Volume Dependence of N-Body Bound States

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in collaboration with Dean Lee

INT Workshop 18-70W, University of Washington

Seattle, WA

February 9, 2018

arXiv:1701.00279 [hep-lat], to appear in PLB

European Research Council
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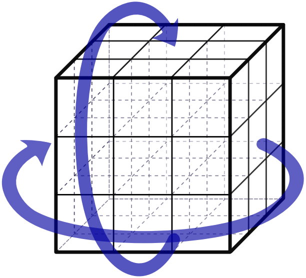
Finite periodic boxes



- physical system enclosed in **finite volume (box)**
- typically used: **periodic boundary conditions**

$\rightsquigarrow$ **volume-dependent energies**

Lüscher formalism

Physical properties encoded in the L-dependent energy levels!

- infinite-volume S-matrix governs discrete finite-volume spectrum
- PBC natural for lattice calculations. . .
- . . . but can also be implemented with other methods

Overview of recent results

1. **Two-body sector**
   - nonzero angular momentum
     SK, Lee, Hammer, PRL **107** 112001 (2011); Annals Phys. **327** 1450 (2011)
   - moving frames (twisted boundary conditions)
     Davoudi, Savage, PRD **84** 114502 (2011)
   - coupled channels, spin, resonances, ...
     e.g., Döring *et al.*, Eur. Phys. J. A **48** 114 (2012); Briceño *et al.*, Phys. Rev. D **89** 074507 (2014)
   - ...

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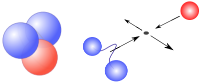
2. **Three-body sector**



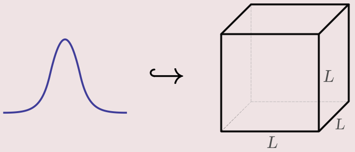
   - Efimov physics (bosons, triton) in finite box
     Kreuzer+Hammer, PLB **673**, 260 (2008); **694**, 424(2011); Kreuzer+Grießhammer, EPJA **48** 93 (2012)
   - topological correction factors
     Bour, SK, Lee, Hammer, Meißner, PRD **84** 091503(R) (2011); Rokash *et al.*, JPG **41** 015105 (2014)
   - explicit result for three bosons at unitarity
     Meißner, Ríos, Rusetsky, PRL **114** 091602 (2015)
   - twisted boundary conditions
     Körber+Luu, PRC **93** 054002 (2016)
   - many formal results (quantization condition)
     Polejaeva+Rusetsky, EPJA **48** 67 (2012)
     Hansen+Sharpe, PRD **90** 116003 (2014), . . . , Briceño, Hansen, Sharpe, PRD **95** 074510 (2017)
     Hammer, Pang, Rusetsky, JHEP **1709** 109; JHEP **1710** 115 (2017)
     Mai+Döring, EPJA **53** 240 (2017)

Two-body review

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

binding momentum κ

$\leftrightarrow$ intrinsic length scale



Asymptotic wavefunction overlap

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

M. Lüscher, Commun. Math. Phys. **104** 177 (1986)

- for S-wave states, one finds $\Delta B(L) = -3\pi|\gamma|^2 \dfrac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$
- in general, the prefactor is a polynomial in $1/\kappa L$

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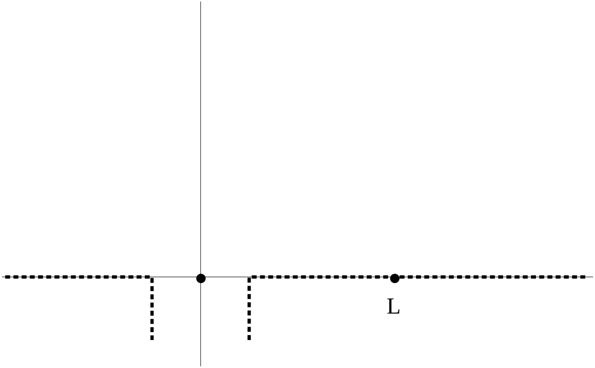

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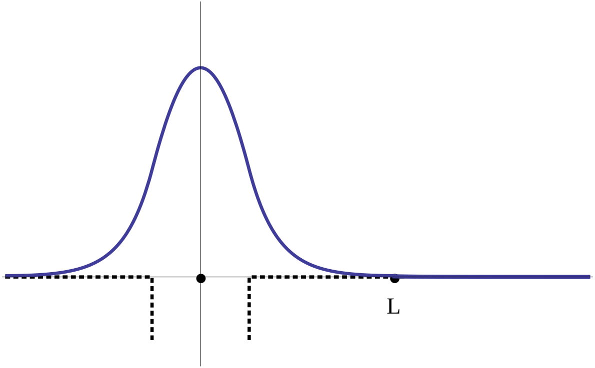

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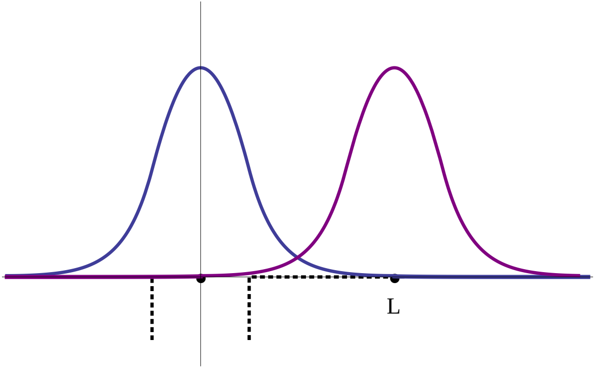

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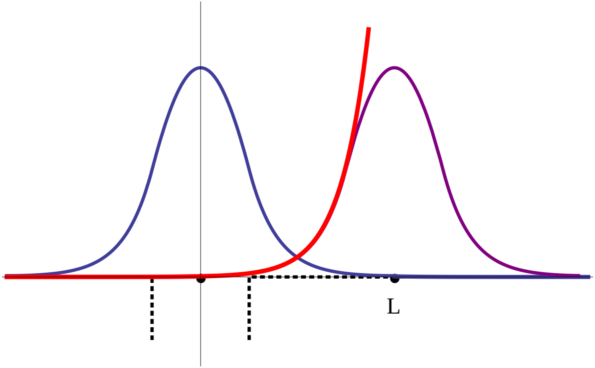

It's all determined by the tail!

Two-body review

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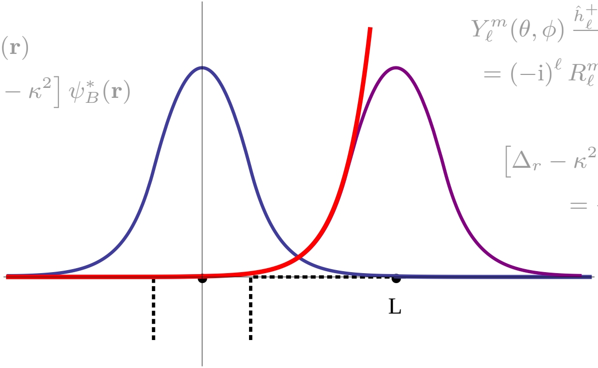
$$\psi_B^*(\mathbf{r}) V(\mathbf{r}) = \left[\Delta_r - \kappa^2\right] \psi_B^*(\mathbf{r})$$



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

$$\left[\Delta_r - \kappa^2\right] \frac{\mathrm{e}^{-\kappa r}}{r} = -4\pi\delta^{(3)}(\mathbf{r})$$

It's all determined by the tail!

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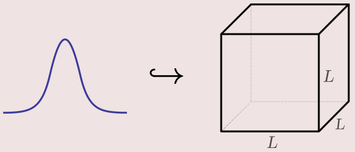

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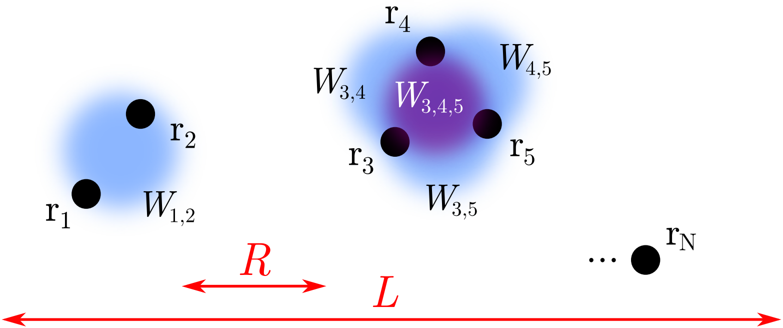
N-body setup

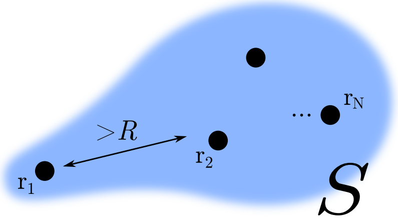
- 2- up to N-body interactions: $V_{1\cdots N}(\mathbf{r}_1,\cdots\mathbf{r}_N;\mathbf{r}'_1,\cdots\mathbf{r}'_N)=$
$$\sum_{i<j}W_{i,j}(\mathbf{r}_i,\mathbf{r}_j;\mathbf{r}'_i,\mathbf{r}'_j)1_{\not{i},\not{j}}+\sum_{i<j<k}W_{i,j,k}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k;\mathbf{r}'_i,\mathbf{r}'_j,\mathbf{r}'_k)1_{\not{i},\not{j},\not{k}}+\cdots$$
- can be local or nonlocal (as written above)
- all with finite range, set $R=\max\{R_{i,j},\cdots\}$, assume $L\gg R$



Cluster separation

1. **consider one particle (WLOG the first) separated from all others**

$\hookrightarrow S = \{(\mathbf{r}_1, \cdots \mathbf{r}_N) : |\mathbf{r}_1 - \mathbf{r}_i| > R \quad \forall i = 2, \cdots N\}$



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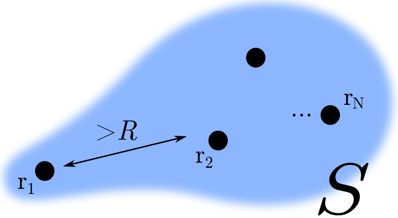

2. **look at Hamiltonian restricted to S:**

$$\hat{H}\big|_S = \sum_{i=2}^{N} \left[\hat{K}_i - \hat{K}^{\mathrm{CM}}_{2\cdots N} + \hat{V}_{2\cdots N}\right] + \hat{K}^{\mathrm{rel}}_{1|N-1}$$ no interaction $\hat{V}_{1\ldots}$!

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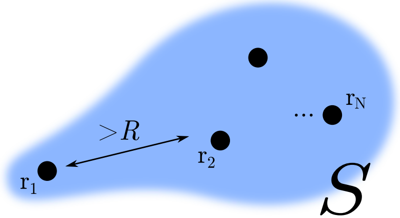

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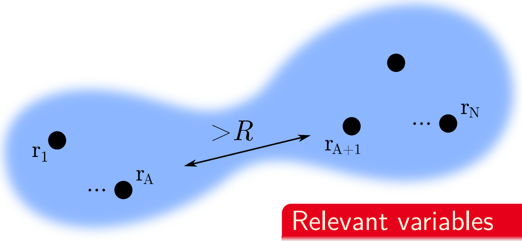
3. **separation ansatz:** $\Psi(\mathbf{r}_1, \cdots \mathbf{r}_N) = \sum_\alpha f_\alpha(\mathbf{r}_2, \cdots \mathbf{r}_N) g_\alpha(\mathbf{r}_{1|N-1})$

   - overall Schrödinger equation: $\hat{H}\Psi\big|_S = -B_N \Psi\big|_S$
   - lowest f_0 is eigenstate of sub-Hamiltonian with energy $-B_{N-1}$
   - $\rightsquigarrow$ g_0 is Bessel function with scale set by $B_N - B_{N-1}$

General case

4. **now separate A particles from the rest and follow the same steps**



Relevant variables

$$\mathbf{r}_{A|N-A} = \frac{m_1\mathbf{r}_1+\cdots+m_A\mathbf{r}_A}{m_1+\cdots+m_A} - \frac{m_{A+1}\mathbf{r}_{A+1}+\cdots+m_N\mathbf{r}_N}{m_{A+1}+\cdots+m_N}$$

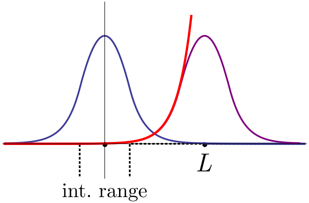
$$\frac{1}{\mu_{A|N-A}} = \frac{1}{m_1+\cdots+m_A} + \frac{1}{m_{A+1}+\cdots+m_N}$$

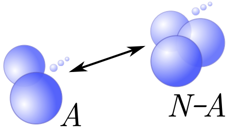
$$\kappa_{A|N-A} = \sqrt{2\mu_{A|N-A}(B_N - B_A - B_{N-A})}$$

$$\psi_N^B(\mathbf{r}_1,\cdots\mathbf{r}_N) \propto \psi_A^B(\mathbf{r}_1,\cdots\mathbf{r}_A)\psi_{N-A}^B(\mathbf{r}_{A+1},\cdots\mathbf{r}_N) \times \left(\kappa_{A|N-A}r_{A|N-A}\right)^{1-d/2} K_{d/2-1}\left(\kappa_{A|N-A}r_{A|N-A}\right)$$

<u>note:</u> this assumes both clusters to be bound

volume dependence $\leftrightarrow$ overlap of asymptotic wave functions





$$\kappa_{A|N-A} = \sqrt{2\mu_{A|N-A}(B_N - B_A - B_{N-A})}$$

Volume dependence of N-body bound state

$$\Delta B_N(L) \propto (\kappa_{A|N-A} L)^{1-d/2} \, K_{d/2-1}(\kappa_{A|N-A} L)$$

$$\sim \exp\left(-\kappa_{A|N-A} L\right) / L^{(d-1)/2} \quad \text{as} \quad L \to \infty$$

(L = box size, d no. of spatial dimensions, K_n = Bessel function)

SK and D. Lee, arXiv:1701.00279 [hep-lat]

- channel with smallest $\kappa_{A|N-A}$ determines asymptotic behavior

Analytical examples

Three bosons at unitarity

- two-body interaction with zero range and infinite scattering length
- $\Delta B_3(L) \propto (\kappa_{1|2}L)^{-1/2} K_{1/2}(\kappa_{1|2}L) P(\kappa_{1|2}L)$

$$\sim \exp\left(-\sqrt{\frac{4mB_3}{3}}L\right)\left(\sqrt{\frac{4mB_3}{3}}L\right)^{-1} P(\kappa_{1|2}L)$$

- same exp. dependence as exact result ✓ Meißner *et al.*, PRL **114** 091602 (2015)
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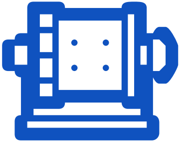
N particles with N-body interaction only

- spinless N-particle bound state with only an N-particle interaction
  $\rightsquigarrow$ no bound cluster substructures!
- $\psi(\mathbf{r}_1, \cdots) \propto (\kappa_{1|N-1} r_{1|N-1})^{1-d(N-1)/2} K_{d(N-1)/2-1}(\kappa_{1|N-1} r_{1|N-1})$
- again agrees with prediction ✓, read off $P(x) = x^{-d(N-2)/2}$

Generator code



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- numerical code to check derived volume dependence
- published with paper, using "scientific copyleft" terms
- fully general: arbitrary dimensions, number of particles
- automatic code generation for each specific system

setup $\longrightarrow$ **Haskell $\longrightarrow$ MATLAB/Octave** $\longrightarrow$ output

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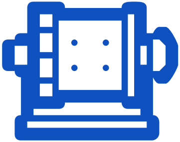

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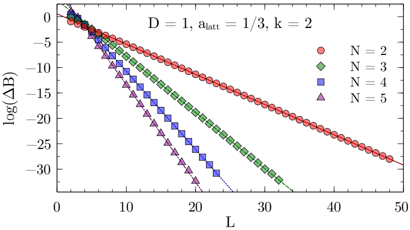
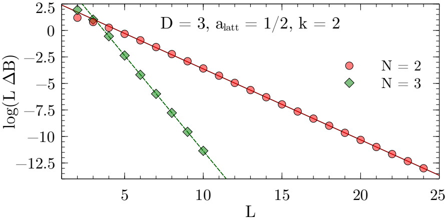
A case for functional programming

- **tell computer what you want, not how to calculate it**
- no loops, only recursion $\rightsquigarrow$ ideal for certain problems
- no mutable variables, only functions
- Haskell compiles to maschine code, can be linked with C/C++
- (NB: full-thruster Mathematica uses functional techniques as well)

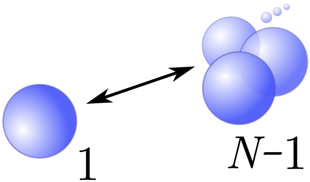
Numerical results





$\hookrightarrow$ **straight lines** $\leftrightarrow$ **excellent agreement with prediction**

N	B_N	$L_{\text{min}} \ldots L_{\text{max}}$	κ_{fit}	$\kappa_{1\|N-1}$
$d = 1,\ V_0 = -1.0,\ R = 1.0$				
2	0.356	$20 \ldots 48$	0.59536(3)	0.59625
3	1.275	$15 \ldots 32$	1.1062(14)	1.1070
4	2.859	$12 \ldots 24$	1.539(3)	1.541
5	5.163	$12 \ldots 20$	1.916(21)	1.920
$d = 3,\ V_0 = -5.0,\ R = 1.0$				
2	0.449	$15 \ldots 24$	0.6694(2)	0.6700
3	2.916	$4 \ldots 14$	1.798(3)	1.814

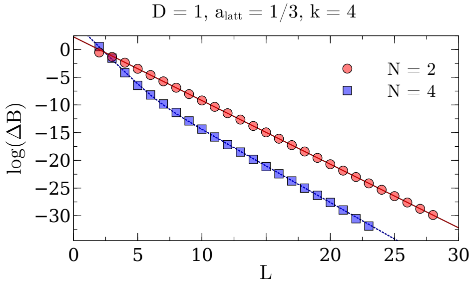


More complicated example

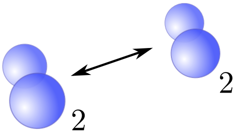
Typically, one exponential dominates, but not necessarily:

Setup

1. attractive two-body force $\rightsquigarrow B_2 < 0$
2. add repulsive three-body force
3. add attractive four-body force $\rightsquigarrow B_4 < 0$



$\kappa_{\text{fit}} = 1.318 \qquad \kappa_{2|2} = 1.282$



- **three-body system unbound**
- asymptotic slope from $2|2$ separation

Finite-volume shift and ANC

recall: $\psi_N^B(\mathbf{r}_1, \cdots \mathbf{r}_N) \propto \psi_A^B(\cdots)\psi_{N-A}^B(\cdots) \times \psi_{\text{asympt}}(r_{A|N-A})$

$$\psi_{\text{asympt}}(r_{A|N-A}) = \gamma \sqrt{\frac{2\kappa_{A|N-A}}{\pi}} (r_{A|N-A})^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} r_{A|N-A})$$

γ = asymptotic normalization coefficient (ANC)

Finite-volume energy shift

$$\Delta B_N(L) = \frac{(-1)^{\ell+1}\sqrt{\frac{2}{\pi}} f(d) |\gamma|^2}{\mu_{A|N-A}} \kappa_{A|N-A}^{2-d/2} L^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} L)$$

$\hookrightarrow$ **extract ANC from volume dependence**

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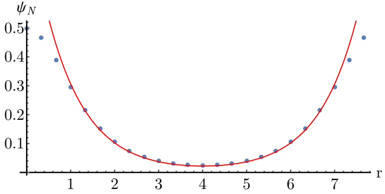


for comparison, extract ANC from finite-volume wavefunction

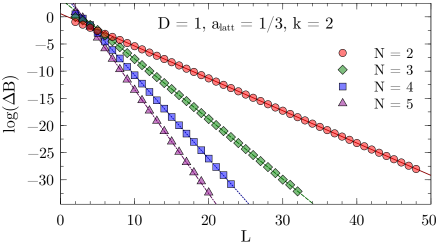
(mind the PBC)

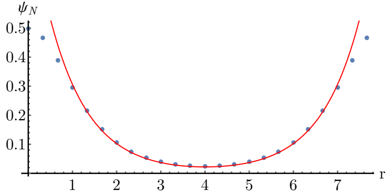
ANC comparison

Compare ANC result to direct extrapolation from wavefunction:

N	B_N	L_{max}	$\lvert\gamma\rvert_{\text{FV}}$	$\lvert\gamma\rvert_{\text{WF}}$
$d = 1,\ V_0 = -1.0,\ R = 1.0$				
2	0.356	48	0.8652(4)	0.8627(4)
3	1.275	32	1.650(27)	1.638(16)
4	2.859	24	2.54(6)	2.56(8)
5	5.163	20	3.65(62)	3.63(18)
$d = 2,\ V_0 = -1.5,\ R = 1.5$				
2	0.338	36	1.923(2)	1.921(9)
3	1.424	24	5.204(4)	5.24(2)
4	3.449	14	11.2(4)	10.99(4)
$d = 3,\ V_0 = -5.0,\ R = 1.0$				
2	0.449	24	1.891(3)	1.89(1)
3	2.916	14	7.459(97)	7.83(11)

$\hookrightarrow$ **good agreement ✔**

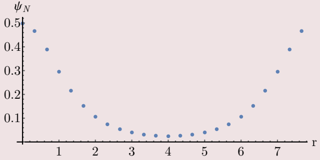


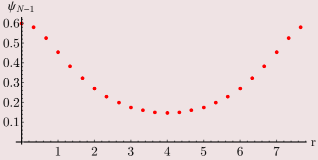


Single-volume extrapolation

Strategy

1. extract N-body and $(N-A)$-body wavefunctions





- look along a given fixed direction, account for periodic boundary
- divide $\psi_N(r)$ by $\psi_{N-1}(0)$ to adjust normalization

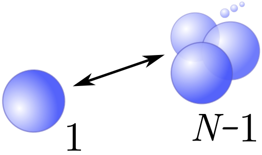
2. get ANC from ratio of tail to known asymptotic form

3. use $\Delta B_N(L) = \frac{\pm\sqrt{\frac{2}{\pi}}f(d)|\gamma^2|}{\mu_{A|N-A}}\kappa_{A|N-A}^{2-d/2}L^{1-d/2}K_{d/2-1}(\kappa_{A|N-A}L)$

- sign determined by angular momentum (or leading parity)
- $\kappa_{A|N-A}$ extracted as part of ANC fit, initial value from energies at L

Single-volume extrapolation

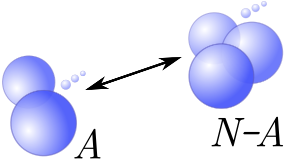
N	B_N	L	$\Delta B_N(L)_{\text{estimate}}$	$\Delta B_N(L)_{\text{actual}}$
		$d=1,\ V_0=-1.0,\ R=1.0$		
2	0.356	8	$-1.32(2)\times10^{-2}$	-1.42×10^{-2}
3	1.275	8	$-3.9(4)\times10^{-3}$	-3.75×10^{-3}
4	2.859	8	$-4.3(7)\times10^{-4}$	-4.69×10^{-4}
5	5.163	8	$-0.6(2)\times10^{-4}$	-0.64×10^{-4}
		$d=2,\ V_0=-1.5,\ R=1.5$		
2	0.338	8	$-2.5(6)\times10^{-2}$	-2.84×10^{-2}
3	1.424	8	$-5.8(6)\times10^{-3}$	-4.99×10^{-3}
4	3.449	8	$-4.1(6)\times10^{-4}$	-4.01×10^{-4}
		$d=3,\ V_0=-5.0,\ R=1.0$		
2	0.356	8	$-1.3(3)\times10^{-2}$	-1.34×10^{-2}
3	2.916	8	$-6.2(6)\times10^{-5}$	-4.80×10^{-5}



- **overall good agreement with known actual energies !**
- uncertainty included fit error and variation of tail fit range
- in practice, noisy data will give larger uncertainties

Summary and outlook

- leading volume dependence known for **arbitrary bound states**
- reproduces known results, **checked numerically**
- calculate ANCs, **single-volume extrapolations possible!**
- applications to lattice QCD, EFT, cold-atomic systems



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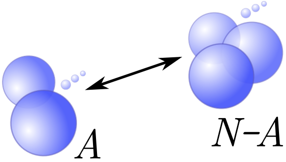

Things to do

- general derivation of power-law correction factors
- connection with / inspiration for general quant. conditions
- include Coulomb interaction
  $\hookrightarrow$ expect asymptotic behavior given by Whittaker function

The end

Thank you!

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