

Composite particles on the lattice

Sebastian König

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

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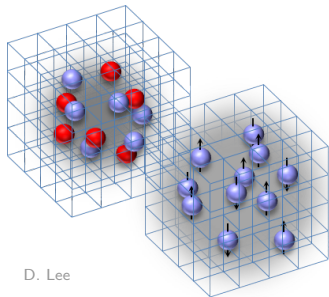
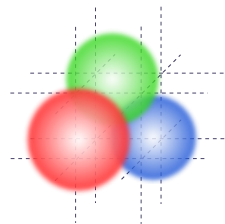
- **Introduction**
- **Part I –**
Mass shift of bound states with angular momentum
[arXiv:1103.4468](#), [1109.4577](#)
- **Part II –**
Topological factors in scattering systems
[arXiv:1107.1272](#)
- **Summary**

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



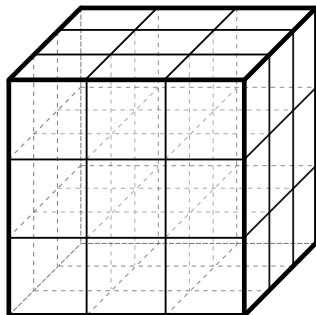
D. Lee

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!

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

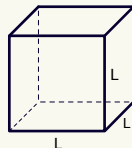
$$p = p(E(L))$$

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

Bound states in boxes

The box

- periodic finite volume
- cube of size L^3



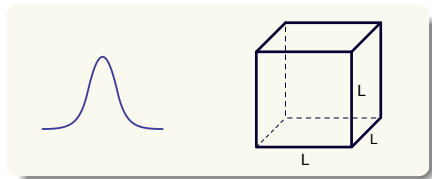
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The bound states

- 2-body bound states
- wavefunction ψ



binding momentum κ \longleftrightarrow intrinsic length scale

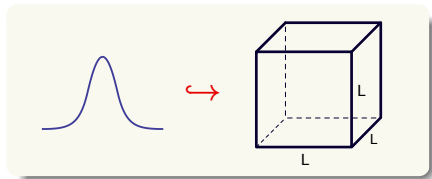
Bound states in boxes

The box

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binding momentum κ \longleftrightarrow intrinsic length scale

The finite volume changes the properties of the system!

Part I

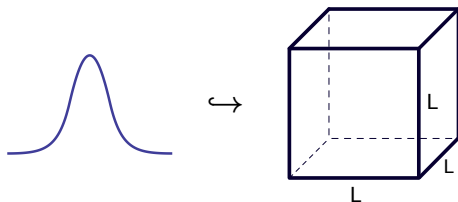
Mass shift of bound states with angular momentum

Starting point

S-wave bound state

Lüscher (1986)

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

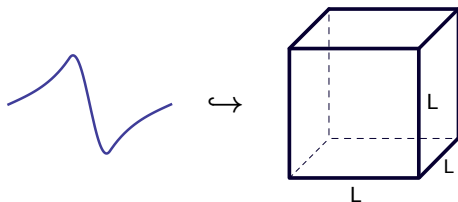


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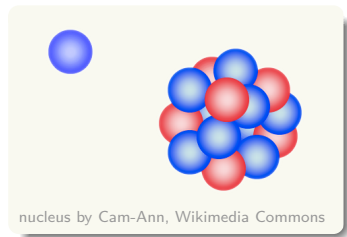


What's the the result for states with angular momentum?

Why care about higher partial waves?

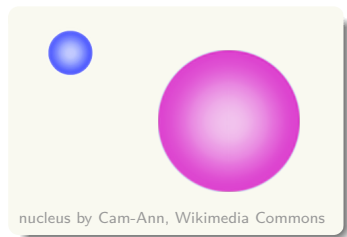
Halo nuclei

- single nucleon weakly bound to a tight core



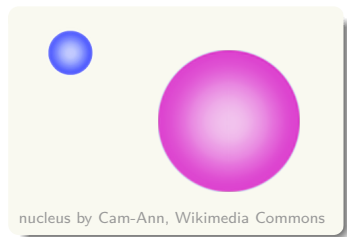
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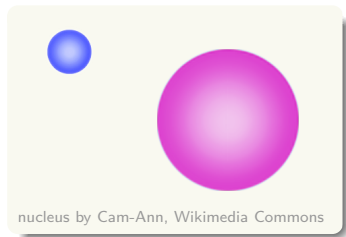


Halo-EFT

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

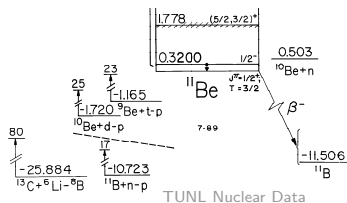
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Halo-EFT

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Example

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

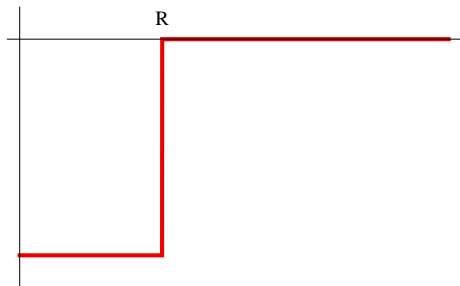
Schrödinger equation

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

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

finite-range interaction:

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



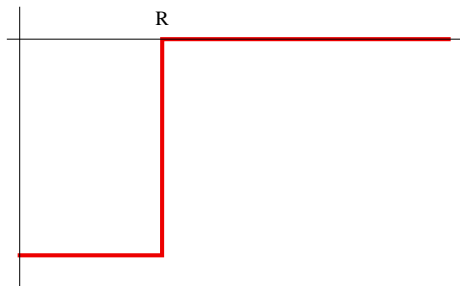
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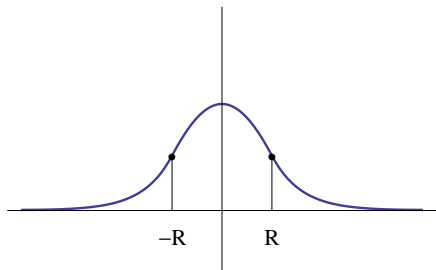
Radial Schrödinger equation

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

Asymptotic wavefunction

Radial Schrödinger equation

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \cancel{2\mu V(r)} - \kappa^2 \right) u_\ell(r) = 0 \text{ for } r > R$$



Asymptotic wavefunction

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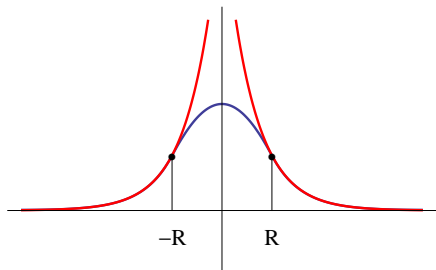
$$\rightsquigarrow u_\ell(r) = i^\ell \gamma \hat{h}_\ell^+(i\kappa r)$$

Riccati-Hankel functions

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

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

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



Periodic finite volume

Periodic boundary conditions

→ infinitely many copies of the potential

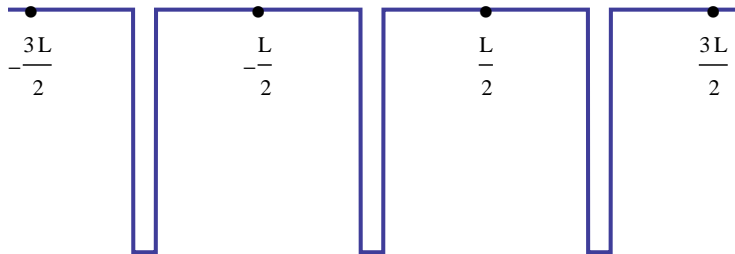
$$V_L(\mathbf{r}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(\mathbf{r} + \mathbf{n}L) \quad , \quad L \gg R$$

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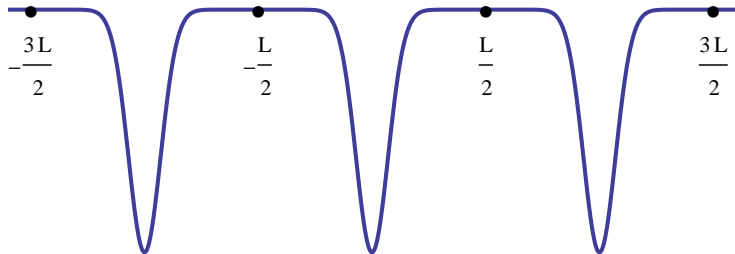
$$V(r) = V_0 \theta(R - r)$$

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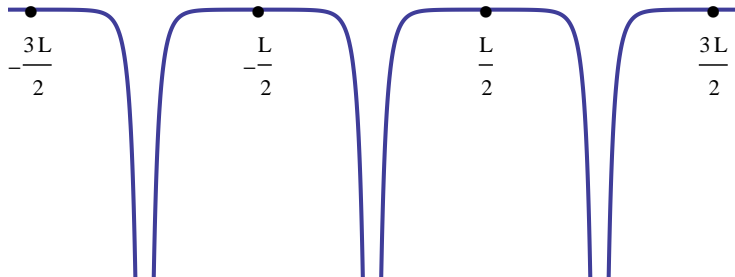
$$V(r) = V_0 \exp(-r^2/R^2)$$

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$$V(r) = V_0 \frac{\exp(-r/R)}{r}$$

Mass shift

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

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

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

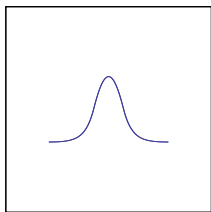
$$\Delta m_B = \frac{\langle \psi | \eta \rangle}{\langle \psi_0 | \psi_0 \rangle} = \sum_{|\mathbf{n}|=1} \int d^3r \psi_B^*(\mathbf{r}) V(\mathbf{r}) \psi_B(\mathbf{r} + \mathbf{n}L) + \mathcal{O}(e^{-\sqrt{2}\kappa L})$$

Overlap integral

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

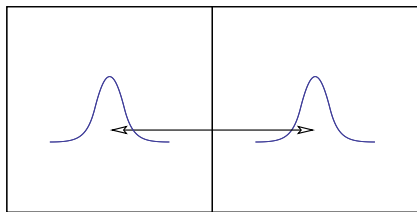
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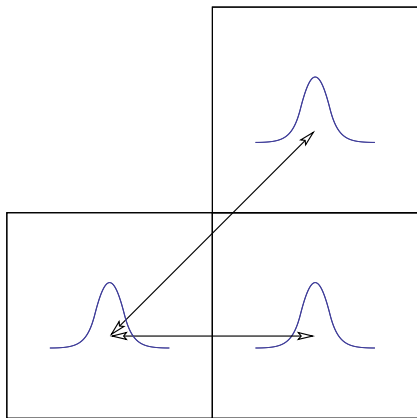
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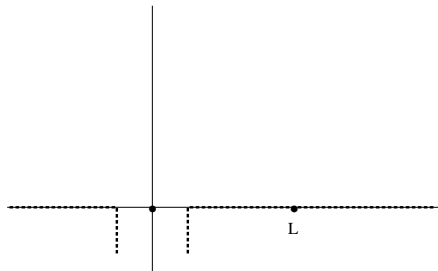
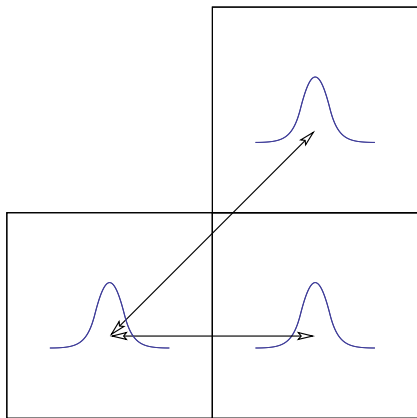
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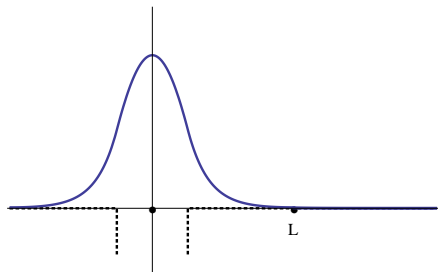
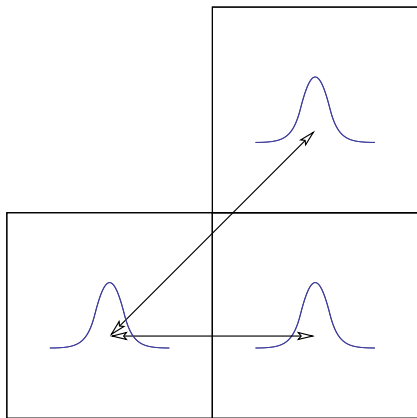
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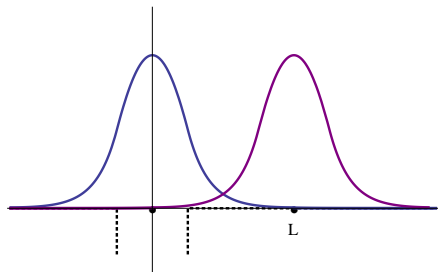
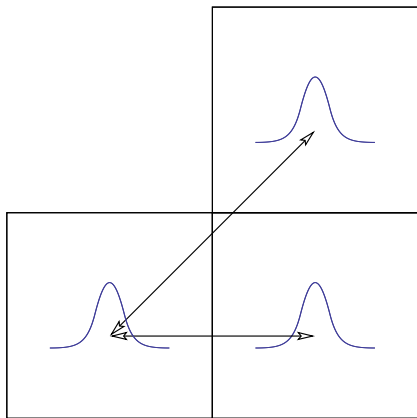
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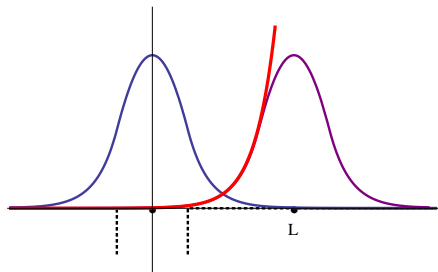
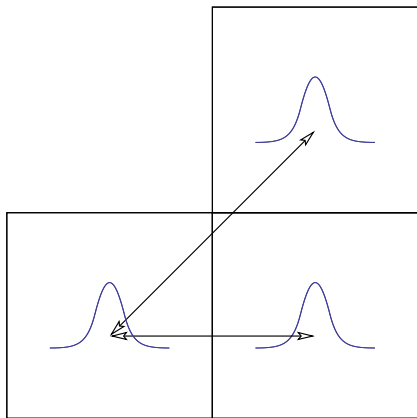
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S-wave result

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

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

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

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S-waves

sum just yields a factor six. . .

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

P-wave result

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

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

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$$\begin{aligned} \frac{\partial}{\partial z} \left[\frac{e^{-\kappa r}}{r} \right] &= \frac{\partial r}{\partial z} \frac{\partial}{\partial r} \left[\frac{e^{-\kappa r}}{r} \right] \\ &= \frac{z}{r} \frac{-\kappa r e^{-\kappa r} - e^{-\kappa r}}{r^2} = \cos \theta \left[\frac{e^{-\kappa r}}{r} \right] \left(-\kappa - \frac{1}{r} \right) \end{aligned}$$

P-wave result

$$\Delta m_B \sim \sum_{|\mathbf{n}|=1} \int d^3r \frac{1}{2\mu} [\Delta_r - \kappa^2] \psi_B^*(\mathbf{r} - \mathbf{n}L) \frac{\partial}{\partial z} \left[\frac{e^{-\kappa r}}{r} \right] + \dots$$

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Lemma

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

Lemma

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

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

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

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

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

Lüscher 1991

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$$\Delta m_B \sim \sum_{|\mathbf{n}|=1} \int d^3r \frac{1}{2\mu} [\Delta_r - \kappa^2] \psi_B^*(\mathbf{r} - \mathbf{n}L) R_\ell^m \left(-\frac{1}{\kappa} \nabla_r \right) \left[\frac{e^{-\kappa r}}{r} \right] + \dots$$

P-wave result

$$\Delta m_B \sim \sum_{|\mathbf{n}|=1} \int d^3r \frac{1}{2\mu} [\Delta_r - \kappa^2] \psi_B^*(\mathbf{r} - \mathbf{n}L) \frac{\partial}{\partial z} \left[\frac{e^{-\kappa r}}{r} \right] + \dots$$

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

$$\begin{aligned} \frac{\partial}{\partial z} \left[\frac{e^{-\kappa r}}{r} \right] &= \frac{\partial r}{\partial z} \frac{\partial}{\partial r} \left[\frac{e^{-\kappa r}}{r} \right] \\ &= \frac{z}{r} \frac{-\kappa r e^{-\kappa r} - e^{-\kappa r}}{r^2} = \cos \theta \left[\frac{e^{-\kappa r}}{r} \right] \left(-\kappa - \frac{1}{r} \right) \end{aligned}$$

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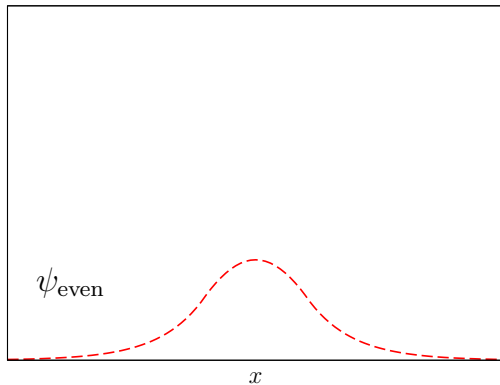
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P-waves

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

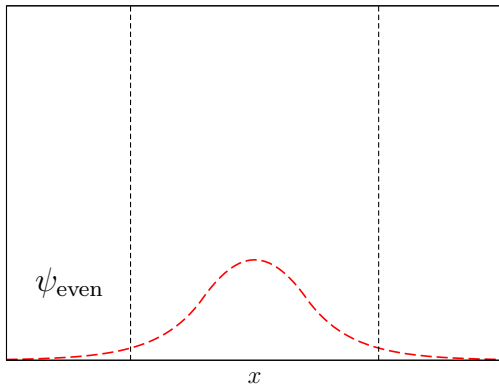
Mass shift for P-wave states exactly reversed compared to S-waves!

Sign of the mass shift



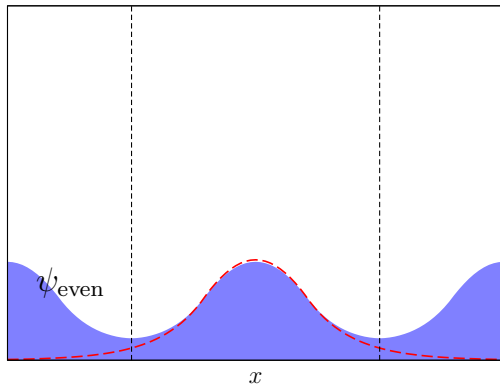
$$\Delta m_B < 0$$

Sign of the mass shift



$$\Delta m_B < 0$$

Sign of the mass shift

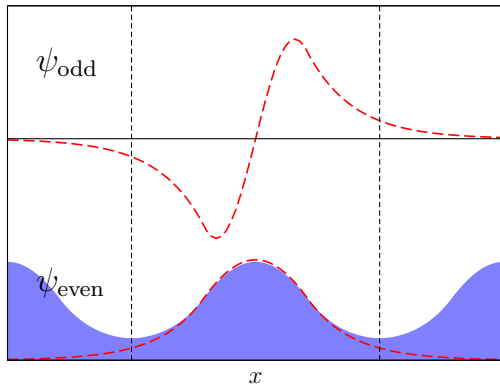


$$\Delta m_B < 0$$

even parity \rightarrow WF profile relaxed \rightarrow less curvature

\rightsquigarrow **more deeply bound**

Sign of the mass shift



$$\Delta m_B > 0$$

$$\Delta m_B < 0$$

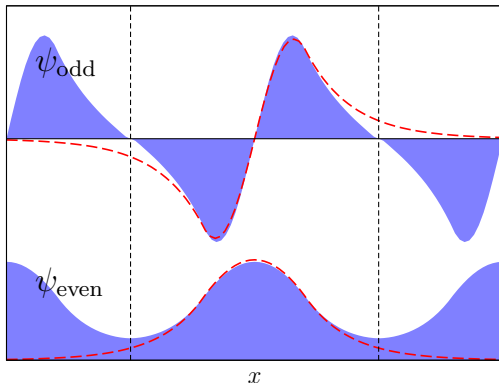
even parity \rightarrow WF profile relaxed \rightarrow less curvature

\rightsquigarrow **more deeply bound**

Sign of the mass shift

odd parity \rightarrow WF profile compressed \rightarrow more curvature

\rightsquigarrow **less bound**



$$\Delta m_B > 0$$

$$\Delta m_B < 0$$

even parity \rightarrow WF profile relaxed \rightarrow less curvature

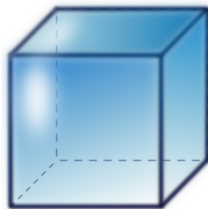
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Broken symmetry

The finite volume breaks the symmetry of the system



rot. group $SO(3)$



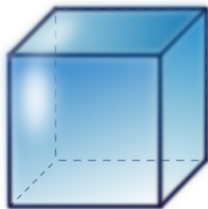
cubic group O

Broken symmetry

The finite volume breaks the symmetry of the system



rot. group $SO(3)$



cubic group O

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

$O \rightarrow 5$ irred. representations

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

calculate mass shift using

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

General result

After integrating by parts, we have

$$\Delta m_B^{(\ell,m)} = (-1)^{\ell+1} \cdot \frac{2\pi\gamma}{\mu} \sum_{|\mathbf{n}|=1} R_\ell^m \left(-\frac{1}{\kappa} \nabla_r \right) \psi_{B,(\ell,m)}^*(\mathbf{r}) \Big|_{\mathbf{r}=\mathbf{n}L} + \dots$$

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General formula

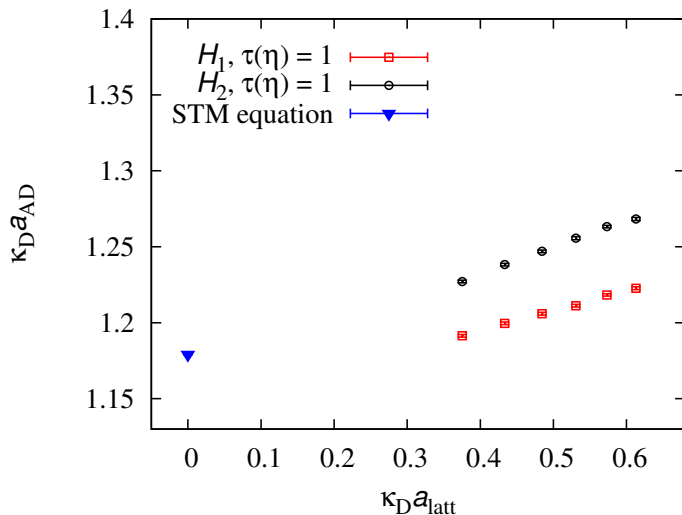
$$\Delta m_B^{(\ell,\Gamma)} = \alpha \left(\frac{1}{\kappa L} \right) \cdot |\gamma|^2 \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}(e^{-\sqrt{2}\kappa L})$$

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

Part II

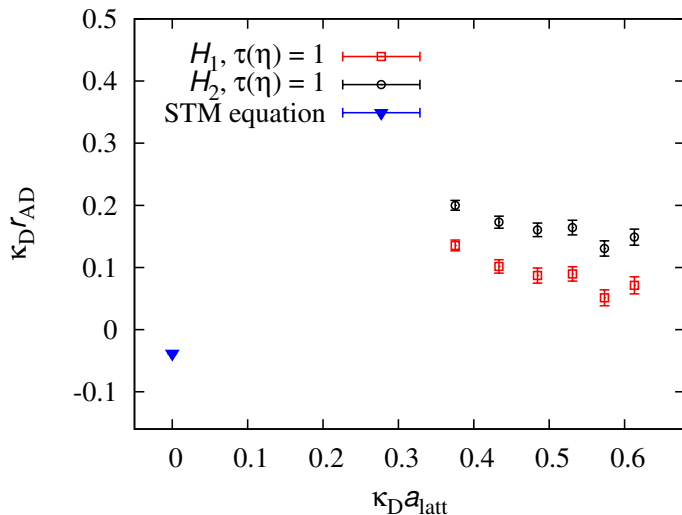
Topological factors in scattering systems

Motivation: atom-dimer scattering



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

Motivation: atom-dimer scattering

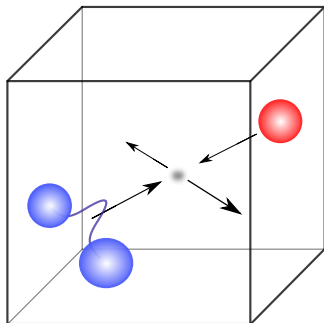


calculation by S. Bour, D. Lee, U.-G. Meißner

Atom-dimer scattering

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

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



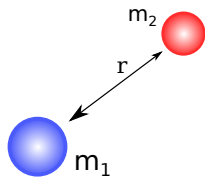
A part of $E(L)$ is due to the binding of the dimer!

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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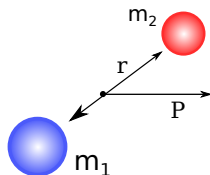
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Now

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

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



Bound states in moving frames

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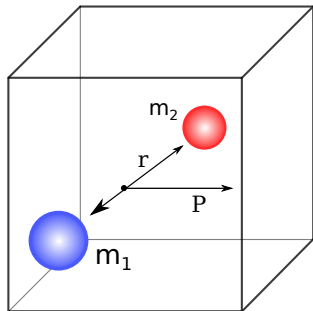
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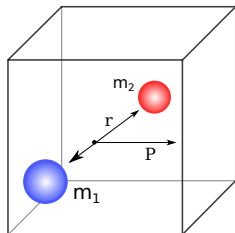
\mathbf{P} = center-of-mass momentum

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



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

Twisted boundary conditions

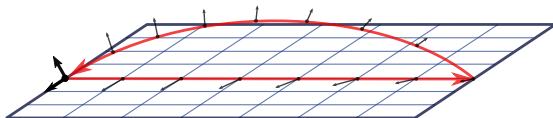


Now $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ has to be periodic!

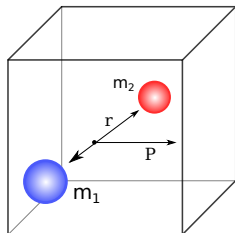
$$\Psi(\mathbf{r}_1 + \mathbf{n}L, \mathbf{r}_2) = e^{i\mathbf{P} \cdot \mathbf{R}} e^{i\alpha L \mathbf{P} \cdot \mathbf{n}} \psi(\mathbf{r} + \mathbf{n}L) = \Psi(\mathbf{r}_1, \mathbf{r}_2)$$

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

“twisted boundary conditions”



Twisted boundary conditions

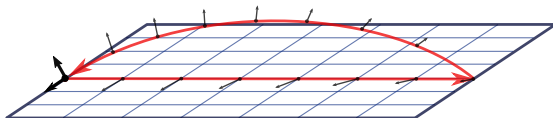


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“twisted boundary conditions”



Question

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

Mass shift for twisted boundary conditions

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

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

S-wave result

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

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The mass shift vanishes in certain moving frames!

→ Davoudi & Savage, arXiv:1108.5371

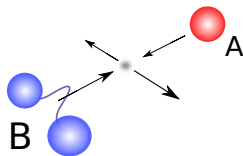
Scattering states

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

Scattering wavefunction

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

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



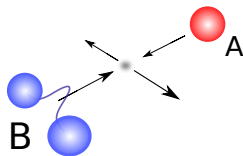
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Topological volume factor

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

Topological correction factors

Topological volume factor

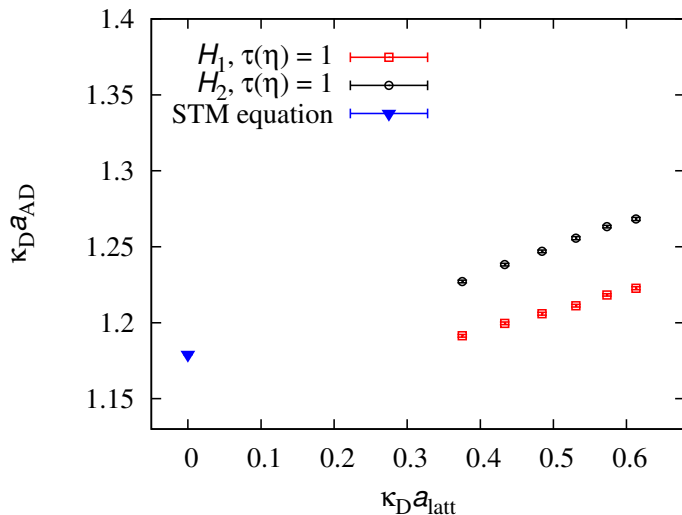
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Final result:

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

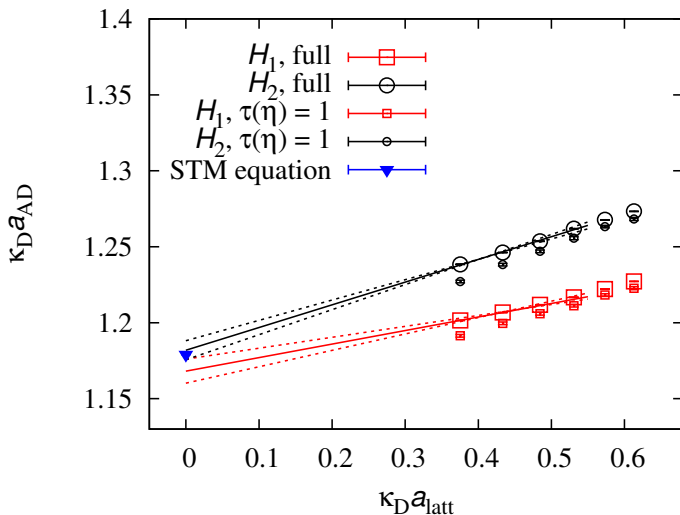
Subtract this correction from measured energy levels! \Rightarrow

Corrected atom-dimer results

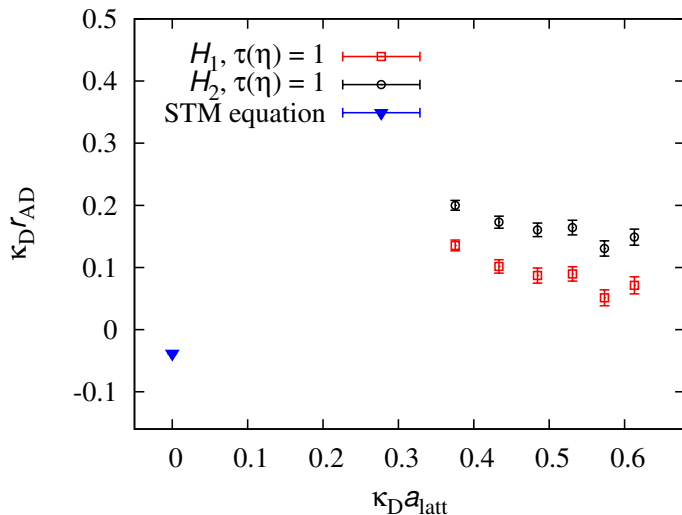


calculation by S. Bour, D. Lee, U.-G. Meißner

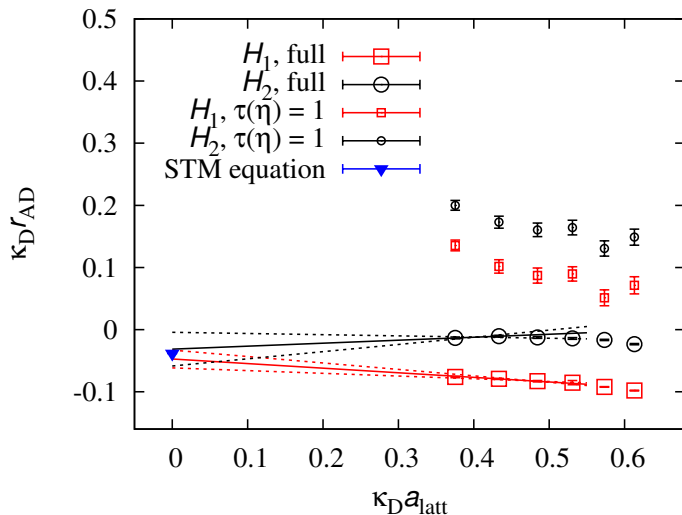
Corrected atom-dimer results



Corrected atom-dimer results



Corrected atom-dimer results



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 with simple numerical calculations.
- Mass shift of composite particles has to be corrected for in scattering calculations.

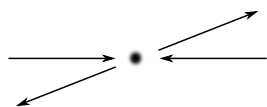
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Thanks for your attention!

Spares

Asymptotic normalization constant



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

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

Effective range expansion

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

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

- shallow bound states: $p = i\kappa \rightarrow 0$

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

Overlap integral details (I)

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 details (II)

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

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

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

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

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

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

Trace formula

Insert asymptotic form once more to get:

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

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

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

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

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

Mass shift for cubic group states

- 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

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

↓

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

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

Cubic group splitting for $\ell = 2$

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

T_2 representation

$$|T_2^+, 2; 1\rangle = -\frac{1}{\sqrt{2}} (|2, -1\rangle + |2, 1\rangle)$$

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

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

E representation

$$|E^+, 2; 1\rangle = |2, 0\rangle$$

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

Mass shift up to $\ell = 3$

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

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

Basis polynomials

Solid harmonics

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

$$R_0^0 \sim 1$$

$$R_1^{-1} \sim x - iy \quad , \quad R_1^0 \sim z \quad , \quad R_1^{+1} \sim x + iy$$

$$R_2^{-2} \sim (x - iy)^2 \quad , \quad R_2^{-1} \sim (x - iy)z \quad , \quad R_2^0 \sim 2z^2 - x^2 - y^2 \quad , \quad \dots$$

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

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

where

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

Then

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

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

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

Numerical checks (I)

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

Lattice Hamiltonian

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

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

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



Numerical checks (II)

i2j

- 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

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

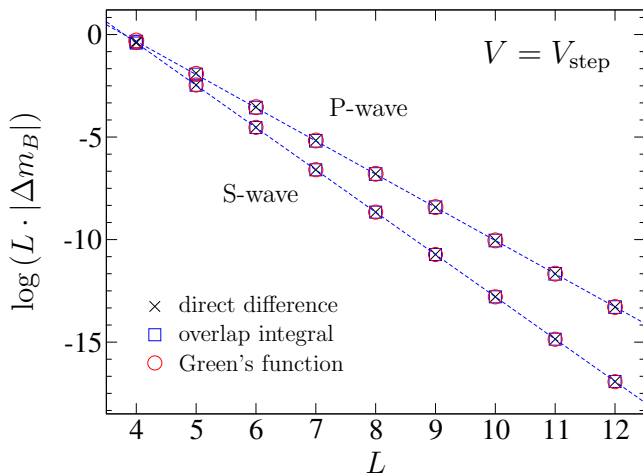
to reduce discretization errors!

Lattice Green's function

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

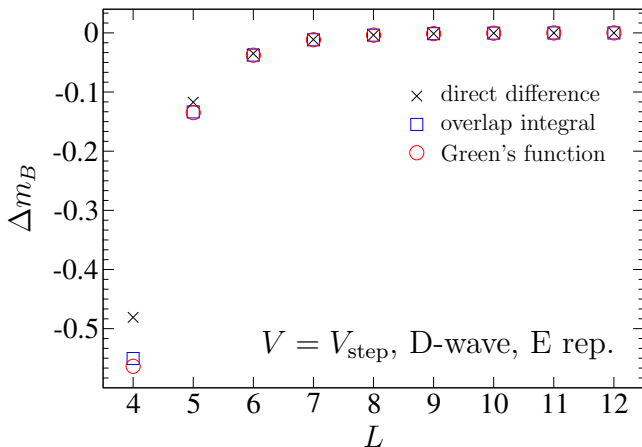
Numerical checks (III)

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



Numerical checks (IV)

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



Numerical checks (V)

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

