

Bound states in a box

Sebastian König

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

Dr. Klaus Erkelenz Preis – Kolloquium

HISKP, Universität Bonn

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Past and present future

The Bonn potential – K. Erkelenz *et al.*

- based on field theoretical approach
- designed to be used in nuclear structure calculations

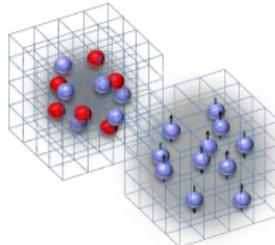


Chiral effective interactions



Modern structure calculations

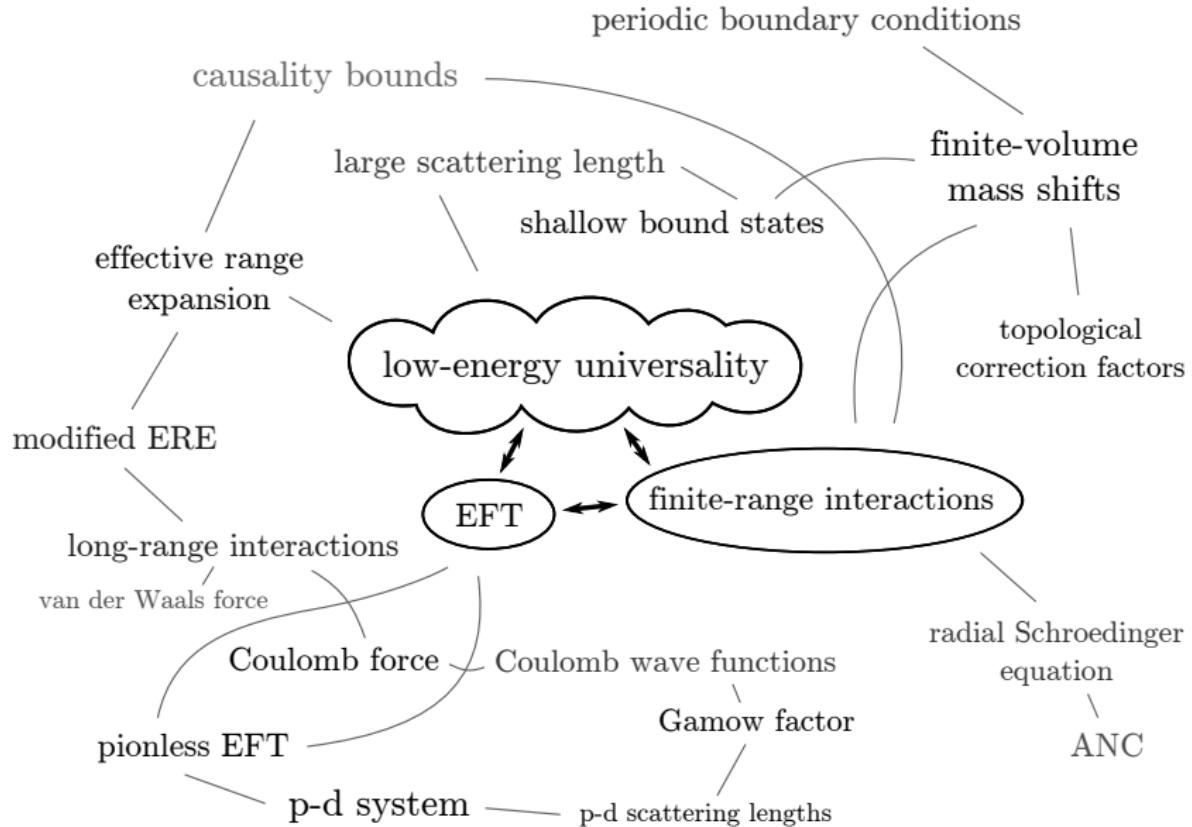
Nuclear Lattice



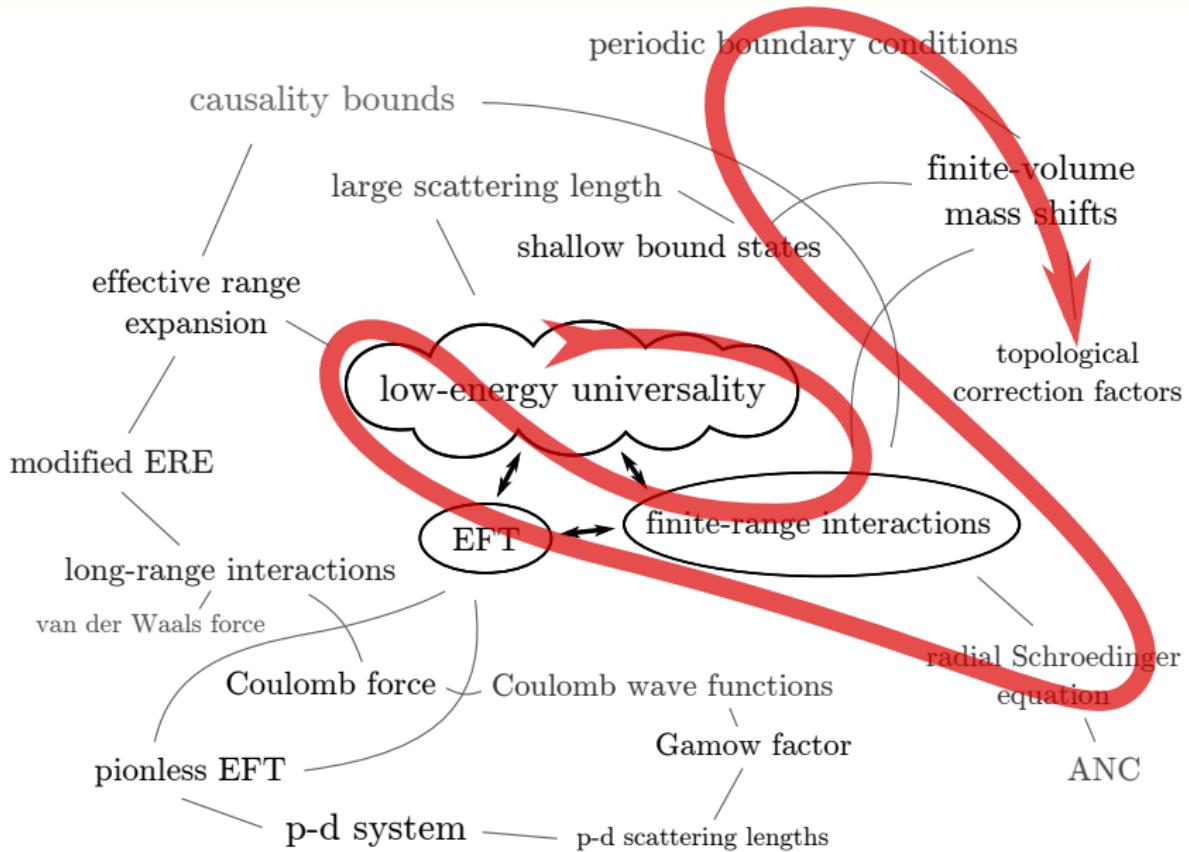
- No-core shell model
- Coupled cluster etc.
- SRG-evolved interactions
- ...

Epelbaum, Krebs, Lähde, Lee, Meißner

Outline



Outline

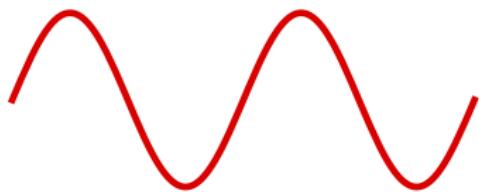


Prelude

Low-energy universality and finite-range interactions

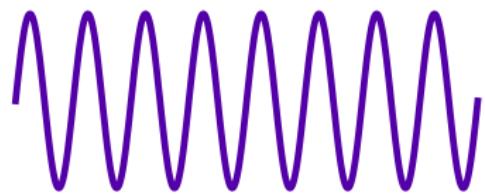
Low-energy universality

low energy → large wavelength



↪ **low resolution**

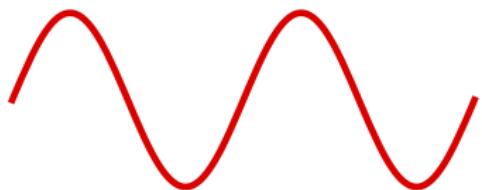
high energy → short wavelength



↪ **high resolution**

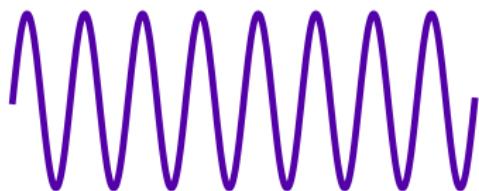
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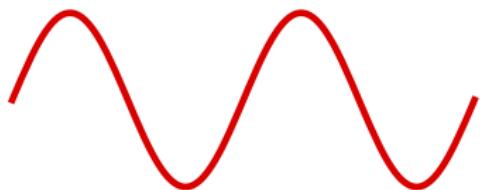
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Resolution and diffraction



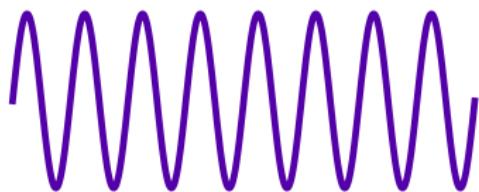
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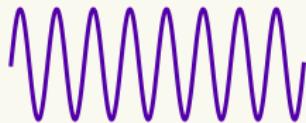
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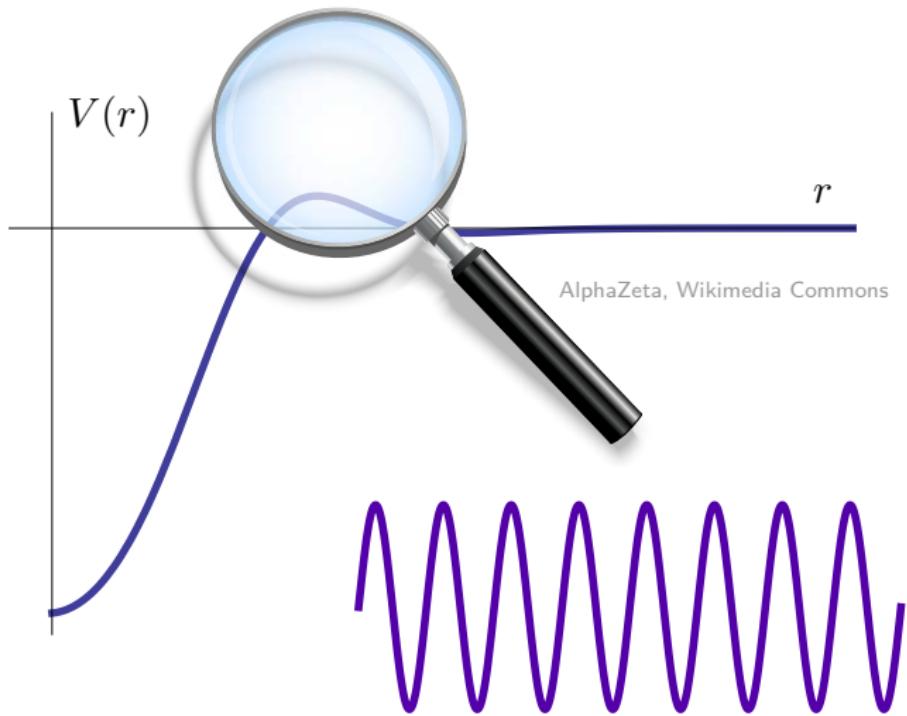


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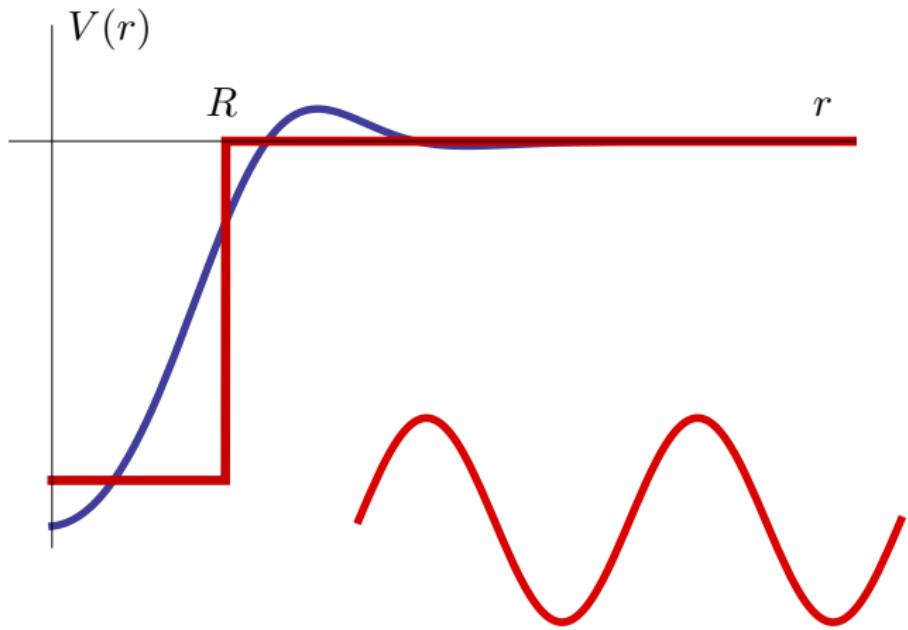
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Low-energy universality



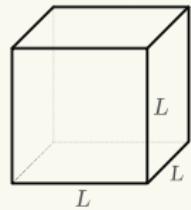
Low-energy universality



Bound states in a box

The box

- periodic finite volume
- cube of size L^3



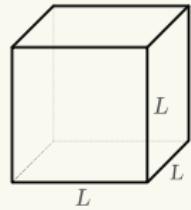
Bound states in a box

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The bound states

- 2-body bound states
- wavefunction ψ



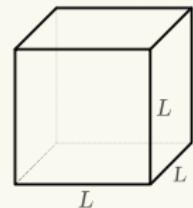
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The finite volume changes the properties of the system!

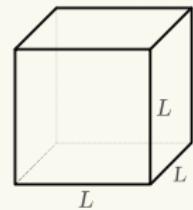
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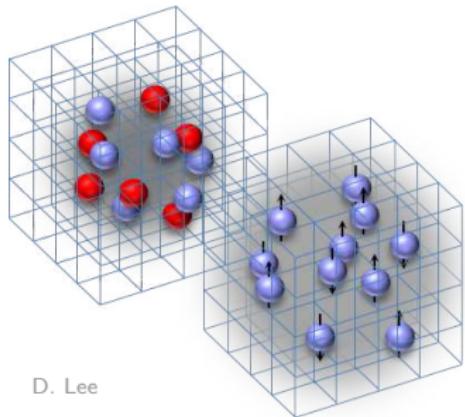
Important for numerical calculations → **Lattice**

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



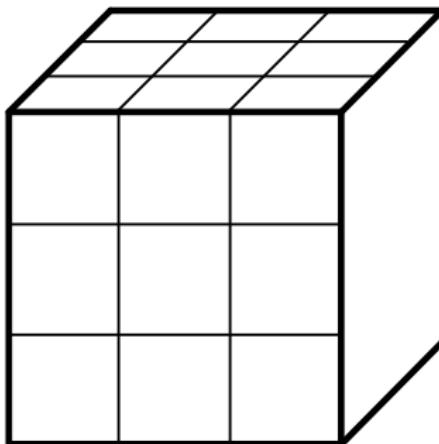
D. Lee

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

- $a \rightarrow 0$: continuum limit
- $L \rightarrow \infty$: 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**

Outline

- **Overview ✓**
- **Part I –**

Mass shift of bound states with angular momentum
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- **Summary**

Part I

Mass shift of bound states with angular momentum

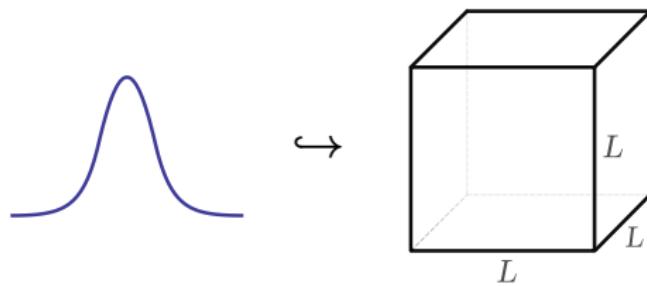
- Lüscher's result for S-waves
- Bound states in a finite volume
- General result for arbitrary partial waves
- Sign of the mass shift
- Numerical tests

Starting point

S-wave bound state

Lüscher (1986)

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

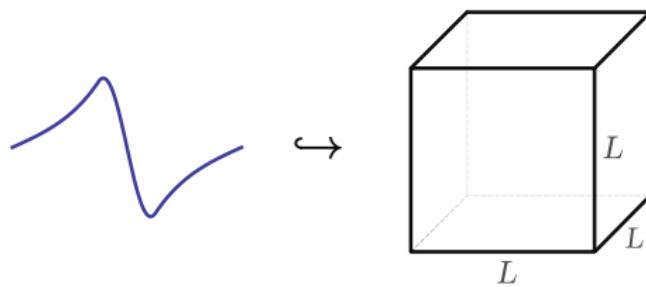


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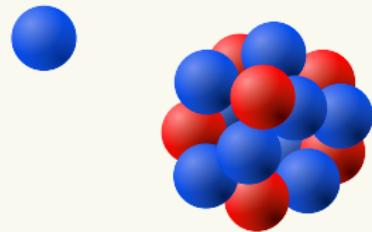


What's the result for states with angular momentum?

Why care about higher partial waves?

Halo nuclei

- single nucleon weakly bound to a tight core



nucleus by Cam-Ann, Wikimedia Commons

Halo nuclei

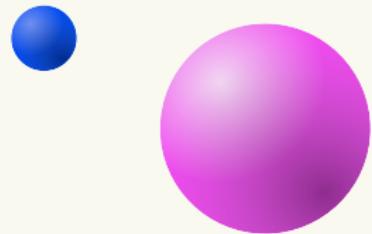
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- can be described as an effective 2-body state



nucleus by Cam-Ann, Wikimedia Commons

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Halo-EFT

expansion in $R_{\text{core}}/R_{\text{halo}} \rightarrow$ effective field theory

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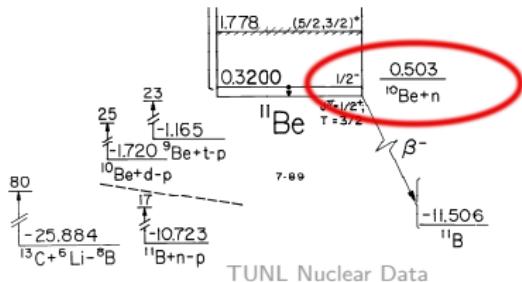
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nucleus by Cam-Ann, Wikimedia Commons

Halo-EFT

expansion in $R_{\text{core}}/R_{\text{halo}} \rightarrow$ effective field theory



Example

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

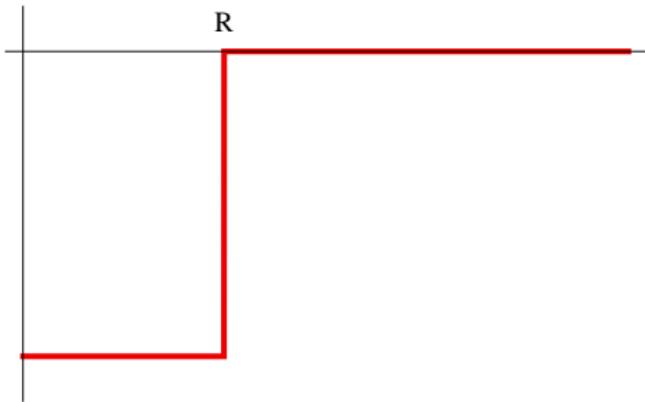
Schrödinger equation

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

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

finite-range interaction:

$$V(r) = 0 \text{ for } r > R$$



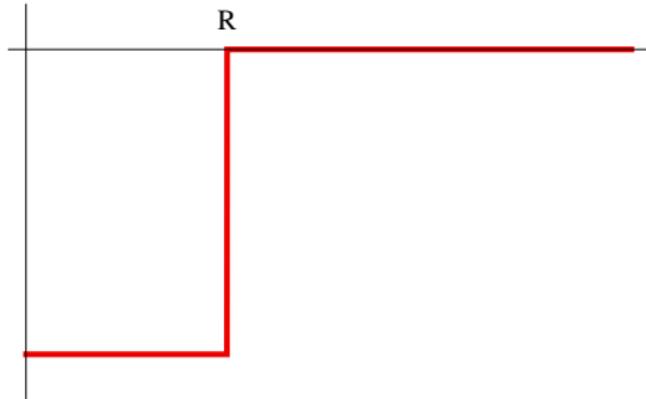
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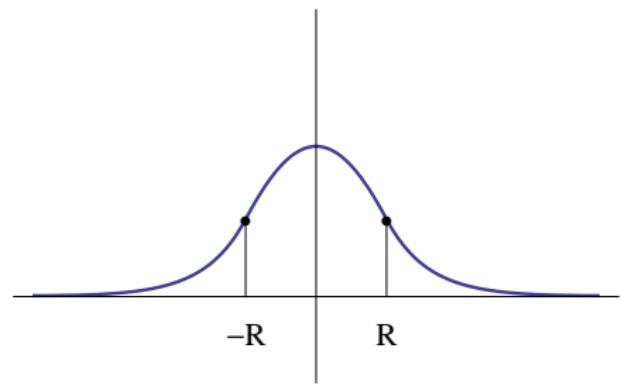
Radial Schrödinger equation

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

Asymptotic wavefunction

Radial Schrödinger equation

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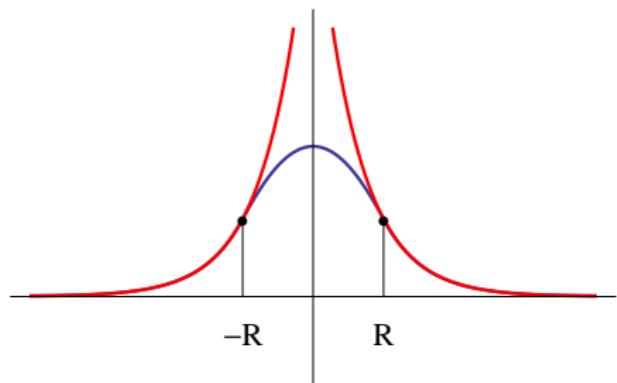
$$\rightsquigarrow u_\ell(r) = i^\ell \gamma \hat{h}_\ell^+(i\kappa r)$$

Riccati–Hankel functions

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

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

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



Finite volume

Periodic boundary conditions

→ infinitely many copies of the potential

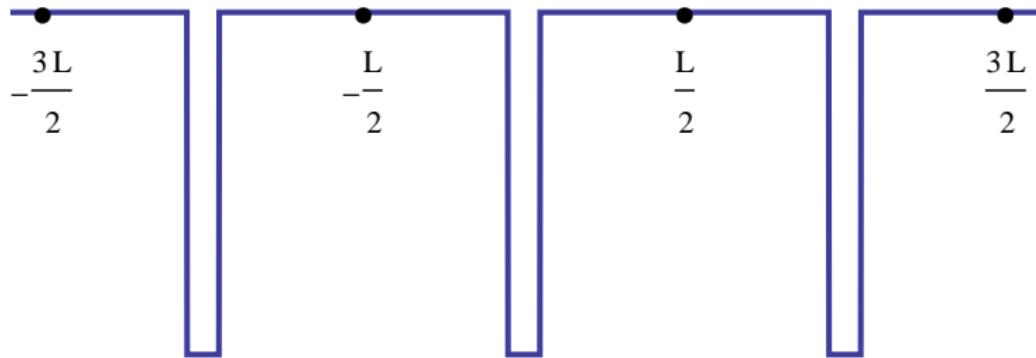
$$V_L(\mathbf{r}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(\mathbf{r} + \mathbf{n}L) \quad , \quad L \gg R$$

Finite volume

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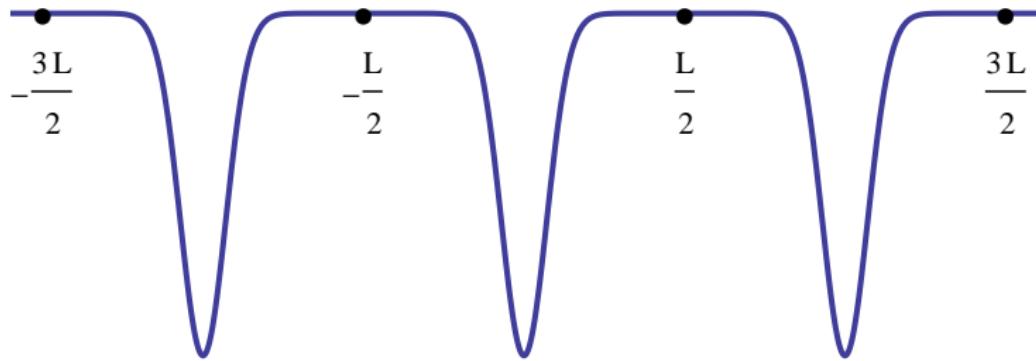
$$V(r) = V_0 \theta(R - r)$$

Finite volume

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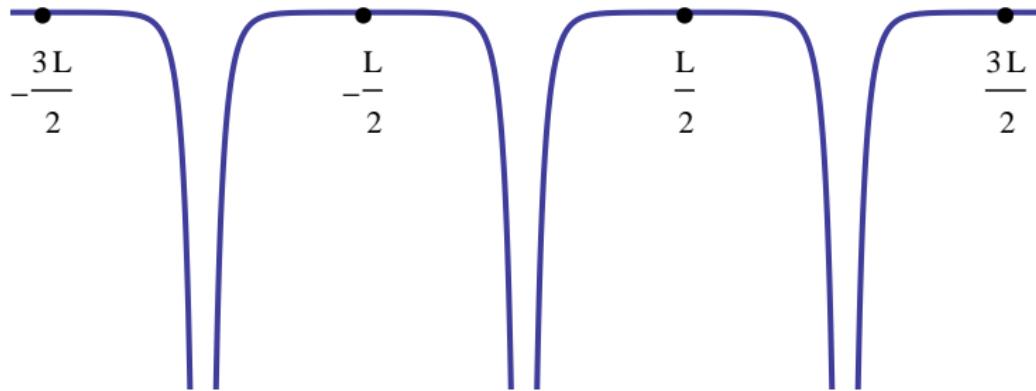
$$V(r) = V_0 \exp(-r^2/R^2)$$

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Finite volume

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

Mass shift

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

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The wavefunction $\psi(\mathbf{r})$ has to be periodic, too!

$$\psi(\mathbf{r} + \mathbf{n}L) = \psi(\mathbf{r})$$

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

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

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

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Result

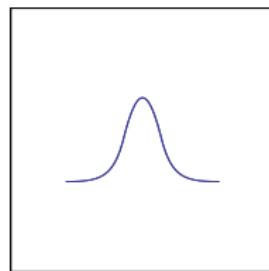
$$\Delta m_B = \frac{\langle \psi | \eta \rangle}{\langle \psi_0 | \psi_0 \rangle} = \sum_{|\mathbf{n}|=1} \int d^3r \psi_B^*(\mathbf{r}) V(\mathbf{r}) \psi_B(\mathbf{r} + \mathbf{n}L) + \mathcal{O}(e^{-\sqrt{2}\kappa L})$$

Finite volume mass shift

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

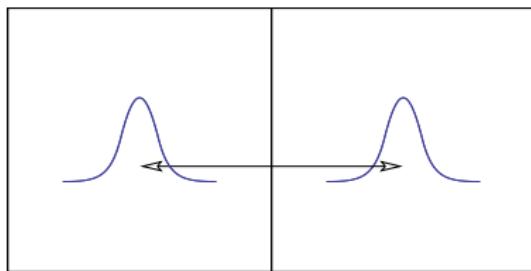
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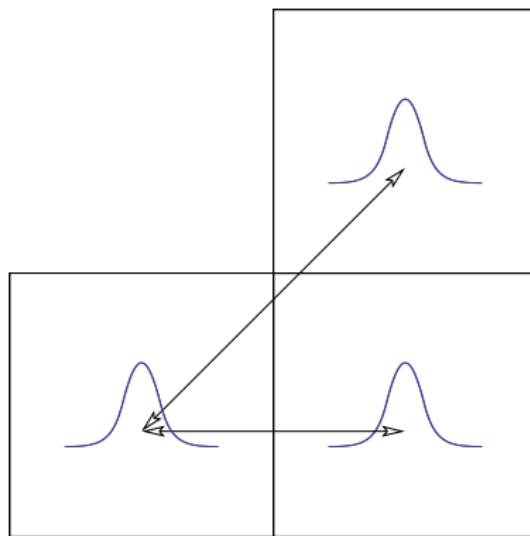
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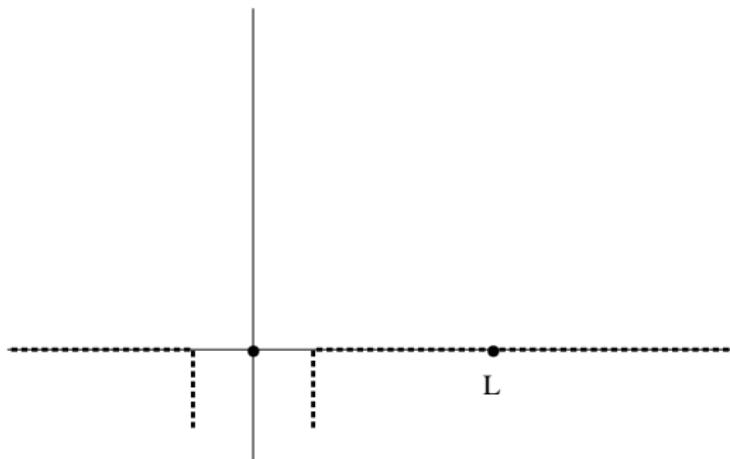
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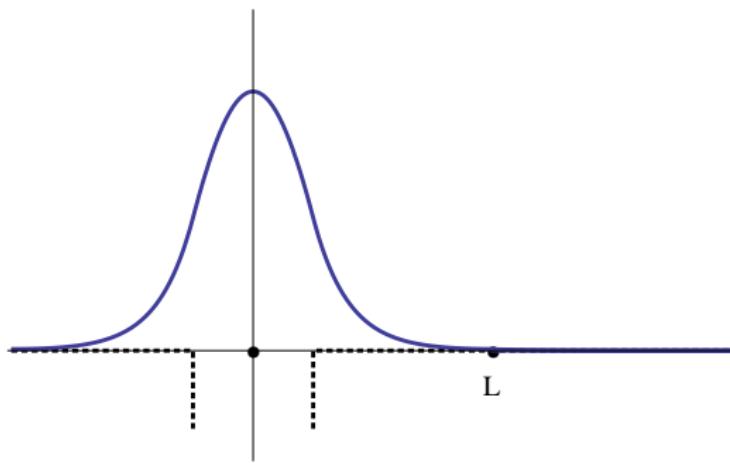
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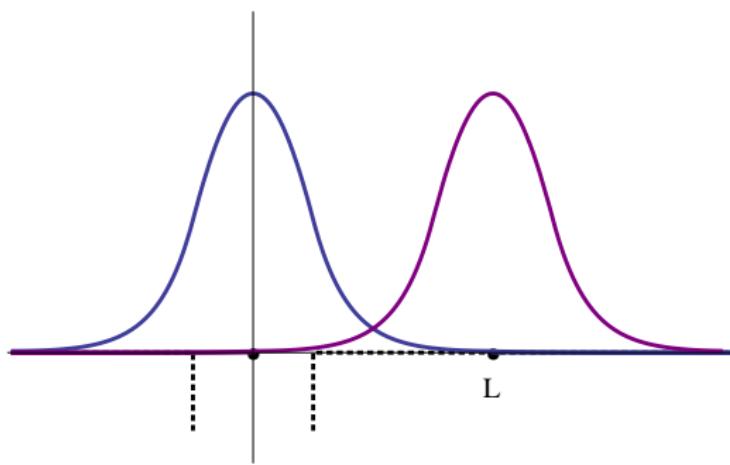
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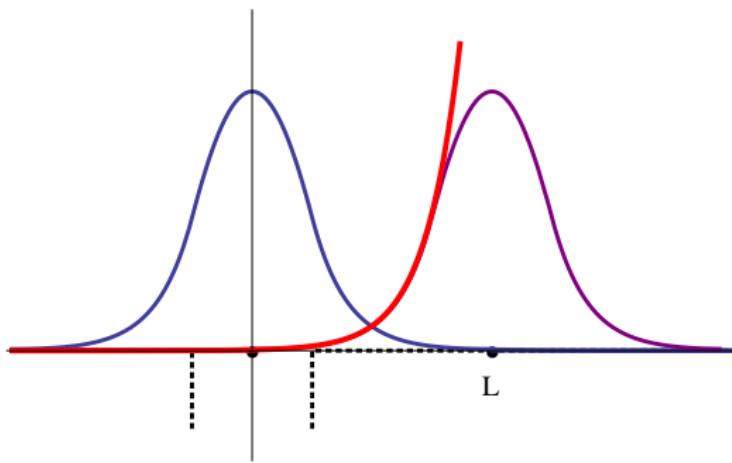
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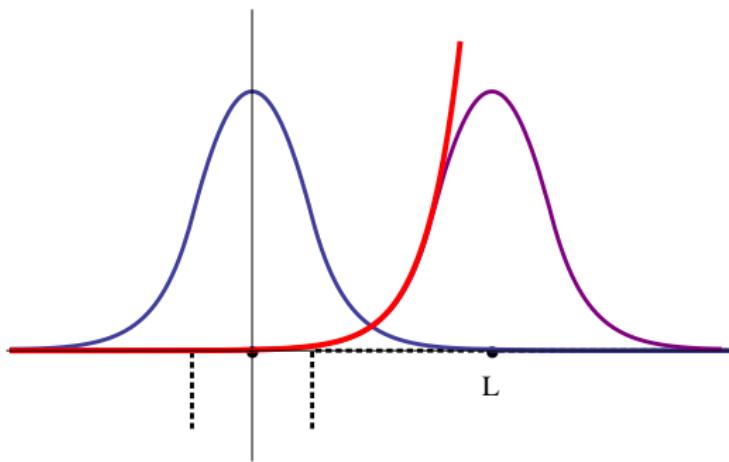
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It's all determined by the tail!



Finite volume mass shift

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

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

Finite volume mass shift

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

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$$[\Delta_r - \kappa^2] \frac{e^{-\kappa r}}{r} = -4\pi \delta^{(3)}(\mathbf{r}) \rightarrow \text{Green's function}$$

Finite volume mass shift

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

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

$$[\Delta_r - \kappa^2] \frac{e^{-\kappa r}}{r} = -4\pi \delta^{(3)}(\mathbf{r}) \rightarrow \text{Green's function}$$

S-waves

sum just yields a factor six...

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

Higher partial waves

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

Lemma

$$Y_\ell^m(\theta, \phi) \frac{\hat{h}_\ell^+(\mathbf{i}\kappa r)}{r} = (-i)^\ell R_\ell^m \left(-\frac{1}{\kappa} \boldsymbol{\nabla}_r \right) \left[\frac{e^{-\kappa r}}{r} \right]$$

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

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Lüscher 1991

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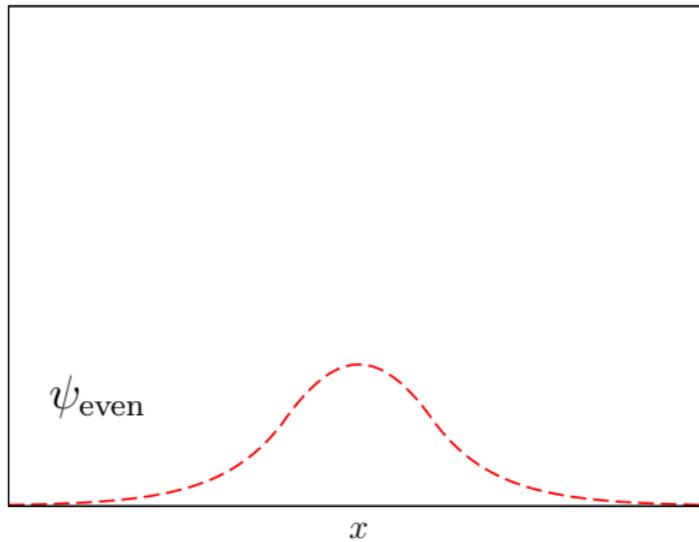
Lüscher 1991

P-waves

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

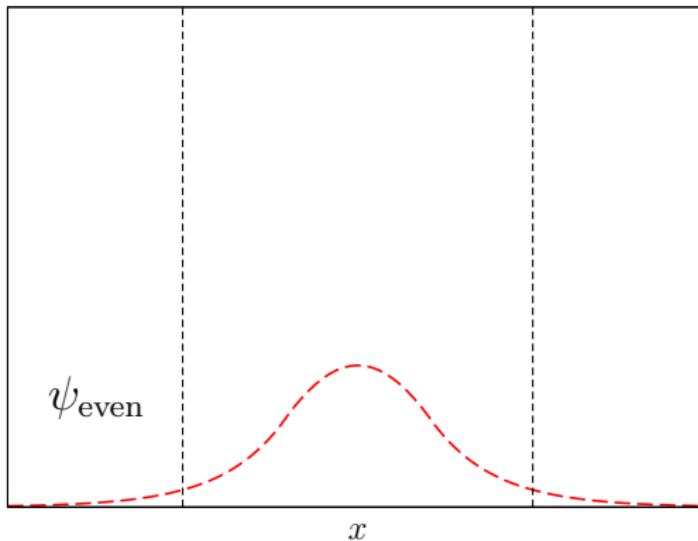
Mass shift for P-wave states exactly reversed compared to S-waves!

Sign of the mass shift



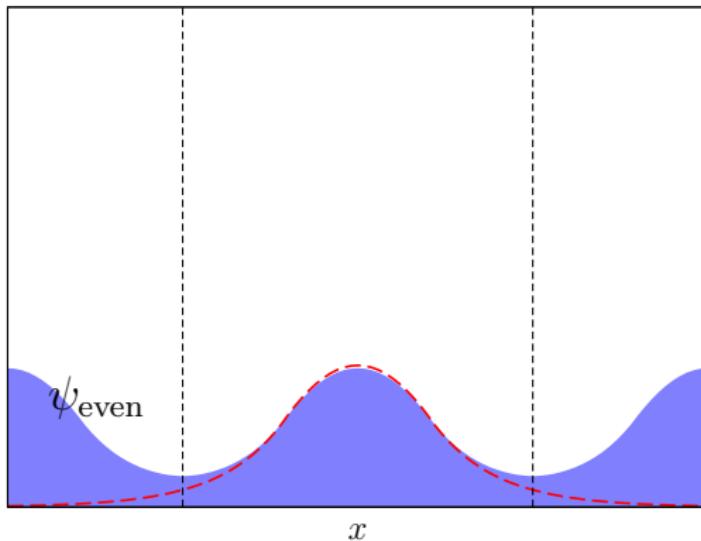
$$\Delta m_B < 0$$

Sign of the mass shift



$$\Delta m_B < 0$$

Sign of the mass shift

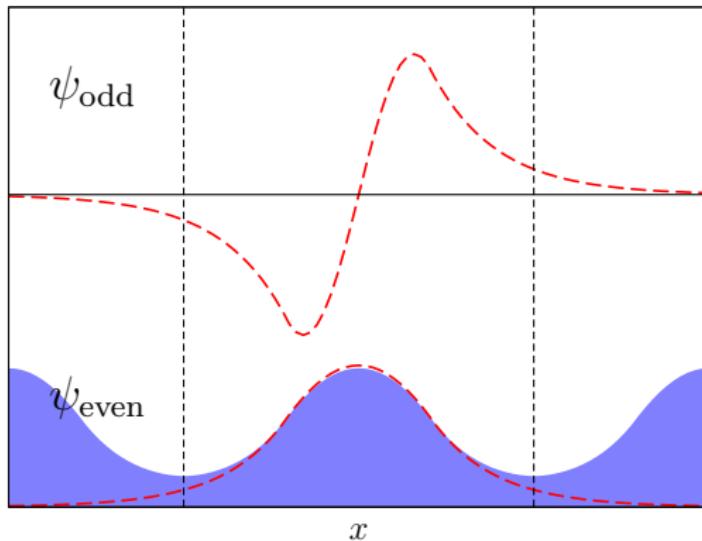


$$\Delta m_B < 0$$

even parity \rightarrow WF profile relaxed \rightarrow less curvature

\rightsquigarrow **more deeply bound**

Sign of the mass shift



$$\Delta m_B > 0$$

$$\Delta m_B < 0$$

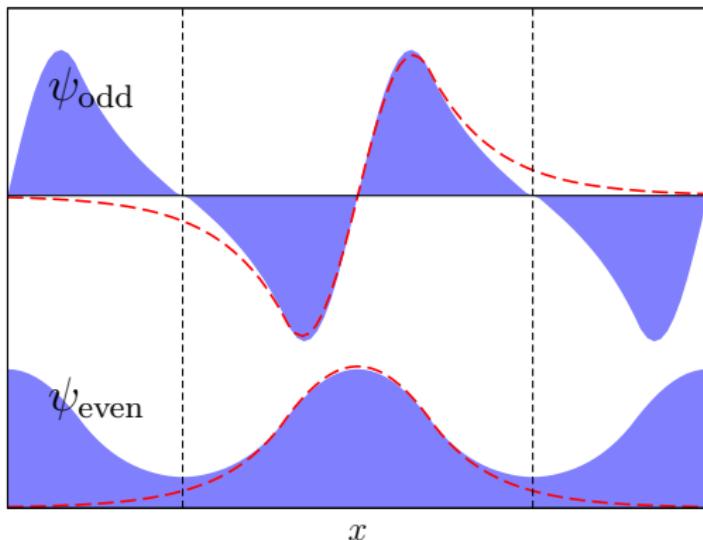
even parity \rightarrow WF profile relaxed \rightarrow less curvature

\rightsquigarrow **more deeply bound**

Sign of the mass shift

odd parity \rightarrow WF profile compressed \rightarrow more curvature

\rightsquigarrow **less bound**



$$\Delta m_B > 0$$

even parity \rightarrow WF profile relaxed \rightarrow less curvature

\rightsquigarrow **more deeply bound**

Final result

General formula

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

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

Final result

General formula

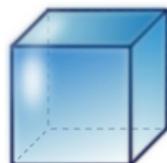
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broken
symmetry!



rotation group $SO(3)$



cubic group O

Numerical checks

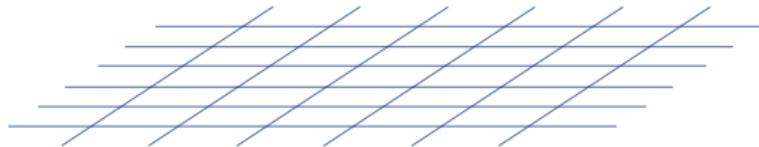
Results can be checked with a very simple calculation...

Lattice Hamiltonian

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

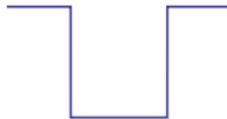
$$\hat{E}(\hat{\mathbf{q}}) = \frac{1}{\hat{\mu}} \sum_{l=1,2,3} (1 - \cos \hat{q}_i) = \frac{1}{2\hat{\mu}} \sum_{l=1,2,3} \hat{q}_l^2 \left[1 + \mathcal{O}(\hat{q}_l^2) \right]$$

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 $L_\infty = 40$

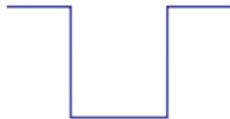


Methods to calculate mass shift

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

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- Replace

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

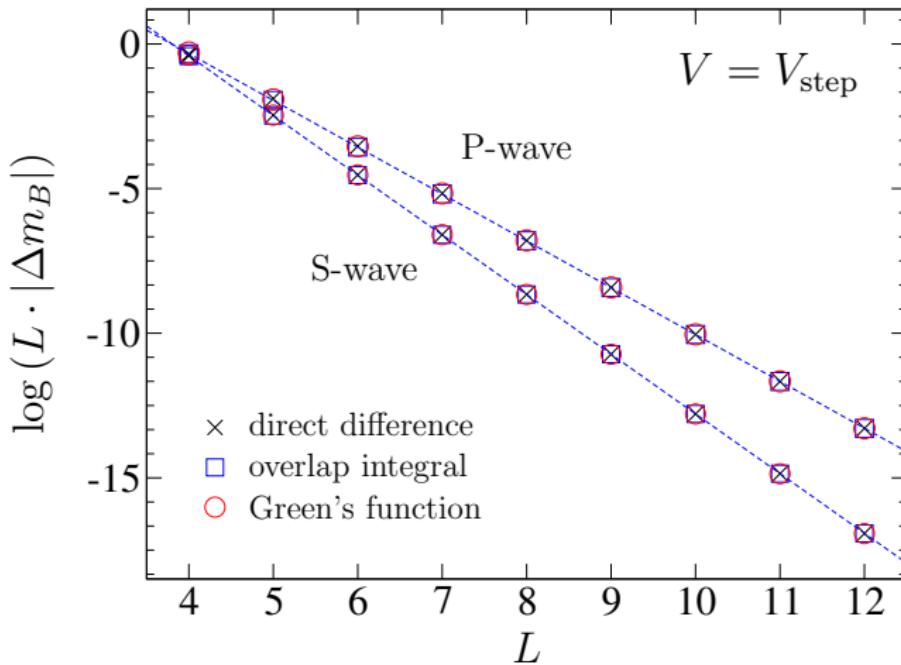
to reduce discretization errors!

Lattice Green's function

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

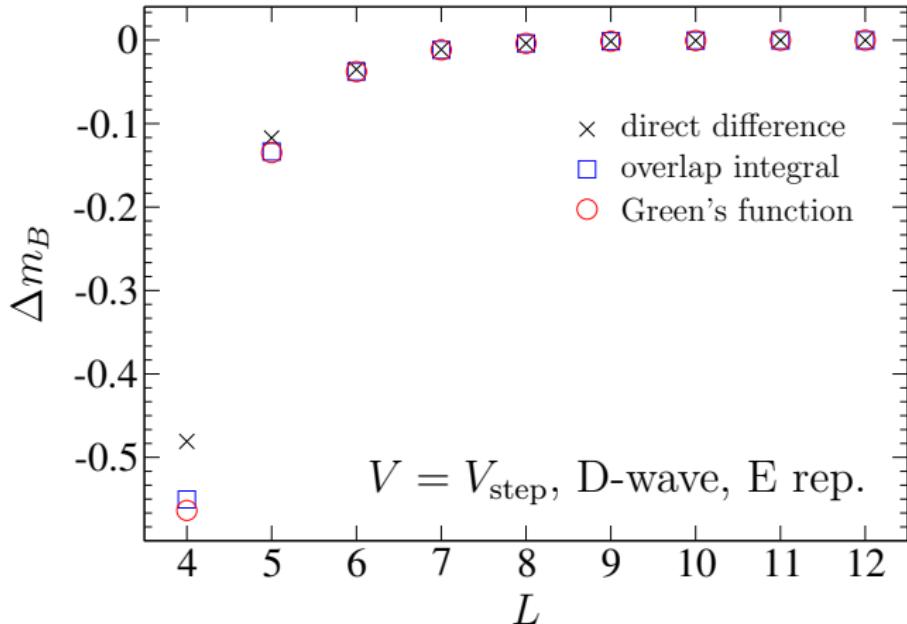
Numerical checks

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



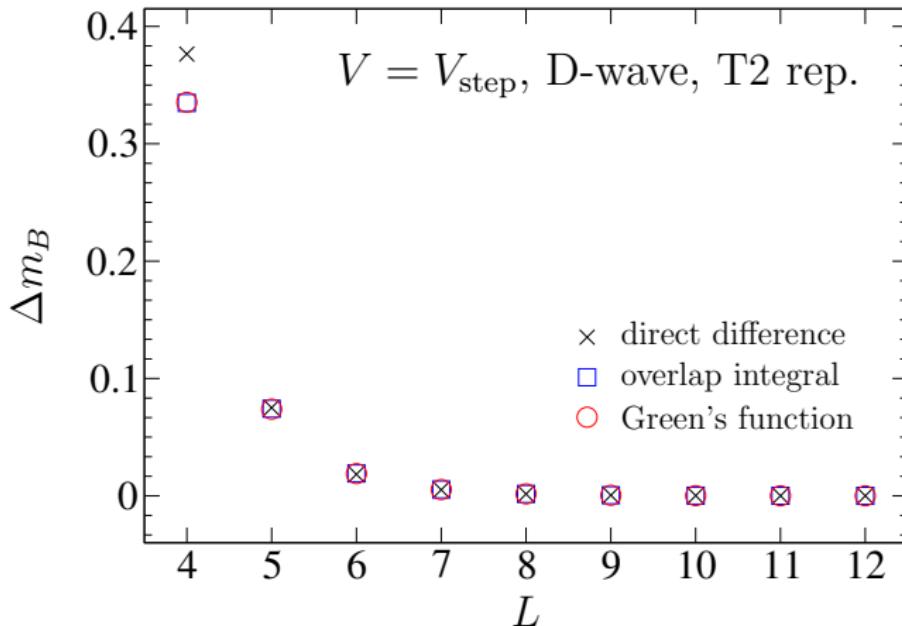
Numerical checks

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



Numerical checks

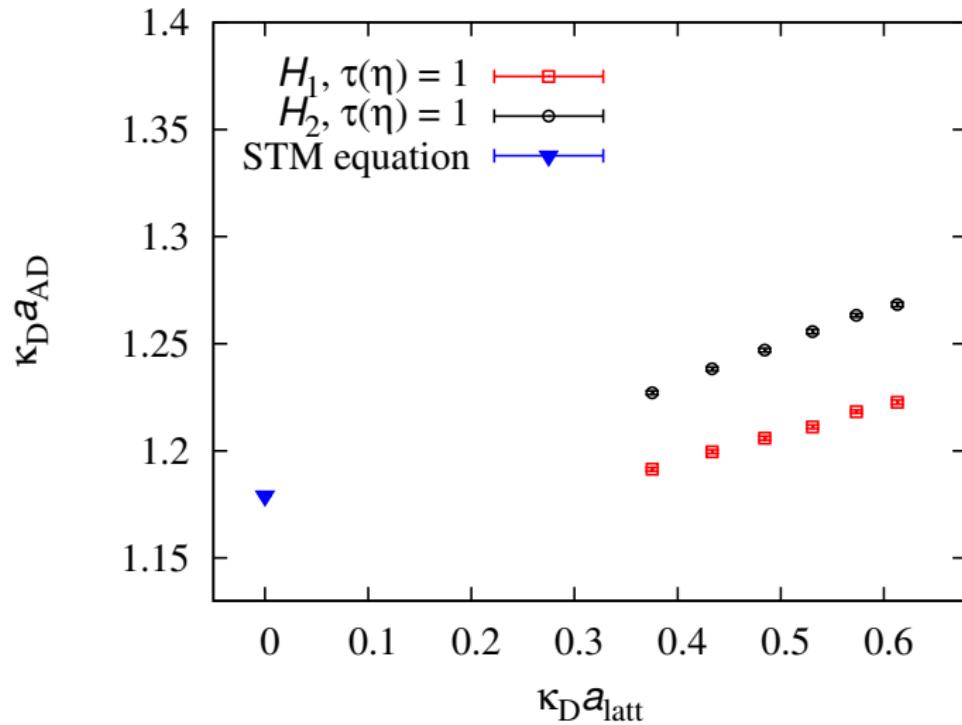
$$\Delta m_B = -^{1/2} \left(15 + \frac{90}{\kappa L} + \dots \right) \cdot |\gamma|^2 \frac{e^{-\kappa L}}{\mu L}$$



Part II

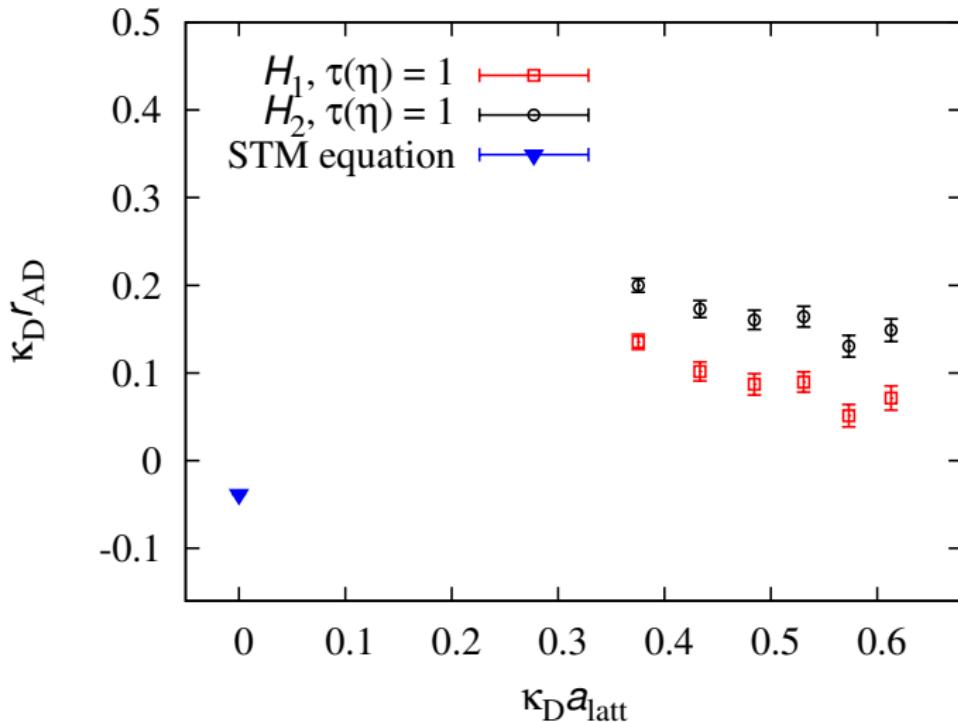
Topological factors in scattering systems

Motivation: atom-dimer scattering



calculation by S. Bour, D. Lee, U.-G. Mei  ner

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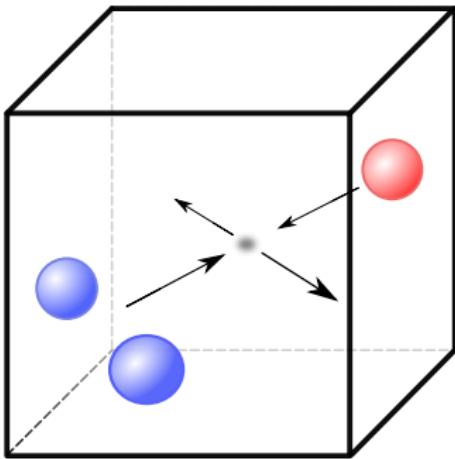


calculation by S. Bour, D. Lee, U.-G. Mei  ner

Atom-dimer scattering

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

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



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

Part II

Topological factors in scattering systems

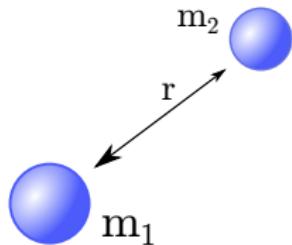
- Motivation ✓
- Moving bound states in a finite volume
- Mass shift for twisted boundary conditions
- Corrections for scattering states
- Conclusion: corrected atom-dimer results

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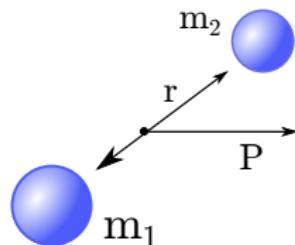
wavefunction $\psi(\mathbf{r})$, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$

Now

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

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

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



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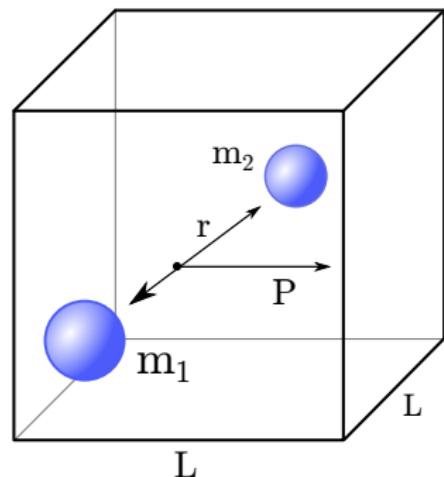
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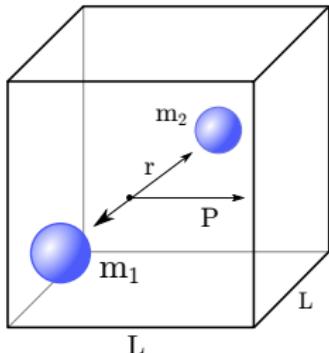
\mathbf{P} = center-of-mass momentum

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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!

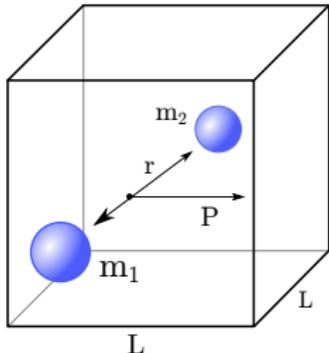
$$\Psi(\mathbf{r}_1 + \mathbf{n}L, \mathbf{r}_2) = e^{i\mathbf{P}\cdot\mathbf{R}} e^{i\alpha L \mathbf{P}\cdot\mathbf{n}} \psi(\mathbf{r} + \mathbf{n}L) = \Psi(\mathbf{r}_1, \mathbf{r}_2)$$

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

“twisted boundary conditions”



Twisted boundary conditions



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“twisted boundary conditions”



Question

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

Mass shift for twisted boundary conditions

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

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S-wave result

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

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

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The mass shift vanishes in certain moving frames!

→ Davoudi & Savage, arXiv:1108.5371

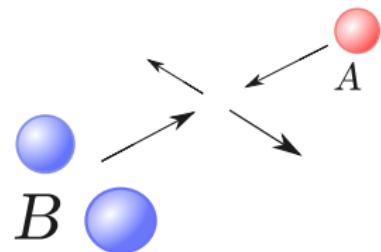
Scattering states

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

Scattering wavefunction

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

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



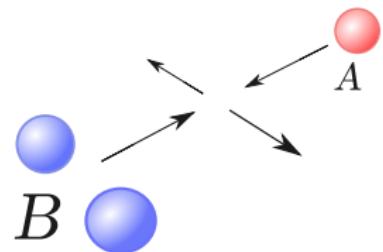
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Topological correction factors

Topological volume factor

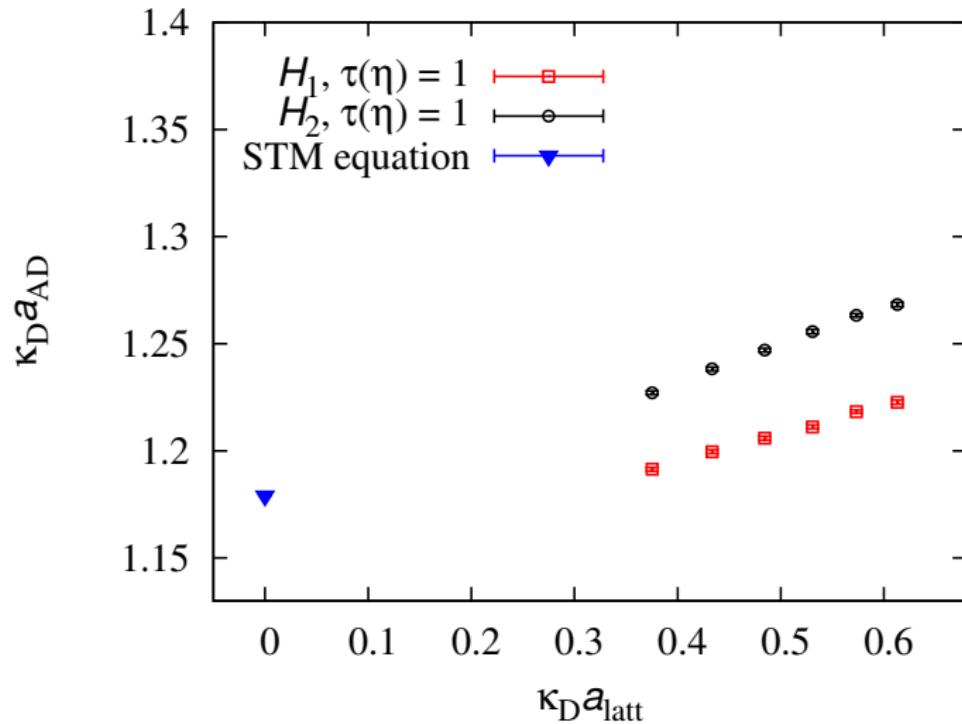
$$\tau(\eta) = \frac{1}{N} \sum_{\vec{k}} \frac{\sum_{l=1,2,3} \cos(2\pi\alpha k_l)}{3(\vec{k}^2 - \eta)^2} , \quad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

Final result:

$$E_{AB}(p, L) - E_{AB}(p, \infty) = \tau_A(\eta) \Delta E_0^A(L) + \tau_B(\eta) \Delta E_0^B(L)$$

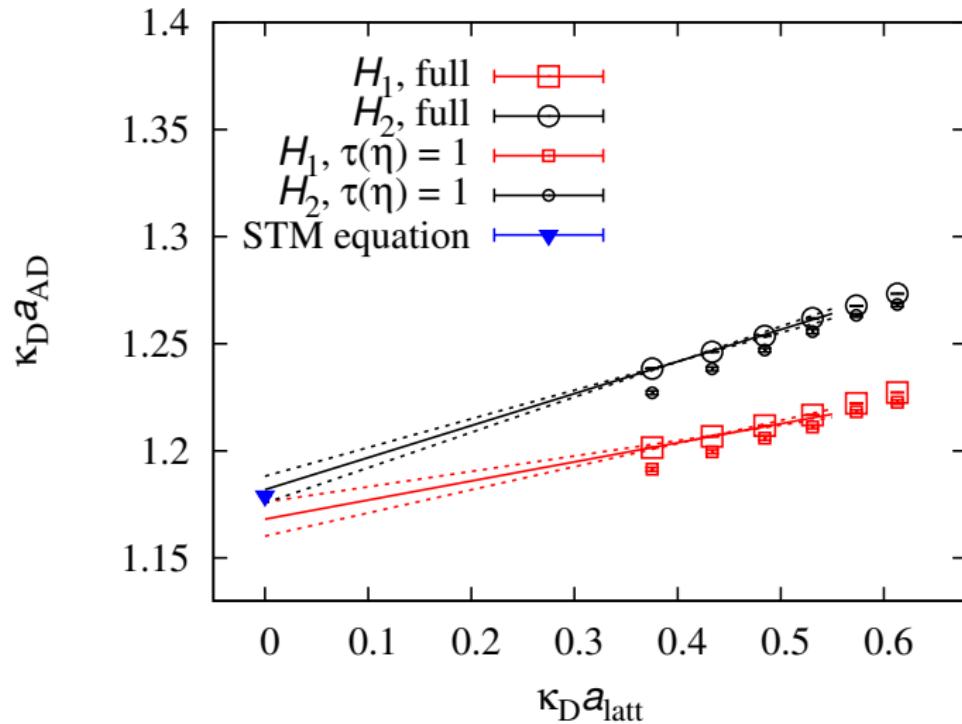
Subtract this correction from measured energy levels! \Rightarrow

Corrected atom-dimer results



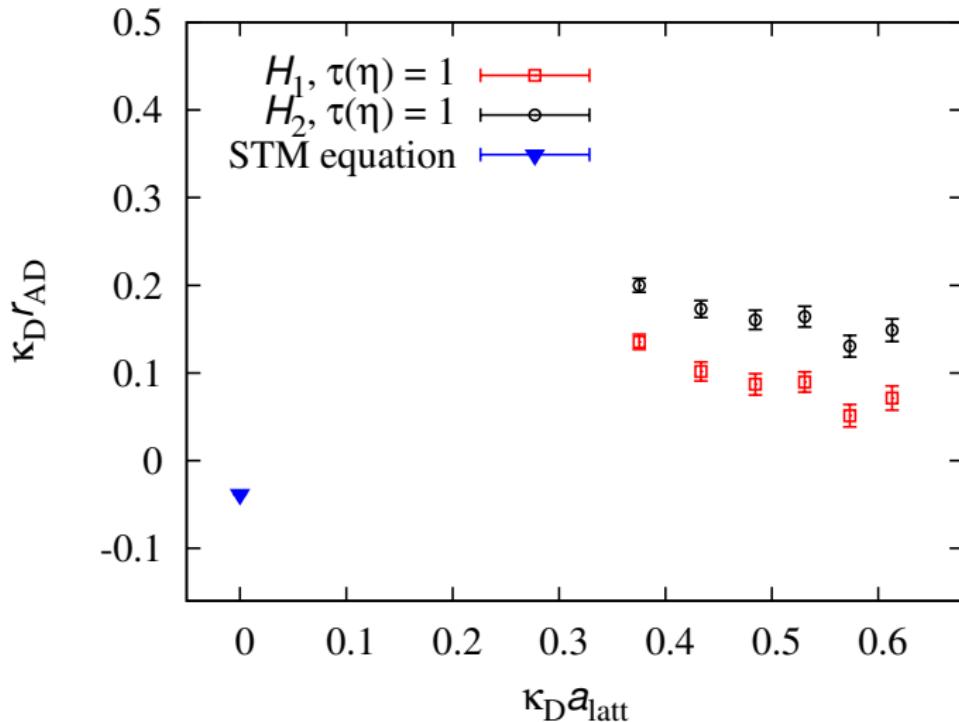
calculation by S. Bour, D. Lee, U.-G. Mei  ner

Corrected atom-dimer results



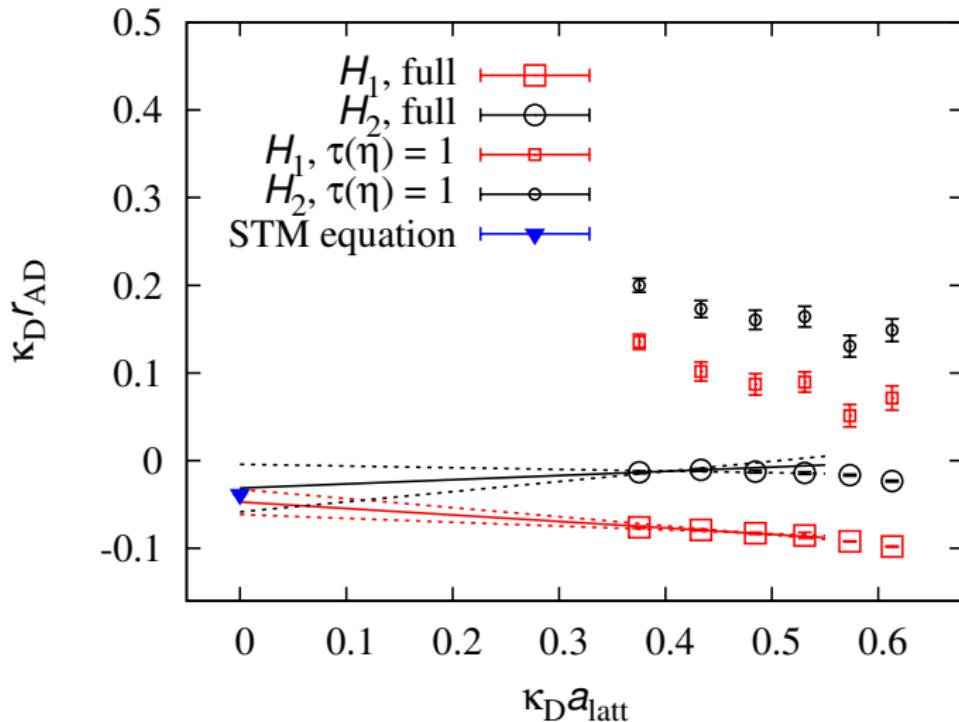
calculation by S. Bour, D. Lee, U.-G. Meißner

Corrected atom-dimer results



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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.

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Thanks for your attention!