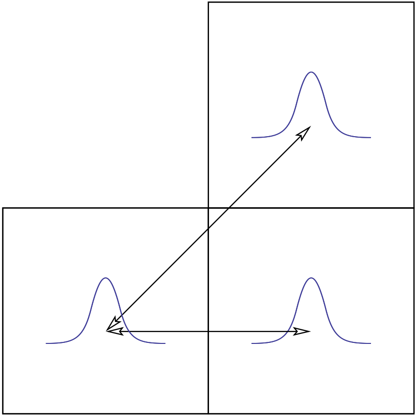

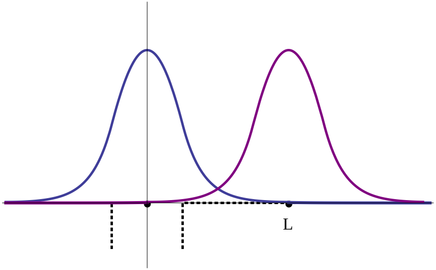

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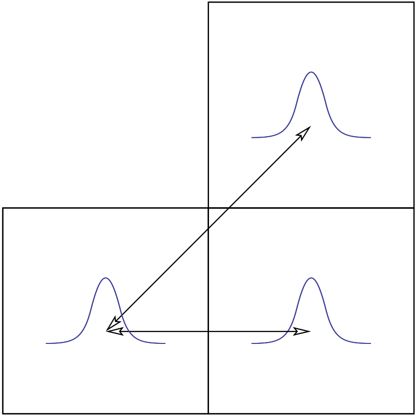

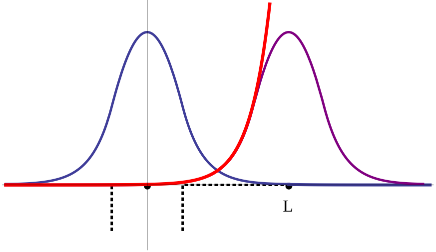

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$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \, \psi_B^*(\mathbf{r} - \mathbf{n}L) \, V(\mathbf{r} - \mathbf{n}L) \, Y_\ell^m(\theta, \phi) \frac{\mathrm{i}^\ell \gamma \hat{h}_\ell^+(\mathrm{i}\kappa r)}{r} + \cdots$$

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S-waves $\rightarrow \; Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \; , \; \hat{h}_0^+(\mathrm{i}\kappa r) = \mathrm{e}^{-\kappa r}$

Finite volume

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \, \frac{\gamma}{\sqrt{16\pi\mu}} \left[\Delta_r - \kappa^2\right] \psi_B^*(\mathbf{r} - \mathbf{n}L) \, \frac{\mathrm{e}^{-\kappa r}}{r} + \cdots$$

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$\left[\Delta_r - \kappa^2\right] \dfrac{\mathrm{e}^{-\kappa r}}{r} = -4\pi\delta^{(3)}(\mathbf{r}) \;\rightarrow$ **Green's function**

Finite volume

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \, \frac{\gamma}{\sqrt{16\pi\mu}} \left[\Delta_r - \kappa^2\right] \psi_B^*(\mathbf{r} - \mathbf{n}L) \, \frac{\mathrm{e}^{-\kappa r}}{r} + \cdots$$

S-waves $\rightarrow \; Y_0^0(\theta,\phi) = \dfrac{1}{\sqrt{4\pi}} \;\; , \;\; \hat{h}_0^+(\mathrm{i}\kappa r) = \mathrm{e}^{-\kappa r}$

$\left[\Delta_r - \kappa^2\right] \dfrac{\mathrm{e}^{-\kappa r}}{r} = -4\pi\delta^{(3)}(\mathbf{r})$ $\rightarrow$ **Green's function**

S-waves

sum just yields a factor six...

$$\Delta m_B^{(0,0)} = -3|\gamma|^2 \, \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right)$$

P-wave result

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \, \frac{1}{2\mu} \Big[\Delta_r - \kappa^2 \Big] \psi_B^*(\mathbf{r} - \mathbf{n}L) \, Y_\ell^m(\theta, \phi) \frac{\mathrm{i}^\ell \gamma \hat{h}_\ell^+(\mathrm{i}\kappa r)}{r} + \cdots$$

P-waves $\rightarrow$ $Y_1^0(\theta, \phi) \sim \cos\theta = \frac{z}{r}$, $\hat{h}_1^+(\mathrm{i}\kappa r) \sim \left(1 + \frac{1}{\kappa r}\right) \frac{\mathrm{e}^{-\kappa r}}{r}$

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$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r \, \frac{1}{2\mu} \Big[\Delta_r - \kappa^2 \Big] \psi_B^*(\mathbf{r} - \mathbf{n}L) \, Y_\ell^m(\theta, \phi) \frac{\mathrm{i}^\ell \gamma \hat{h}_\ell^+(\mathrm{i}\kappa r)}{r} + \cdots$$

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$$R_\ell^m(\mathbf{r}) = r^\ell Y_\ell^m(\hat{\mathbf{r}})$$

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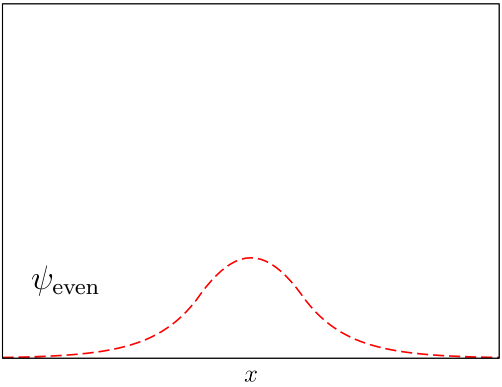
P-waves

$$\Delta m_B^{(1,0)} = \Delta m_B^{(1,\pm 1)} = 3|\gamma|^2\, \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

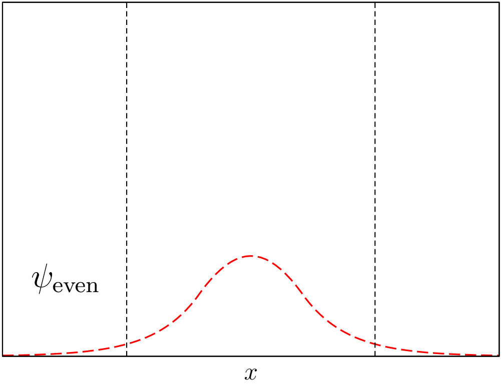
Mass shift for P-wave states exactly reversed compared to S-waves!

Sign of the mass shift



$\Delta m_B < 0$

Sign of the mass shift



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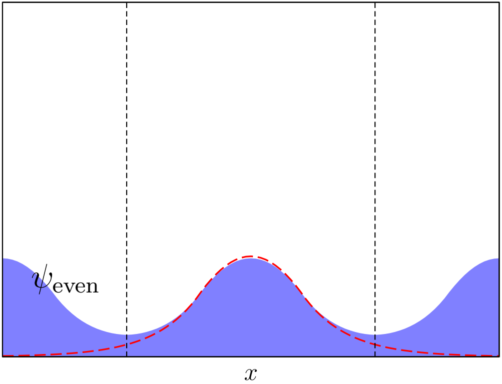
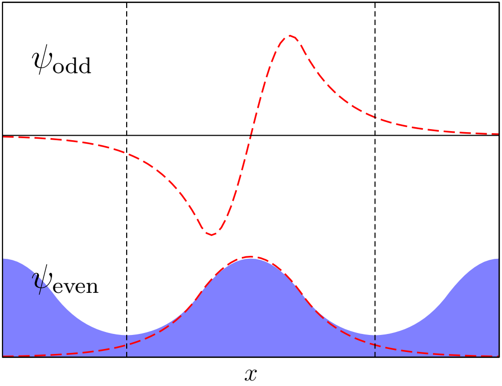


$\Delta m_B < 0$

even parity $\rightarrow$ WF profile relaxed $\rightarrow$ less curvature

$\rightsquigarrow$ **more deeply bound**

Sign of the mass shift



$\Delta m_B > 0$

$\Delta m_B < 0$

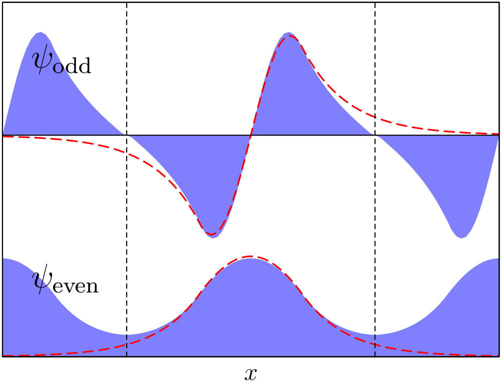
even parity $\rightarrow$ WF profile relaxed $\rightarrow$ less curvature

$\rightsquigarrow$ **more deeply bound**

Sign of the mass shift

odd parity → WF profile compressed → more curvature

⇝ **less bound**



$\Delta m_B > 0$

$\Delta m_B < 0$

even parity → WF profile relaxed → less curvature

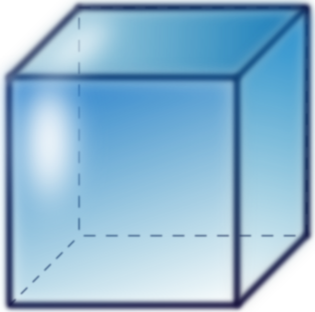
⇝ **more deeply bound**

Broken symmetry

The finite volume breaks the symmetry of the system

rotation group $SO(3)$

$\longrightarrow$



cubic group O

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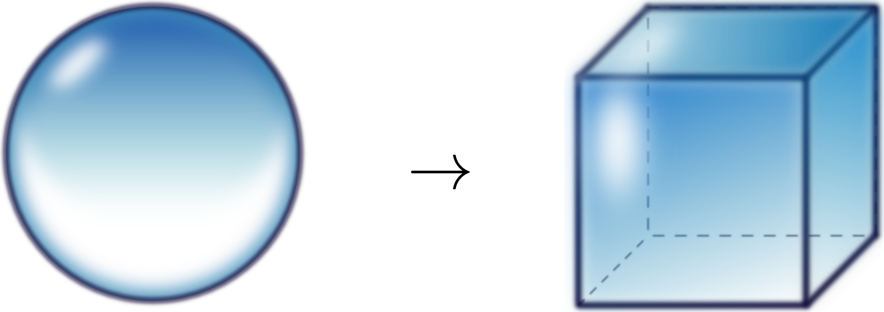

rotation group $SO(3)$ $\longrightarrow$ **cubic group** O

Irreducible representations of $SO(3)$ are reducible with respect to O!

The cubic group

- finite subgroup (24 elements) of $SO(3)$
- five irreducible representations

Γ	A_1	A_2	E	T_1	T_2
$\dim\Gamma$	1	1	2	3	3

Rewrite the mass shift

$$\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r\, \psi_B^*(\mathbf{r})\, V(\mathbf{r})\, \psi_B(\mathbf{r}+\mathbf{n}L) + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

$$\downarrow$$

$$\Delta m_B^{(\Gamma,\ell;i)} = \langle \Gamma,\ell;i|\hat{V} \sum_{|\mathbf{n}|=1} \hat{T}(\mathbf{n}L)|\Gamma,\ell;i\rangle + \cdots$$

$$|\Gamma,\ell;i\rangle = \sum_m C^{\Gamma}_{\ell i m}\, |\ell,m\rangle$$

Example

$$D^2 = T_2^+ \oplus E^+$$

T_2 representation

$$\left|T_2^+, 2; 1\right\rangle = -\frac{1}{\sqrt{2}}\left(|2,-1\rangle + |2,1\rangle\right)$$
$$\left|T_2^+, 2; 2\right\rangle = \frac{\mathrm{i}}{\sqrt{2}}\left(|2,-1\rangle - |2,1\rangle\right)$$
$$\left|T_2^+, 2; 3\right\rangle = -\frac{1}{\sqrt{2}}\left(|2,-2\rangle - |2,2\rangle\right)$$

E representation

$$\left|E^+, 2; 1\right\rangle = |2,0\rangle$$
$$\left|E^+, 2; 2\right\rangle = \frac{1}{\sqrt{2}}\left(|2,-2\rangle + |2,2\rangle\right)$$

Result

General formula

$$\Delta m_B^{(\ell,\Gamma)} = \alpha\left(\tfrac{1}{\kappa L}\right) \cdot |\gamma|^2 \, \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

ℓ	Γ	$\alpha(x)$
0	A_1^+	-3
1	T_1^-	$+3$
2	T_2^+	$30x + 135x^2 + 315x^3 + 315x^4$
2	E^+	$-1/2\left(15 + 90x + 405x^2 + 945x^3 + 945x^4\right)$

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Trace formula

$$\sum_{m=-\ell}^{\ell} \Delta m_B^{(\ell,m)} = \sum_{\Gamma,i=1}^{\dim\Gamma} \Delta m_B^{(\ell,\Gamma;i)} = (-1)^{\ell+1}(2\ell+1)\cdot 3|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \ldots$$

Numerical checks

Results can be checked with a very simple calculation…

Lattice Hamiltonian

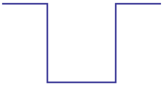
$$\hat{H}_0 = \sum_{\hat{\mathbf{n}}} \left[\frac{3}{\hat{\mu}} a^\dagger(\hat{\mathbf{n}}) a(\hat{\mathbf{n}}) - \frac{1}{2\hat{\mu}} \sum_{l=1,2,3} \left(a^\dagger(\hat{\mathbf{n}}) a(\hat{\mathbf{n}} + \hat{\mathbf{e}}_l) + a^\dagger(\hat{\mathbf{n}}) a(\hat{\mathbf{n}} - \hat{\mathbf{e}}_l) \right) \right]$$

$$\hat{E}(\hat{\mathbf{q}}) = \frac{1}{\hat{\mu}} \sum_{l=1,2,3} (1 - \cos \hat{q}_i) = \frac{1}{2\hat{\mu}} \sum_{l=1,2,3} \hat{q}_l^2 \left[1 + \mathcal{O}(\hat{q}_l^2) \right]$$

lattice units: $\hat{L} = L/a$, $\hat{E} = E \cdot a$, etc. , $a =$ lattice spacing

Numerical checks

- Interaction: $V_{\text{step}}(r) = -V_0\,\theta(R-r)$
- Approximate infinite volume with $L_\infty = 40$



Methods to calculate mass shift

1. $\Delta m_B = E_B(L_\infty) - E_B(L)$ (direct difference)
2. $\Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r\, \psi_B^*(\mathbf{r})\, V(\mathbf{r})\, \psi_B(\mathbf{r}+\mathbf{n}L)$ (overlap integral)
3. $\Delta m_B = \alpha\left(\frac{1}{\kappa L}\right) \cdot |\gamma|^2\, \frac{\mathrm{e}^{-\kappa L}}{\mu L}$ (Green's function)

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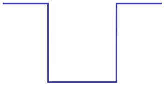

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- Replace

$$\mathrm{e}^{-\hat{\kappa}\hat{L}}/\hat{L} \longrightarrow 4\pi \hat{G}_{\hat{\kappa}}(\hat{L},0,0)$$

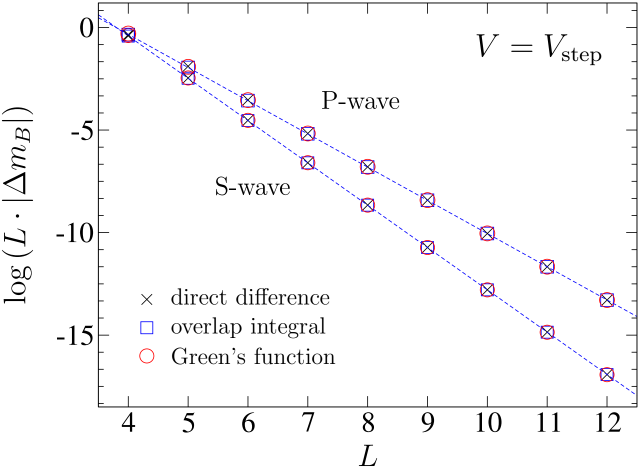
to reduce discretization errors!

Lattice Green's function

$$\hat{G}_{\hat{\kappa}}(\hat{\mathbf{n}}) = \frac{1}{L^3}\sum_{\hat{\mathbf{q}}} \frac{\mathrm{e}^{-\mathrm{i}\hat{\mathbf{q}}\cdot\hat{\mathbf{n}}}}{Q^2(\hat{\mathbf{q}}) + \hat{\kappa}^2}$$

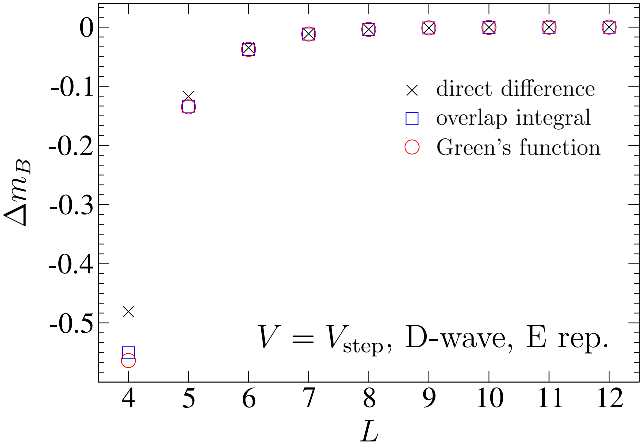
Numerical checks

$$\Delta m_B = \pm 3 \cdot |\gamma|^2 \, \frac{\mathrm{e}^{-\kappa L}}{\mu L}$$



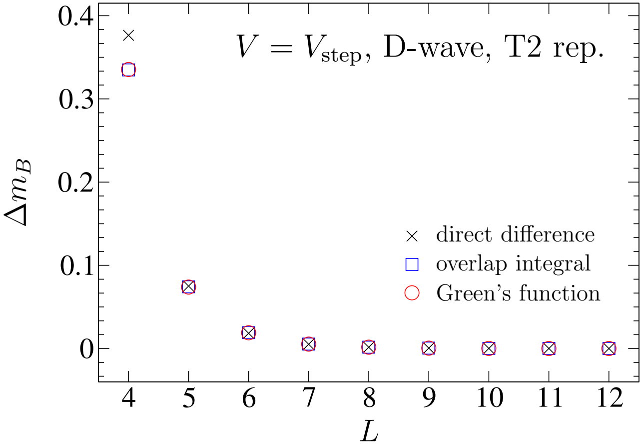
Numerical checks

$$\Delta m_B = \left(\frac{30}{\kappa L} + \cdots \right) \cdot |\gamma|^2 \, \frac{e^{-\kappa L}}{\mu L}$$



Numerical checks

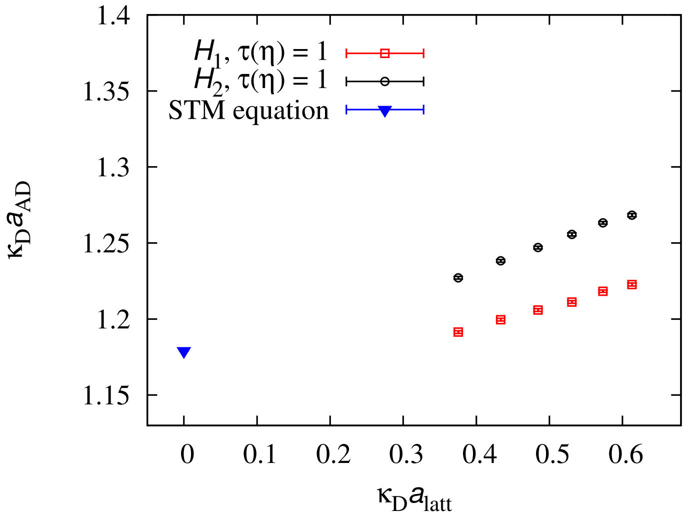
$$\Delta m_B = -{}^1\!/\!{}_2 \left(15 + \frac{90}{\kappa L} + \cdots\right) \cdot |\gamma|^2 \, \frac{\mathrm{e}^{-\kappa L}}{\mu L}$$



Part II

Topological factors in scattering systems

Motivation: atom-dimer scattering



calculation by S. Bour, D. Lee, U.-G. Meißner

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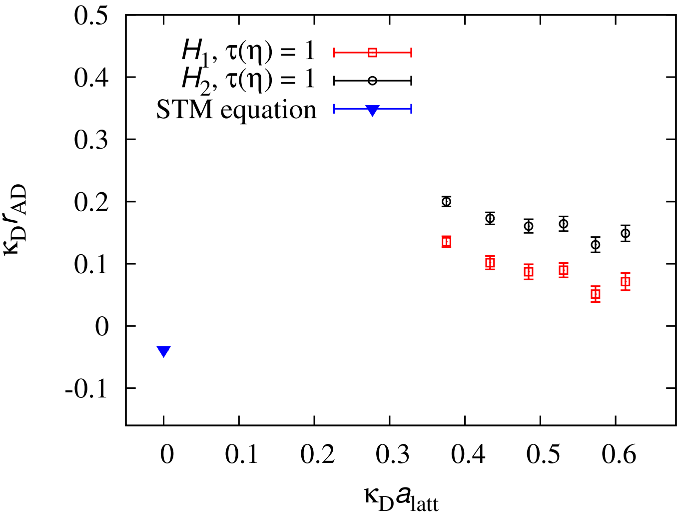

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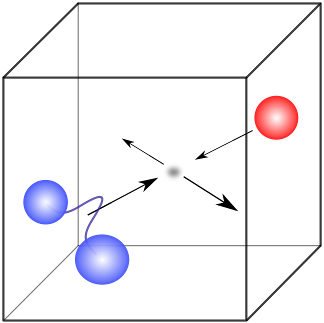
Atom-dimer scattering

$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta) \quad , \quad \eta = \left(\frac{Lp}{2\pi}\right)^2 \quad , \quad p = p(E(L))$$

$$p \cot \delta_0(p) = -\frac{1}{a_{\rm AD}} + \frac{r_{\rm AD}}{2} p^2 + \mathcal{O}(p^4)$$



A part of $E(L)$ is due to the binding of the dimer!

Part II

Topological factors in scattering systems

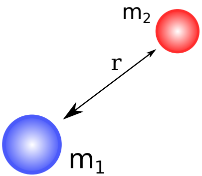
- Motivation ✓
- Moving bound states in a finite volume
- Mass shift for twisted boundary conditions
- Corrections for scattering states
- Conclusion: corrected atom-dimer results

Bound states in moving frames

So far...

considered two-particle state directly in relative coordinates

wavefunction $\psi(\mathbf{r})$, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$



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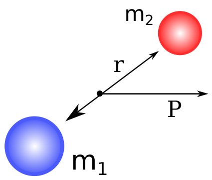
Now

full wavefunction $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{R}}\,\psi(\mathbf{r})$

$\mathbf{P}$ = center-of-mass momentum

$\mathbf{R} = \alpha\mathbf{r}_1 + (1-\alpha)\mathbf{r}_2$, $\alpha = \dfrac{m_1}{m_1 + m_2}$



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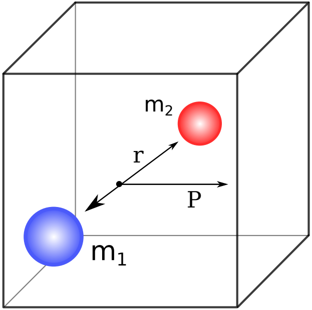
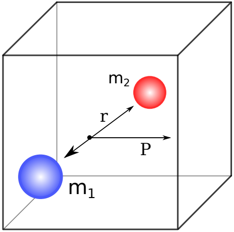


Put system into finite box, impose periodic BC...

Twisted boundary conditions

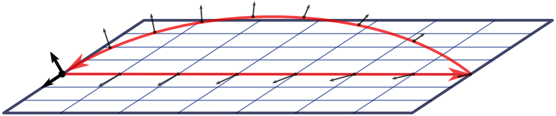


Now $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ has to be periodic!

$$\Psi(\mathbf{r}_1{+}\mathbf{n}L, \mathbf{r}_2) = \mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{R}}\,\mathrm{e}^{\mathrm{i}\alpha L\mathbf{P}\cdot\mathbf{n}}\,\psi(\mathbf{r}{+}\mathbf{n}L) = \Psi(\mathbf{r}_1, \mathbf{r}_2)$$

$$\rightsquigarrow \psi(\mathbf{r}+\mathbf{n}L) = \mathrm{e}^{-\mathrm{i}\alpha L\mathbf{P}\cdot\mathbf{n}}\,\psi(\mathbf{r})$$

“twisted boundary conditions”



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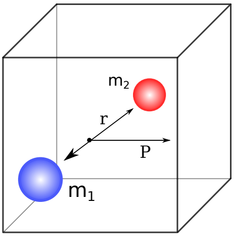

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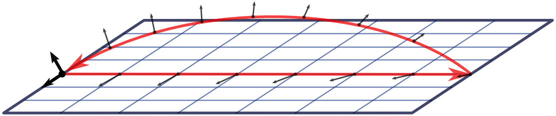

Question

What is the finite-volume mass shift in this case?

Mass shift for twisted boundary conditions

- boundary condition: $\psi(\mathbf{r}+\mathbf{n}L) = \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}\cdot\mathbf{n}}\,\psi(\mathbf{r})$, $\boldsymbol{\theta} = \alpha L \mathbf{P}$
- new ansatz: $\psi_0(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \psi_B(\mathbf{r}+\mathbf{n}L)\,\mathrm{e}^{\mathrm{i}\boldsymbol{\theta}\cdot\mathbf{n}}$

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$$\rightsquigarrow \Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3 r\, \psi_B^*(\mathbf{r})\, V(\mathbf{r})\, \psi_B(\mathbf{r} + \mathbf{n}L)\,\mathrm{e}^{\mathrm{i}\boldsymbol{\theta}\cdot\mathbf{n}} + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

S-wave result

$$\Delta m_B = -|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} \times \sum_{\mathbf{n}=\hat{\mathbf{e}}_x,\hat{\mathbf{e}}_y,\hat{\mathbf{e}}_z} \cos(\boldsymbol{\theta}\cdot\mathbf{n}) + \cdots$$

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$$\sum_{\mathbf{n}} \cos(\boldsymbol{\theta}\cdot\mathbf{n}) = 3 \quad \text{for} \quad \boldsymbol{\theta} = (0,0,0) \;\rightarrow\; \text{consistent} \checkmark$$

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$\sum_{\mathbf{n}} \cos(\boldsymbol{\theta}\cdot\mathbf{n}) = 3$ for $\boldsymbol{\theta} = (0,0,0)$ $\rightarrow$ consistent ✓

The mass shift vanishes in certain moving frames!

→ Davoudi & Savage, arXiv:1108.5371

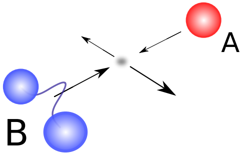
Scattering states

Now consider the scattering of two states A and B...

Scattering wavefunction

$$\langle\vec{r}\,|\Psi_p\rangle = c\sum_{\vec{k}} \frac{e^{i\frac{2\pi\vec{k}}{L}\cdot\vec{r}}}{\left(2\pi\vec{k}/L\right)^2 - p^2}\ ,\ E_{AB}(p,L) = \frac{\langle\Psi_p|\,\hat{H}\,|\Psi_p\rangle}{\langle\Psi_p\,|\Psi_p\rangle}$$

- $\Delta E^A_{\vec{k}}(L) \equiv E^A_{\vec{k}}(L) - E^A_{\vec{k}}(\infty) = 0$
- $\Delta E^B_{\vec{k}}(L) = -|\gamma|^2\,\frac{\mathrm{e}^{-\kappa L}}{\mu L} \times \sum_{l=1,2,3} \cos(2\pi\alpha_B k_l)$



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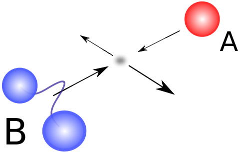


Topological volume factor

$$\tau(\eta) = \frac{1}{\mathcal{N}}\sum_{\vec{k}} \frac{\sum_{l=1,2,3}\cos(2\pi\alpha k_l)}{3\left(\vec{k}^2-\eta\right)^2} \quad , \quad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

Topological correction factors

Topological volume factor

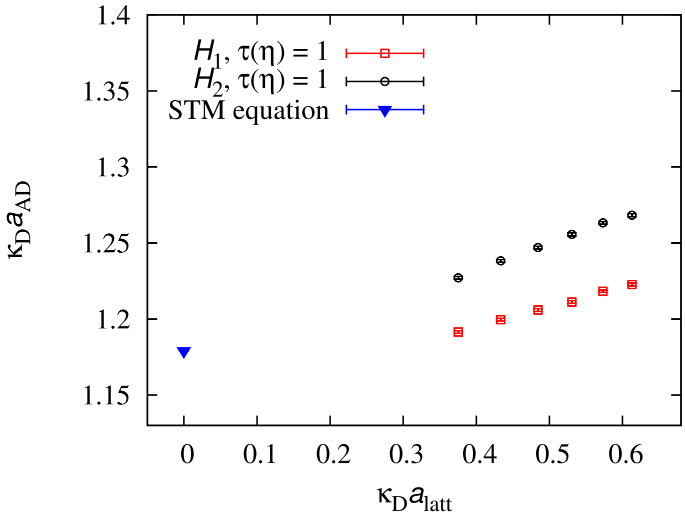
$$\tau(\eta) = \frac{1}{\mathcal{N}} \sum_{\vec{k}} \frac{\sum_{l=1,2,3} \cos(2\pi\alpha k_l)}{3\left(\vec{k}^2 - \eta\right)^2} \quad , \quad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

Final result:

$$E_{AB}(p,L) - E_{AB}(p,\infty) = \tau_A(\eta)\,\Delta E^A_{\vec{0}}(L) + \tau_B(\eta)\,\Delta E^B_{\vec{0}}(L)$$

Subtract this correction from measured energy levels! $\Rightarrow$

Corrected atom-dimer results



calculation by S. Bour, D. Lee, U.-G. Meißner

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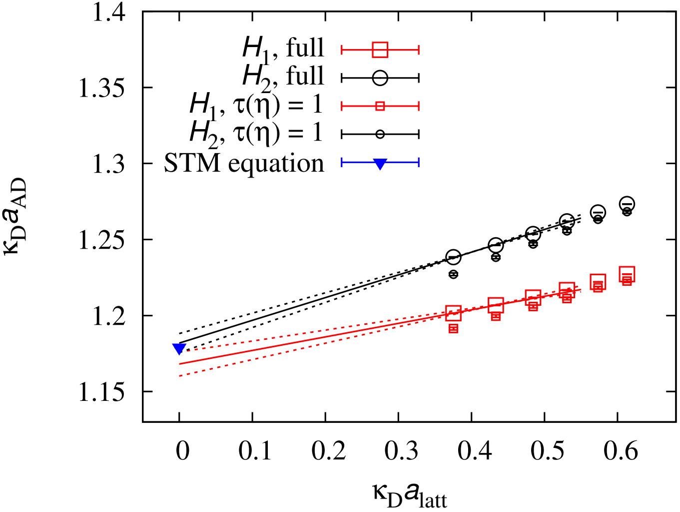

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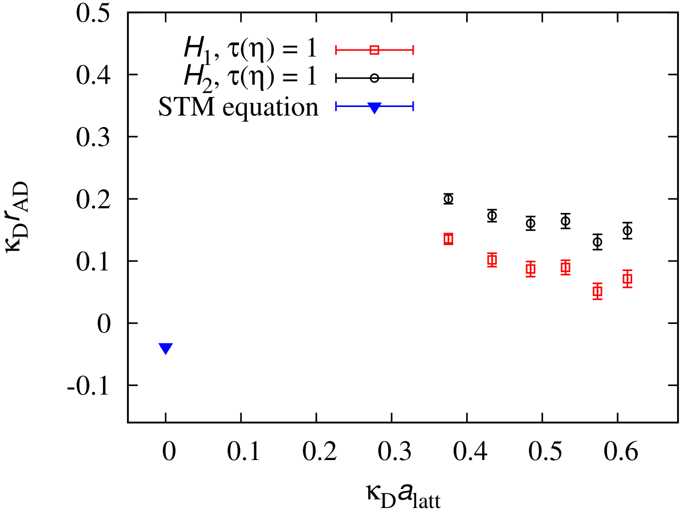

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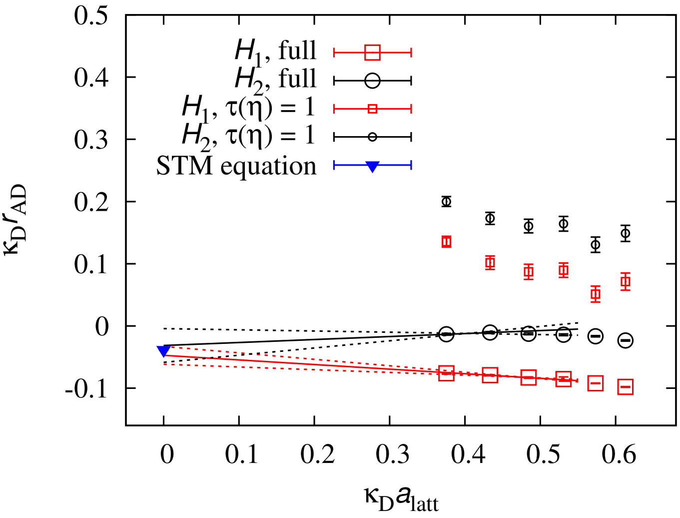

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Summary

- Mass shift can be calculated for bound states with arbitrary ℓ.
- Sign of the shift can be related to parity of the states.
- Predictions can be tested by numerical calculations.
- Mass shift of composite particles has to be corrected for in scattering calculations.

Summary

- Mass shift can be calculated for bound states with arbitrary ℓ.
- Sign of the shift can be related to parity of the states.
- Predictions can be tested by numerical calculations.
- Mass shift of composite particles has to be corrected for in scattering calculations.

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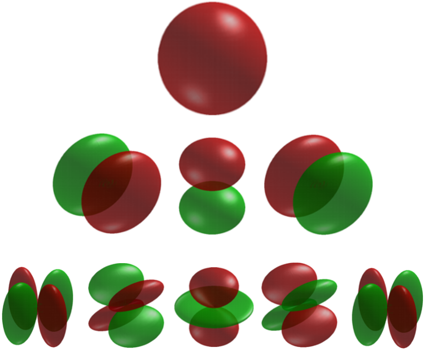
Thanks for your attention!

Spares

Angular momentum

wavefunction ψ → probability $P(V) = \int_V |\psi|^2 \mathrm{d}V$

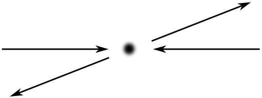
angular momentum → angular distribution



I. Sarxos, taken from Wikimedia Commons

$\ell = 0$	S-wave
$\ell = 1$	P-wave
$\ell = 2$	D-wave

Asymptotic normalization constant



$$\boxed{u_\ell(r) = \mathrm{i}^\ell \gamma \, \hat{h}_\ell^+(i\kappa r)} \quad , \quad \mathrm{Res}_{p\to \mathrm{i}\kappa} \, f_\ell(p) \sim \gamma^2$$

scattering amplitude $f_\ell(p) \sim T_\ell(p) = \langle p|\hat{T}|p\rangle_\ell$

Effective range expansion

$$f_\ell(p) \propto \frac{p^{2\ell}}{p^{2\ell+1}\left[\cot\delta_\ell(p) - \mathrm{i}\right]}$$

$$p^{2\ell+1}\cot\delta_\ell(p) = -\frac{1}{a_\ell} + \frac{1}{2} r_\ell \, p^2 + \cdots$$

- shallow bound states: $p = \mathrm{i}\kappa \to 0$

$$r_\ell + \frac{2\kappa^{2\ell}}{\gamma^2} = \mathcal{O}(\kappa) \ \text{ for } \ \ell \geq 1 \quad , \quad r_0 + \frac{2}{\gamma^2} - \frac{1}{\kappa} = \mathcal{O}(\kappa) \ \text{ for } \ \ell = 0$$

Overlap integral

It holds that

$$
\begin{aligned}
H_L\psi_0(\mathbf{r}) &= \left(H_0 + \sum_{\mathbf{n}} V(\mathbf{r}+\mathbf{n}L)\right)\sum_{\mathbf{n}'}\psi_B(\mathbf{r}+\mathbf{n}'L) \\
&= \sum_{\mathbf{n}'}\left[H_0 + V(\mathbf{r}+\mathbf{n}'L) + \sum_{\mathbf{n}|\mathbf{n}\neq\mathbf{n}'} V(\mathbf{r}+\mathbf{n}L)\right]\psi_B(\mathbf{r}+\mathbf{n}'L) \\
&= -E_B(\infty)\sum_{\mathbf{n}'}\psi_B(\mathbf{r}+\mathbf{n}'L) + \sum_{\mathbf{n}\neq\mathbf{n}'} V(\mathbf{r}+\mathbf{n}L)\,\psi_B(\mathbf{r}+\mathbf{n}'L)\,,
\end{aligned}
$$

hence

$$
\hat{H}_L\,|\psi_0\rangle = -E_B(\infty)\,|\psi_0\rangle + |\eta\rangle\ ,
$$

where

$$
\langle\mathbf{r}|\eta\rangle = \eta(\mathbf{r}) = \sum_{\mathbf{n}\neq\mathbf{n}'} V(\mathbf{r}+\mathbf{n}L)\,\psi_B(\mathbf{r}+\mathbf{n}'L)
$$

Overlap integral

$$|\psi\rangle = \alpha\,|\psi_0\rangle + |\psi'\rangle \quad \text{with} \quad |\psi'\rangle = \mathcal{O}(\mathrm{e}^{-\kappa L}) \quad \text{, choose } \alpha \text{ s.t.} \quad \langle\psi'|\psi_0\rangle = 0$$

$$\begin{aligned}\langle\psi|\,\hat{H}_L\,|\psi_0\rangle &= -E_B(\infty)\,\langle\psi|\psi_0\rangle + \langle\psi|\eta\rangle = -E_B(\infty)\,\langle\psi_0|\psi_0\rangle + \langle\psi|\eta\rangle \\ &= -E_B(L)\,\langle\psi|\psi_0\rangle = -E_B(L)\,\langle\psi_0|\psi_0\rangle\end{aligned}$$

$$\Rightarrow\;\; E_B(\infty) - E_B(L) = \Delta m_B = \frac{\langle\psi|\eta\rangle}{\langle\psi_0|\psi_0\rangle}$$

$$\langle\psi|\eta\rangle = \langle\psi_0|\eta\rangle + \langle\psi'|\eta\rangle = \langle\psi_0|\eta\rangle + \mathcal{O}(\mathrm{e}^{-2\kappa L})$$

- Infinite normalization constant drops out!
- Only consider nearest neighbours!

$$\Rightarrow\;\; \Delta m_B = \sum_{|\mathbf{n}|=1} \int \mathrm{d}^3r\,\psi_B^*(\mathbf{r})\,V(\mathbf{r})\,\psi_B(\mathbf{r}+\mathbf{n}L) + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

Trace formula

Insert asymptotic form once more to get:

$$\Delta m_B^{(\ell,m)} = (-1)^{\ell+1} \cdot \frac{2\pi|\gamma|^2}{\mu} \sum_{|\mathbf{n}|=1} R_\ell^m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r\right) R_\ell^{*m}\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r\right) \left[\frac{\mathrm{e}^{-\kappa r}}{r}\right]\Bigg|_{\mathbf{r}=\mathbf{n}L} + \ldots$$

From $$\sum_{m=-\ell}^{\ell} R_\ell^m(\mathbf{r}) R_\ell^{*m}(\mathbf{r}) = \frac{2\ell+1}{4\pi}\, r^{2\ell}$$

we get $$\sum_{m=-\ell}^{\ell} R_\ell^m\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r\right) R_\ell^{*m}\left(-\frac{1}{\kappa}\boldsymbol{\nabla}_r\right) f(r) = \frac{2\ell+1}{4\pi}\frac{1}{\kappa^{2\ell}}\,\Delta^\ell f(r)$$

$$\Delta^\ell\, \frac{\mathrm{e}^{-\kappa r}}{r} = \kappa^{2\ell}\, \frac{\mathrm{e}^{-\kappa r}}{r} \quad \text{for} \quad \mathbf{r} \neq \mathbf{0}$$

$$\Rightarrow \quad \sum_{m=-\ell}^{\ell} \Delta m_B^{(\ell,m)} = (-1)^{\ell+1}(2\ell+1)\cdot 3|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \ldots$$

Mass shift up to $\ell = 3$

$$\Delta m_B^{(\ell,\Gamma)} = \alpha\left(\tfrac{1}{\kappa L}\right)\cdot|\gamma|^2\,\frac{\mathrm{e}^{-\kappa L}}{\mu L}. + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$$

ℓ	Γ	$\alpha(x)$
0	A_1^+	-3
1	T_1^-	$+3$
2	T_2^+	$30x + 135x^2 + 315x^3 + 315x^4$
2	E^+	$-1/2\,(15 + 90x + 405x^2 + 945x^3 + 945x^4)$
3	A_2^-	$315x^2 + 2835x^3 + \cdots + 28350x^6$
3	T_2^-	$-1/2\,(105x + 945x^2 + 5355x^3 + \cdots + 42525x^6)$
3	T_1^-	$1/2\,(14 + 105x + 735x^2 + 3465x^3 + \cdots + 23625x^6)$

Basis polynomials

Solid harmonics

$R_\ell^m(\mathbf{r}) = r^\ell \, Y_\ell^m(\hat{\mathbf{r}})$

$$R_0^0 \sim 1$$

$$R_1^{-1} \sim x - \mathrm{i}y \quad , \quad R_1^0 \sim z \quad , \quad R_1^{+1} \sim x + \mathrm{i}y$$

$$R_2^{-2} \sim (x - \mathrm{i}y)^2 \quad , \quad R_2^{-1} \sim (x - \mathrm{i}y)z \quad , \quad R_2^0 \sim 2z^2 - x^2 - y^2 \quad , \quad \ldots$$

Cubic group basis polynomials

$P_{\ell,\Gamma;i}(\hat{\mathbf{r}})$

$$P_{0,A_1^+} \sim 1$$

$$P_{1,T_1^-} \sim x \quad , \quad y \quad , \quad z$$

$$P_{2,T_2^+} \sim xy \quad , \quad yz \quad , \quad zx \quad ; \quad P_{2,E^+} \sim x^2 - y^2 \quad , \quad y^2 - z^2$$

Leading parity

Define

$$\operatorname{lp} P = (-1)^{d_{\max}}$$

where

$$d_{\max} = \max\{\deg_x P, \deg_y P, \deg_z P\}$$

Then

$$\alpha\left(\frac{1}{\kappa L}\right) \sim (-1)^{d_{\max}+1}\left(\frac{1}{\kappa L}\right)^{\ell - d_{\max}} \quad \text{as} \quad \kappa L \to \infty$$

$$P_{2,T_2^+} \sim xy\ ,\ yz\ ,\ zx \ \Rightarrow d_{\max} = 1$$

$$P_{2,E^+} \sim x^2 - y^2\ ,\ y^2 - z^2 \ \Rightarrow d_{\max} = 2$$