JÜLICH
FORSCHUNGSZENTRUM

Applying Twisted Boundary Conditions for Few-Body Nuclear Systems

C. Körber & T. Luu

12th, April 2016 | Christopher Körber | PhD Student | Forschungszentrum Jülich & University of Bonn

INT — Nuclear Physics from lattice QCD

Mitglied der Helmholtz-Gemeinschaft

Outline

- *Motivation*
- *Implementation*
- *Explanation*
- *Methodology*
- *Numerical Results*
  - *2-Body*
  - *3-Body*

Mitglied der Helmholtz-Gemeinschaft

Finite Volume (FV)

As a tool for

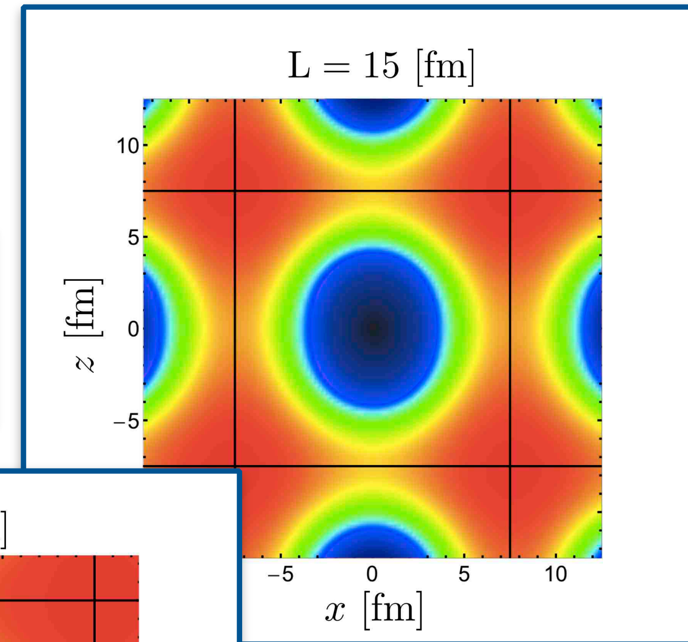
- **Non-perturbative physics**
  Evaluation of path integral
- **Many-body physics**
  Scalability of HMC algorithms
- **Physical finite systems**
  E.g. carbon nanotubes

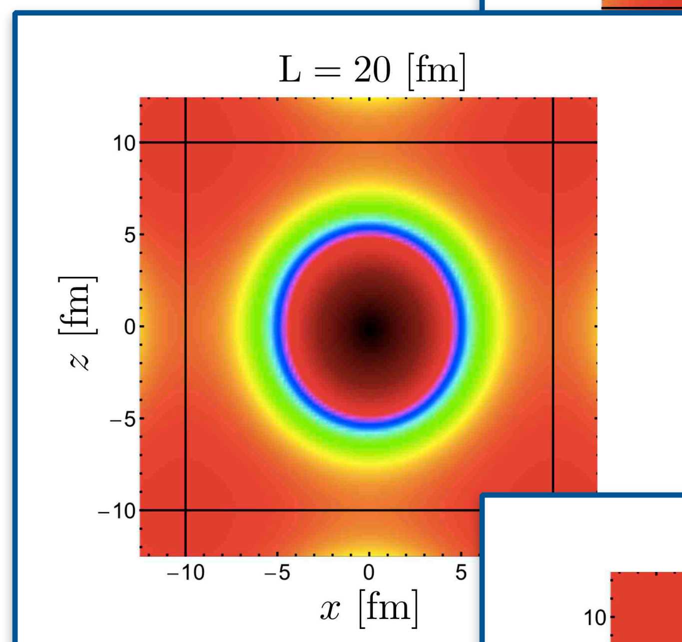
But…

- **Systematic "errors"…**
  … since observables depend on the volume (L)
- **Broken symmetries…**
  … since rotation symmetry is reduced to 'just' cubic rotation symmetry
- **Multiple calculations…**
  … at multiple volumes must be performed to extrapolate to infinite volume

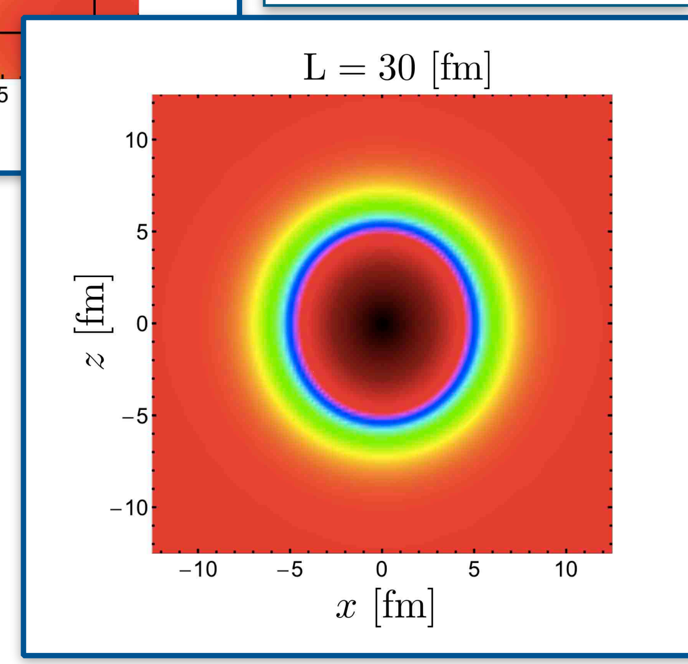
Can this be overcome?

Mass density of deuteron wave function at rest in different volumes





"Two-Nucleon Systems in a Finite Volume …", R. Briceno, Z. Davoudi, T. Luu, M. Savage [arXiv:1309.3556] Phys. Rev. **D88**



Mitglied der Helmholtz-Gemeinschaft

Twisted Boundaries

A 'knob' for reducing FV effects

Reduce FV effects by increasing volume

Bound states scale exponentially in volume…

$$\mathcal{O}(e^{-\lambda L})$$

… but the computational cost increases as well

$$\mathcal{O}\left(N_L^3 \times N_t\right)$$

Change the boundary conditions

Usually LQCD and NLEFT calculations utilize periodic boundary conditions (PBs)

$$\psi(\vec{r} + \vec{e}_i L) = \psi(\vec{r})$$

Anti-periodic boundary conditions

$$\psi(\vec{r} + \vec{e}_i L) = -\psi(\vec{r})$$

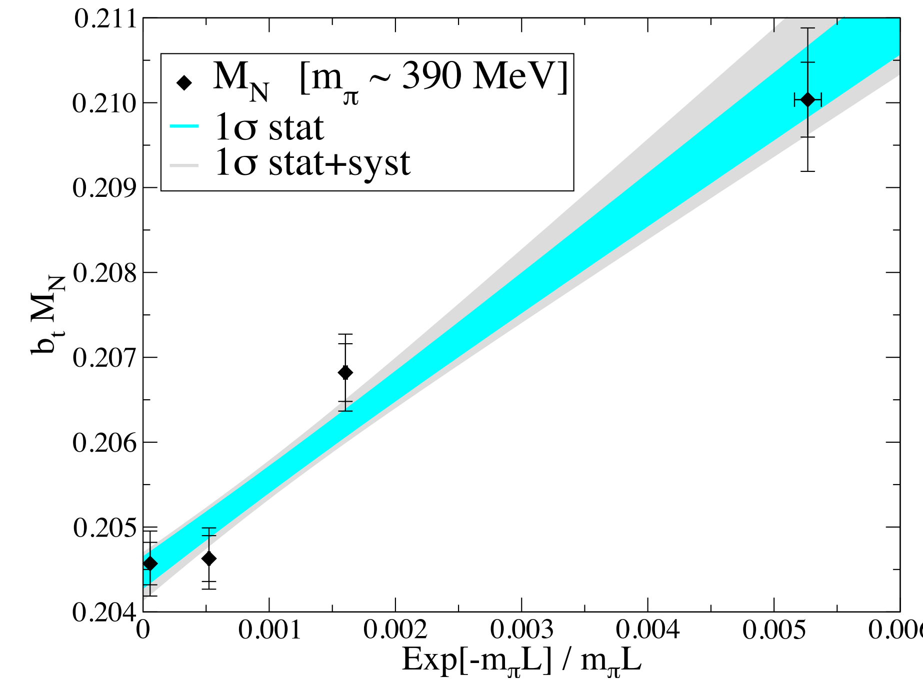
Twisted boundary conditions

$$\psi(\vec{r} + \vec{e}_i L) = e^{i\vec{\phi}\cdot\vec{e}_i}\psi(\vec{r})$$

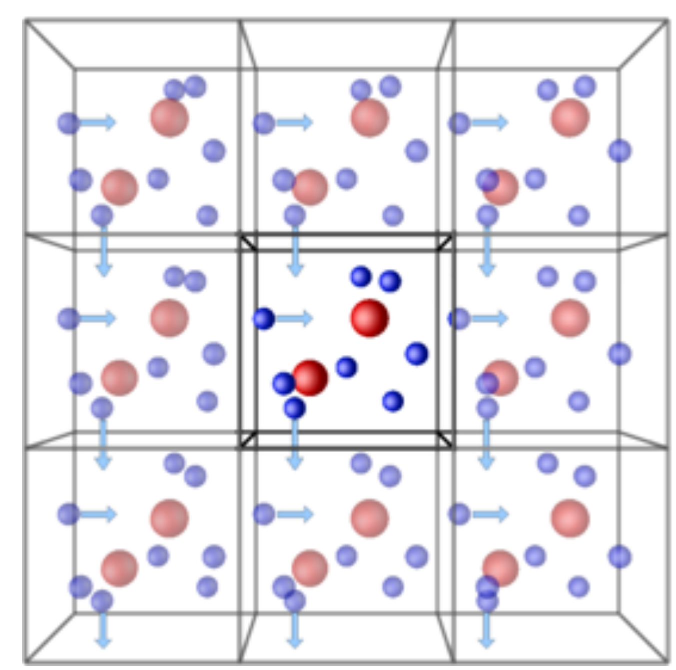
'i-Periodic':

$$e^{i\pi/2} = i$$

"…Volume Dependence of Light Hadron Masses", NPLQCD [arXiv:1104.4101], Phys.Rev. **D84**



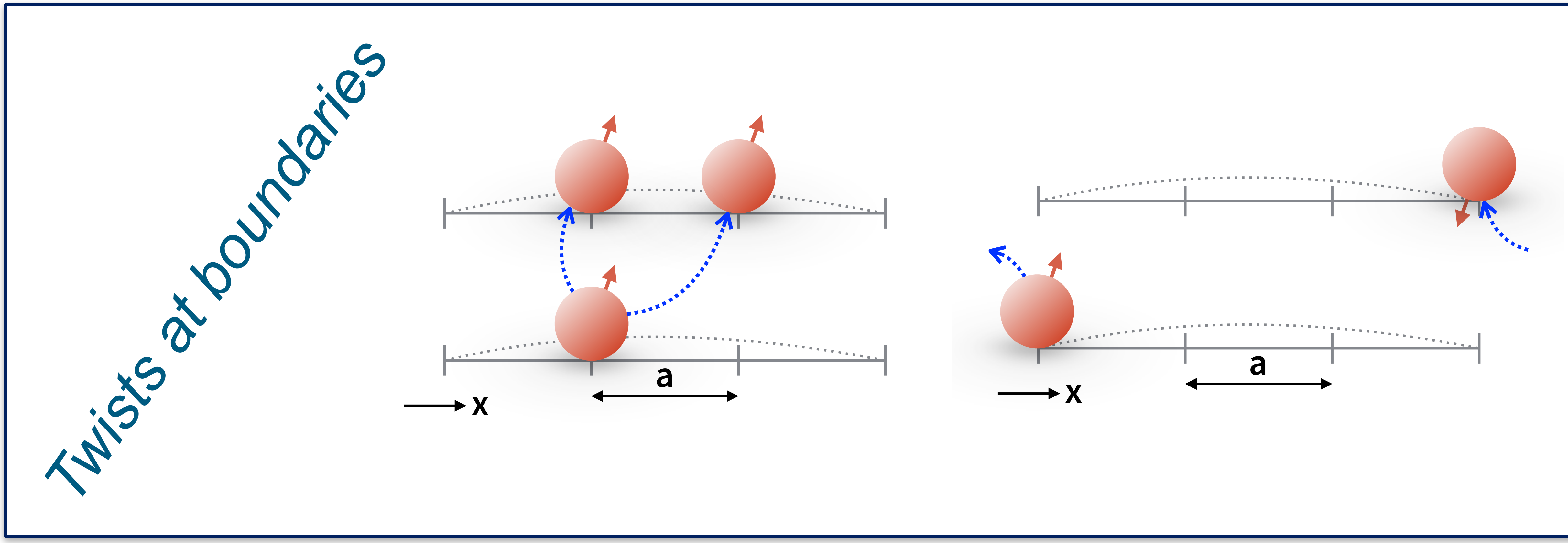
Nucleon mass volume (*L)* dependence.



isaacs.sourceforge

Mitglied der Helmholtz-Gemeinschaft

TBCs — Implementation

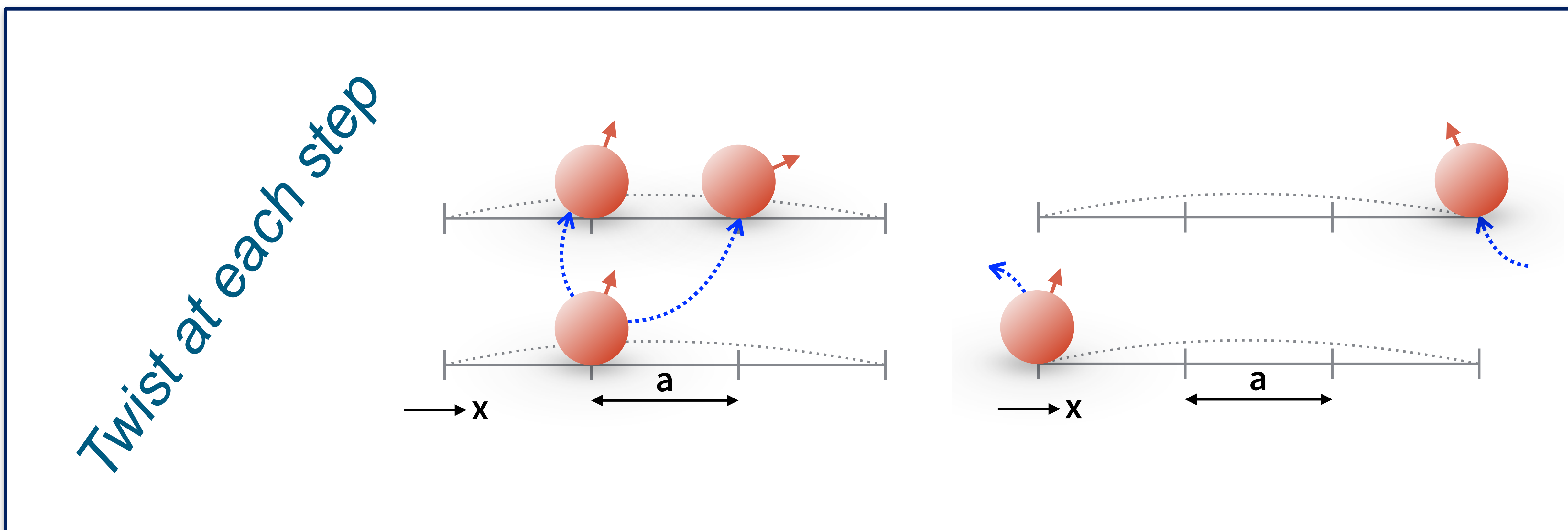


$$\sum_{\vec{n}'\in\mathbb{Z}^3} a^\dagger(\vec{n}'+\vec{l}\,)a(\vec{n}')\,|\vec{n}\rangle = \begin{cases} |\vec{n}+\vec{l}\rangle & , \quad \vec{n}+\vec{l} \in L^3 \\ |(\vec{n}+\vec{l})_{L^3}\rangle\, e^{-i\vec{\phi}\cdot\hat{l}} & , \quad \vec{n}+\vec{l} \notin L^3 \end{cases}$$

Mitglied der Helmholtz-Gemeinschaft

TBCs — Implementation

$$\sum_{\vec{n}' \in \mathbb{Z}^3} a^\dagger(\vec{n}' + \vec{l}\,)a(\vec{n}')\,|\vec{n}\rangle = \begin{cases} |\vec{n}+\vec{l}\rangle\, e^{-i\vec{\phi}\cdot\vec{l}/N_L} & , \quad \vec{n}+\vec{l} \in L^3 \\ |(\vec{n}+\vec{l})_{L^3}\rangle\, e^{-i\vec{\phi}\cdot\vec{l}/N_L} & , \quad \vec{n}+\vec{l} \notin L^3 \end{cases}$$



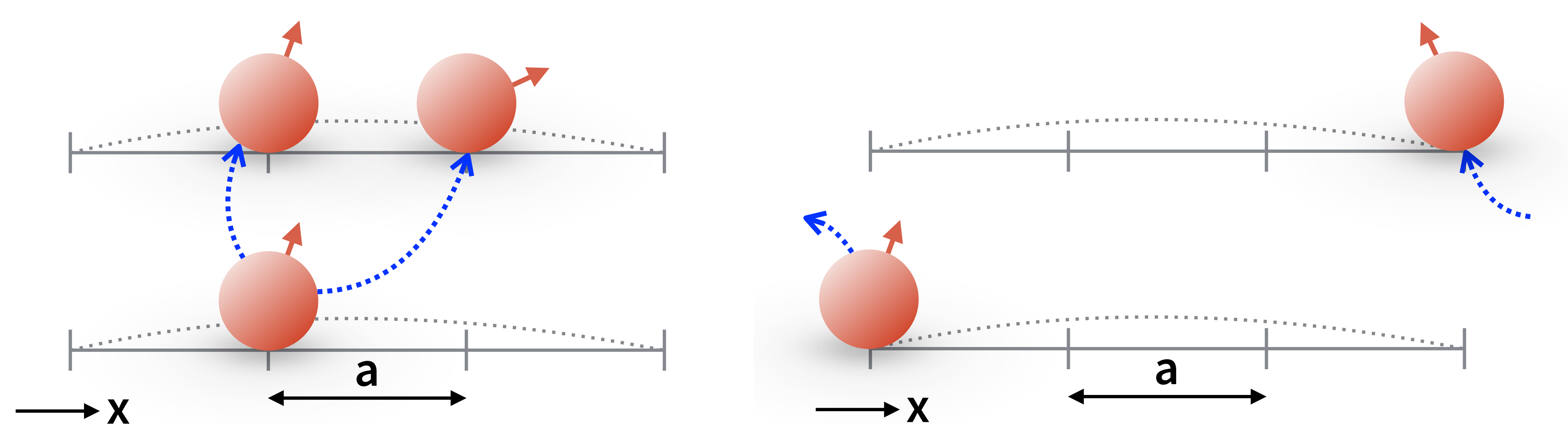
Mitglied der Helmholtz-Gemeinschaft

TBCs — Implementation

Hermitian operators stay hermitian

$$\langle \vec{m}_1^{\vec{\phi}_1}, \cdots ; \vec{m}_N^{\vec{\phi}_N} | O | \vec{n}_1^{\vec{\phi}_1}, \cdots ; \vec{n}_N^{\vec{\phi}_N} \rangle$$
$$= \langle \vec{m}_1^{\vec{0}}, \cdots ; \vec{m}_N^{\vec{0}} | O | \vec{n}_1^{\vec{0}}, \cdots ; \vec{n}_N^{\vec{0}} \rangle \exp\left(i \sum_{i=1}^{N} \vec{\phi}_i / N_L \cdot (\vec{n}_i - \vec{m}_i) \right)$$

Twist at each step



Mitglied der Helmholtz-Gemeinschaft

TBCs — Summary

- **Twists are implemented at each step**
  Well defined momenta (translation invariance)

$$\vec{p} \mapsto \frac{2\pi}{L}\vec{n}_p + \frac{\vec{\phi}}{L} \qquad \vec{n}_p \in \mathbb{Z}^3$$

- **Twist are connected to particle "hops"**
  For each d.o.f. you could use a different twist

$$\vec{\phi}_1, \vec{\phi}_2, \cdots, \vec{\phi}_N$$

- **Twists can change CMS motion**
  Constrained on twist conserve CMS motion

$$\sum_i \vec{\phi}_i = \vec{0}$$

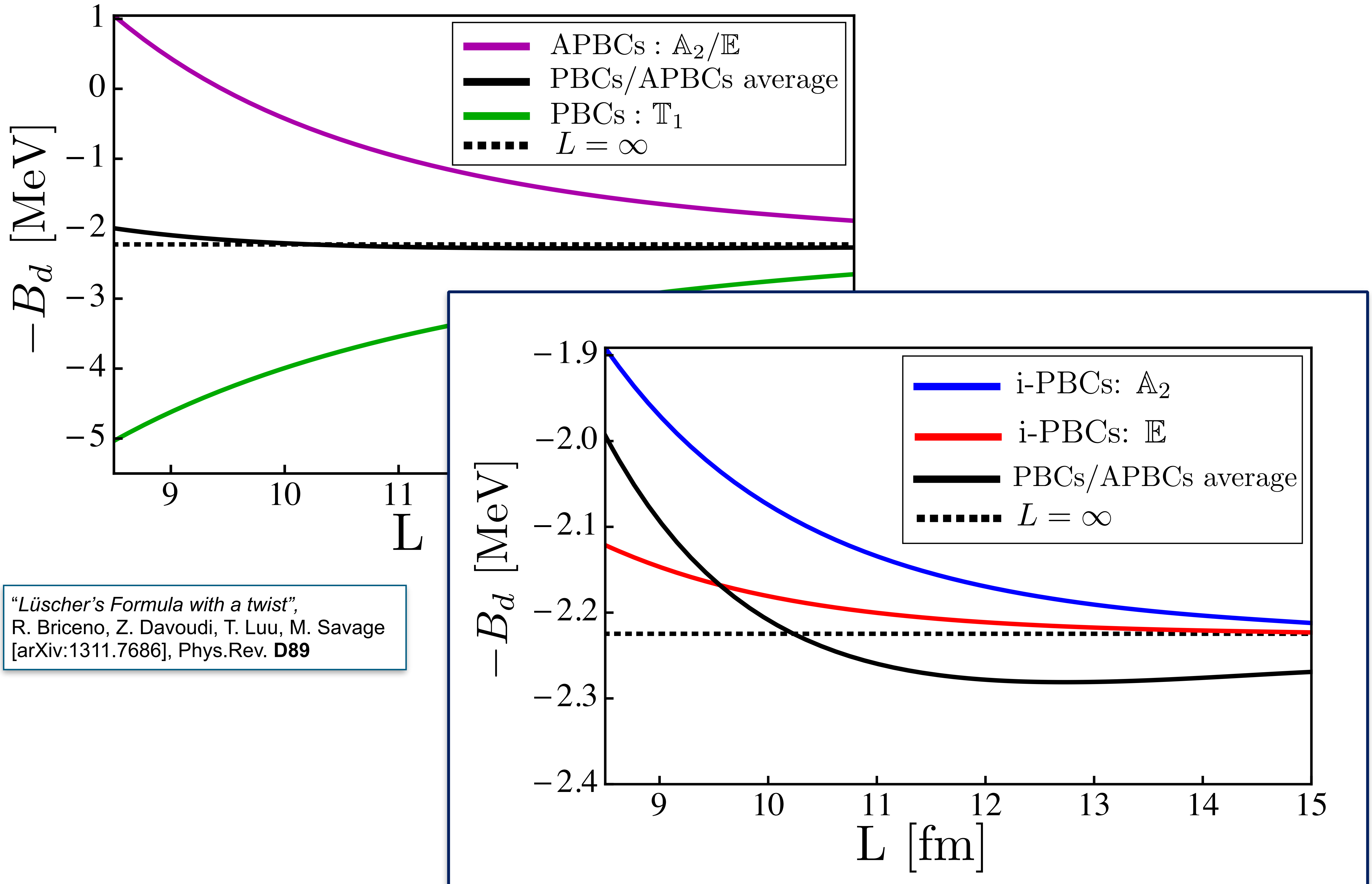
Mitglied der Helmholtz-Gemeinschaft

Analytic Deuteron Results

Why should you use twisted boundaries?

Mitglied der Helmholtz-Gemeinschaft

Analytic Deuteron Results



"Lüscher's Formula with a twist",
R. Briceno, Z. Davoudi, T. Luu, M. Savage
[arXiv:1311.7686], Phys.Rev. **D89**

TBCs — How does this work?

For two-body systems

Schrödinger formalism

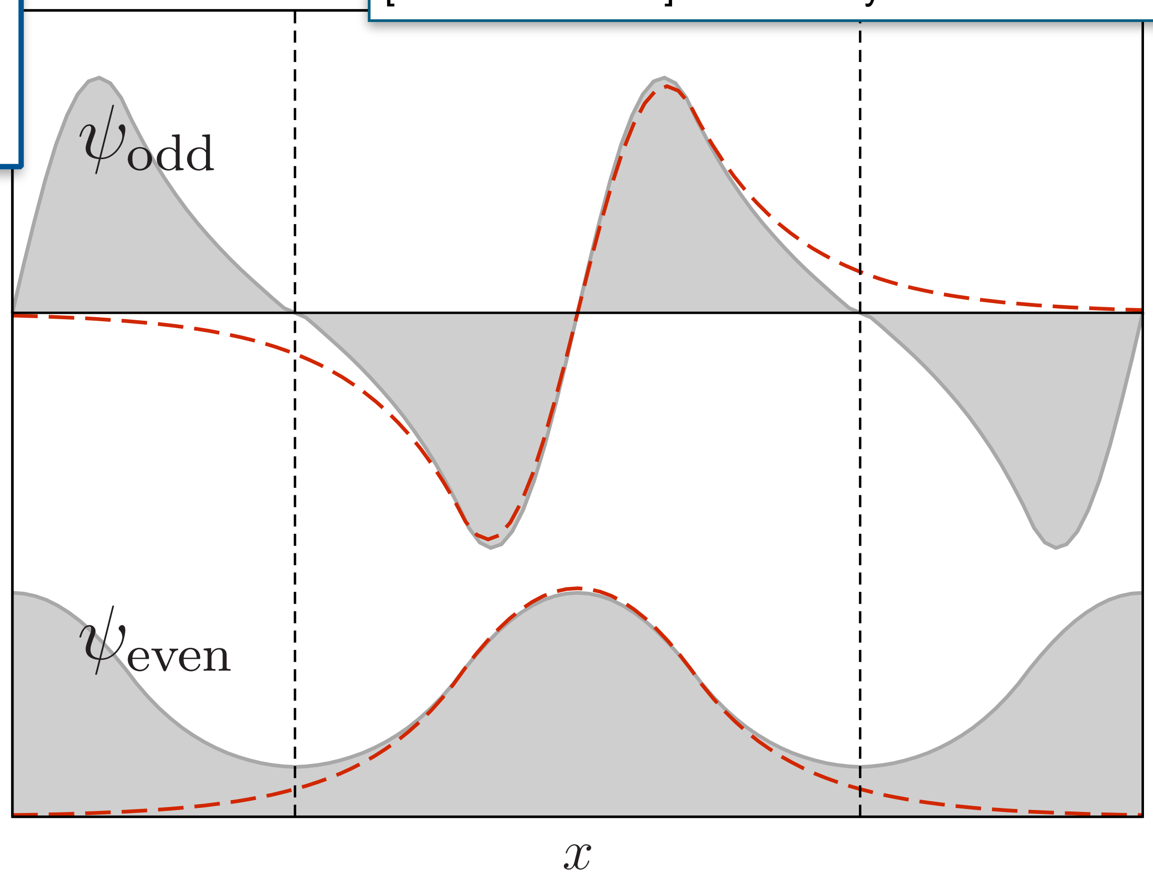
$$\Delta E_L(L,\phi) := \langle \psi_L | \hat{H}_L - E_\infty | \psi_L \rangle$$

"*Volume Dependence of the Energy Spectrum in Massive Quantum Field Theories. 1. Stable Particle States*", M. Lüscher Commun.Math.Phys. **104** (1986) 177

Finite volume wave as copies of infinite volume wave (PB)

$$\langle \vec{r} | \psi_L \rangle = \sum_{\vec{n}\in\mathbb{Z}^3} \langle \vec{r} + \vec{n}L | \psi_\infty \rangle + \mathcal{O}(e^{-\kappa L})$$

"Non-relativistic bound states in a finite volume", H. W. Hammer, S. König, D. Lee [arXiv:1109.4577] Annals Phys. **327**



Mitglied der Helmholtz-Gemeinschaft

JÜLICH FORSCHUNGSZENTRUM

TBCs — How does this work?

For two-body systems

Schrödinger formalism

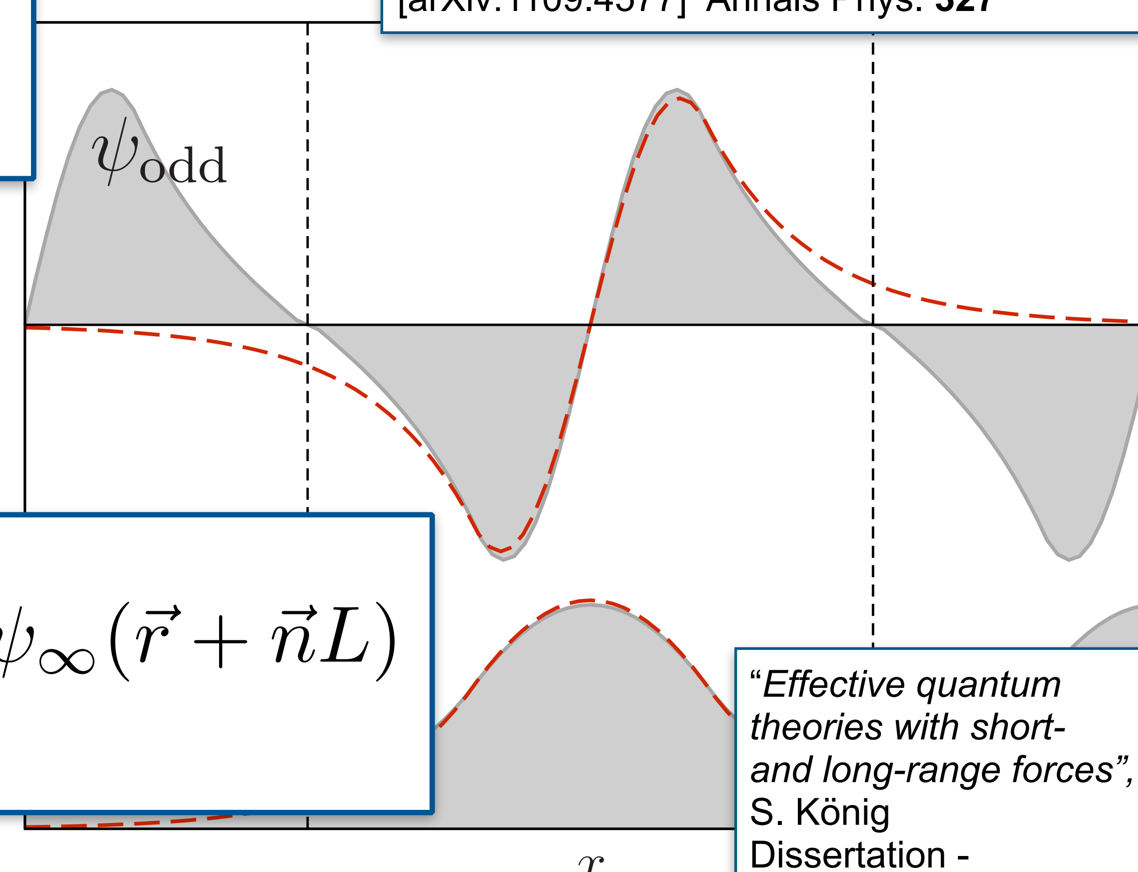
$$\Delta E_L(L,\phi) := \langle \psi_L | \hat{H}_L - E_\infty | \psi_L \rangle$$

"*Volume Dependence of the Energy Spectrum in Massive Quantum Field Theories. 1. Stable Particle States*", M. Lüscher Commun.Math.Phys. **104** (1986) 177

Finite volume wave as copies of infinite volume wave (PB)

$$\langle \vec{r} | \psi_L \rangle = \sum_{\vec{n} \in \mathbb{Z}^3} \langle \vec{r} + \vec{n} L | \psi_\infty \rangle + \mathcal{O}(e^{-\kappa L})$$

"Non-relativistic bound states in a finite volume", H. W. Hammer, S. König, D. Lee [arXiv:1109.4577] Annals Phys. **327**



Energy shift corresponds to different box overlap

$$\Delta E_L^{(LO)}(L) := \sum_{|\vec{n}|=1} \int \mathrm{d}^3\vec{r}\; \psi_\infty^*(\vec{r}) V(r) \psi_\infty(\vec{r} + \vec{n}L)$$

"*Effective quantum theories with short- and long-range forces*", S. König Dissertation - University of Bonn (2013)

Mitglied der Helmholtz-Gemeinschaft

Periodic boundary result: S-Wave

$$\Delta E_L^{(LO)}(L) := \sum_{|\vec{n}|=1} \int \mathrm{d}^3\vec{r}\, \psi_\infty^*(\vec{r}) V(r) \psi_\infty(\vec{r} + \vec{n}L) = -3|\mathcal{A}|^2 \frac{e^{-\kappa L}}{\mu L}$$

$$V(\vec{r}) = 0 \;\Rightarrow\; \psi_\infty(\vec{r}) = \mathcal{A}\sqrt{\frac{1}{4\pi}} \frac{e^{-\kappa r}}{r} \quad \forall\, R < r < L\,, \quad \kappa^2 = -2\mu E_\infty$$

Mitglied der Helmholtz-Gemeinschaft

Periodic boundary result: S-Wave

$$\Delta E_L^{(LO)}(L) := \sum_{|\vec{n}|=1} \int \mathrm{d}^3\vec{r}\, \psi_\infty^*(\vec{r}) V(r) \psi_\infty(\vec{r}+\vec{n}L) = -3|\mathcal{A}|^2 \frac{e^{-\kappa L}}{\mu L}$$

Twisted boundaries

$$\langle \vec{r}^{\vec{\phi}} | \psi_L \rangle = \sum_{\vec{n}\in\mathbb{Z}^3} \langle \vec{r}+\vec{n}L | \psi_\infty \rangle\, e^{-i\vec{n}\cdot\vec{\phi}} + \mathcal{O}(e^{-\kappa L})$$

Twisted boundaries result

"Topological phases for bound states moving in a finite volume", S. Bour, H. Hammer, S. König, D. Lee, U. Meißner [arXiv:1107.1272] Phys.Rev. **D84**

$$\Delta E_L^{(LO)}(L,\vec{\phi}) := \sum_{|\vec{n}|=1} \int \mathrm{d}^3\vec{r}\, \psi_\infty^*(\vec{r}) V(r) \psi_\infty(\vec{r}+\vec{n}L) e^{-i\vec{n}\cdot\vec{\phi}}$$

$$= -|\mathcal{A}|^2 \frac{e^{-\kappa L}}{\mu L} \sum_{i=1}^{3} \cos(\phi_i)$$

Mitglied der Helmholtz-Gemeinschaft

Formalism and Methodology

Mitglied der Helmholtz-Gemeinschaft

Formalism & Error Analysis

For 2-Body Level

$$\boxed{\hat{H}_L \left|\psi\right\rangle = E_L \left|\psi\right\rangle \, , \quad V_L(\vec{n}) = \frac{c}{a^3}\delta_{\vec{n},\vec{0}}}$$

Sources of errors

(Numerical deviation from theoretical prediction)

- ~~**Contact interaction estimate**~~
  (Fitting on Lattice)
- **Solving procedure**
  (Lanczos like iteration)
- **Resolution not sufficient**
  (Discretization errors)

Uncertainty of solving procedure

$$\boxed{=: \delta E_S \simeq 10^{-4} [\, MeV \,]}$$

Same spacing for all computations (?)

JÜLICH FORSCHUNGSZENTRUM

Mitglied der Helmholtz-Gemeinschaft

Lattice effects without twists

Momenta in FV:

$$\vec{r} \in \mathbb{R}^3 \mapsto \vec{r} \in L^3 \qquad \Rightarrow \qquad \vec{p} \in \mathbb{R}^3 \mapsto \frac{2\pi}{L}\vec{n}_p \, , \quad \vec{n}_p \in \mathbb{Z}^3$$

Momenta in discrete space:

Discretization (one step derivative):

$$\partial^2_{x,a} f(\vec{r}) := \frac{1}{a^2}\left(f(\vec{r} + a\vec{e}_x) - 2f(\vec{r}) + f(\vec{r} - a\vec{e}_x)\right)$$

Dispersion relation (one step derivative):

$$\hat{p}_x^2 \left|\vec{p}\right\rangle \mapsto \frac{2\left(1 - \cos(p_x a)\right)}{a^2} \left|\vec{p}\right\rangle$$

Mitglied der Helmholtz-Gemeinschaft

Lattice effects with twists

Momenta in FV:

$$\vec{r} \in \mathbb{R}^3 \mapsto \vec{r} \in L^3 \qquad \Rightarrow \qquad \vec{p} \in \mathbb{R}^3 \mapsto \vec{p}^{\vec{\phi}} = \frac{2\pi}{L}\vec{n}_p + \frac{\vec{\phi}}{L}\,, \quad \vec{n}_p \in \mathbb{Z}^3$$

Momenta in discrete space:

Discretization (one step derivative):

$$\partial_{x,a}^2 f(\vec{r}) := \frac{1}{a^2}\left(e^{i\phi_x a/L} f(\vec{r}+a\vec{e}_x) - 2f(\vec{r}) + e^{-i\phi_x a/L} f(\vec{r}-a\vec{e}_x)\right)$$

Dispersion relation (one step derivative):

$$\hat{p}_x^2 \left|\vec{p}^{\vec{\phi}}\right\rangle \mapsto \frac{2\left(1-\cos(p_x^{\vec{\phi}} a)\right)}{a^2}\left|\vec{p}^{\vec{\phi}}\right\rangle$$

Mitglied der Helmholtz-Gemeinschaft

Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

Mitglied der Helmholtz-Gemeinschaft

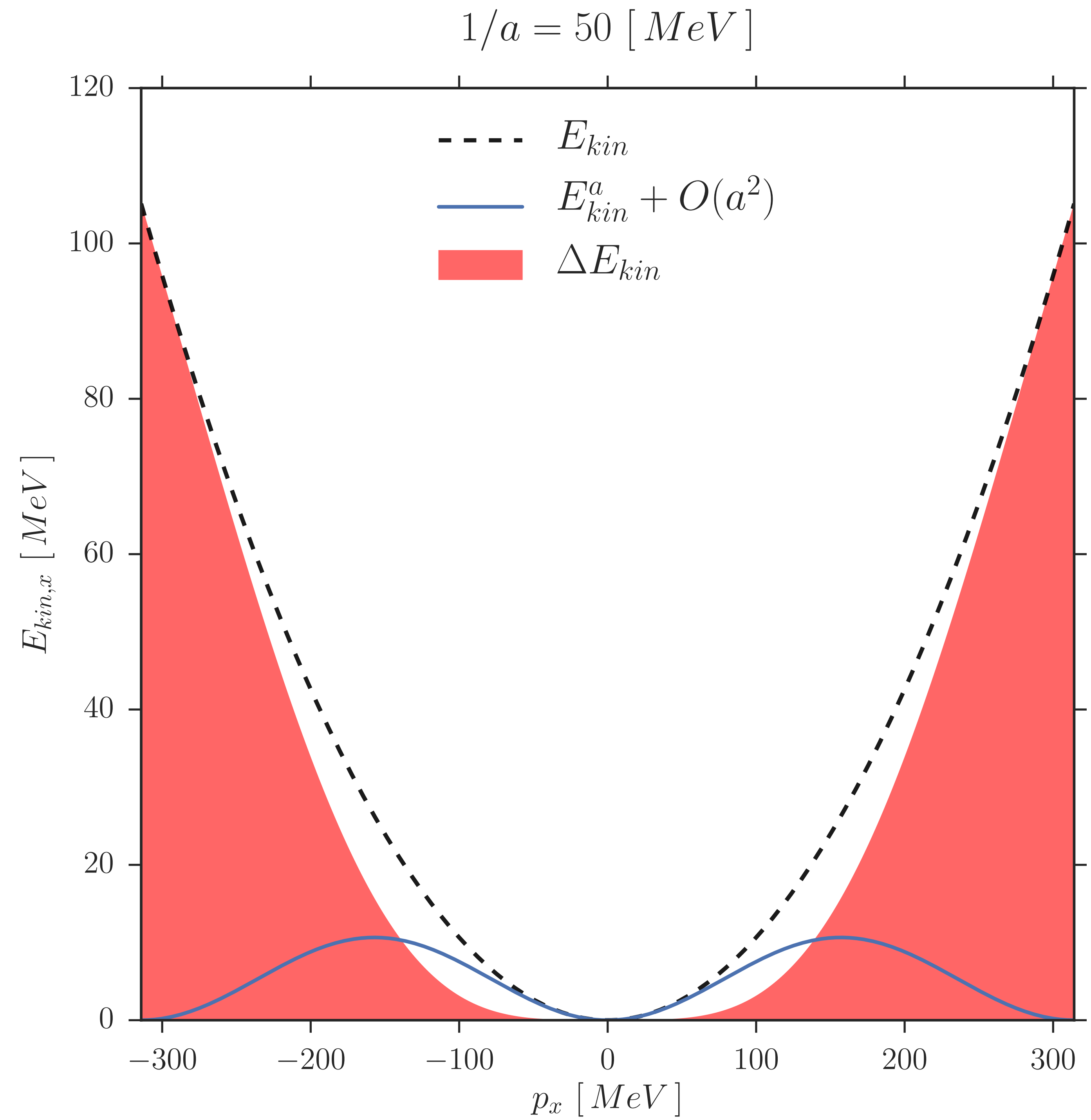
Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

- **Dispersion relations**



Mitglied der Helmholtz-Gemeinschaft

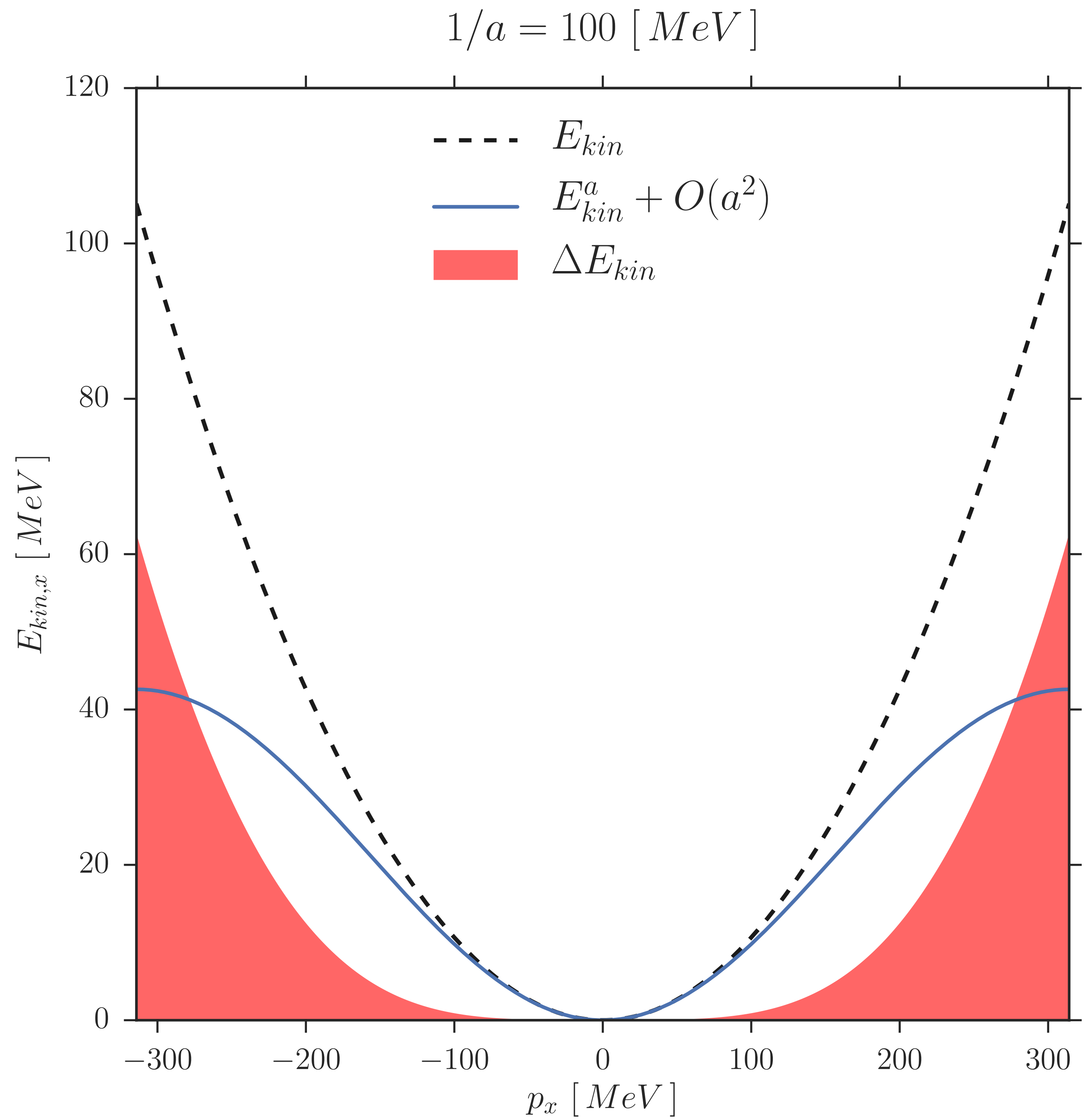
Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

- **Dispersion relations**



Mitglied der Helmholtz-Gemeinschaft

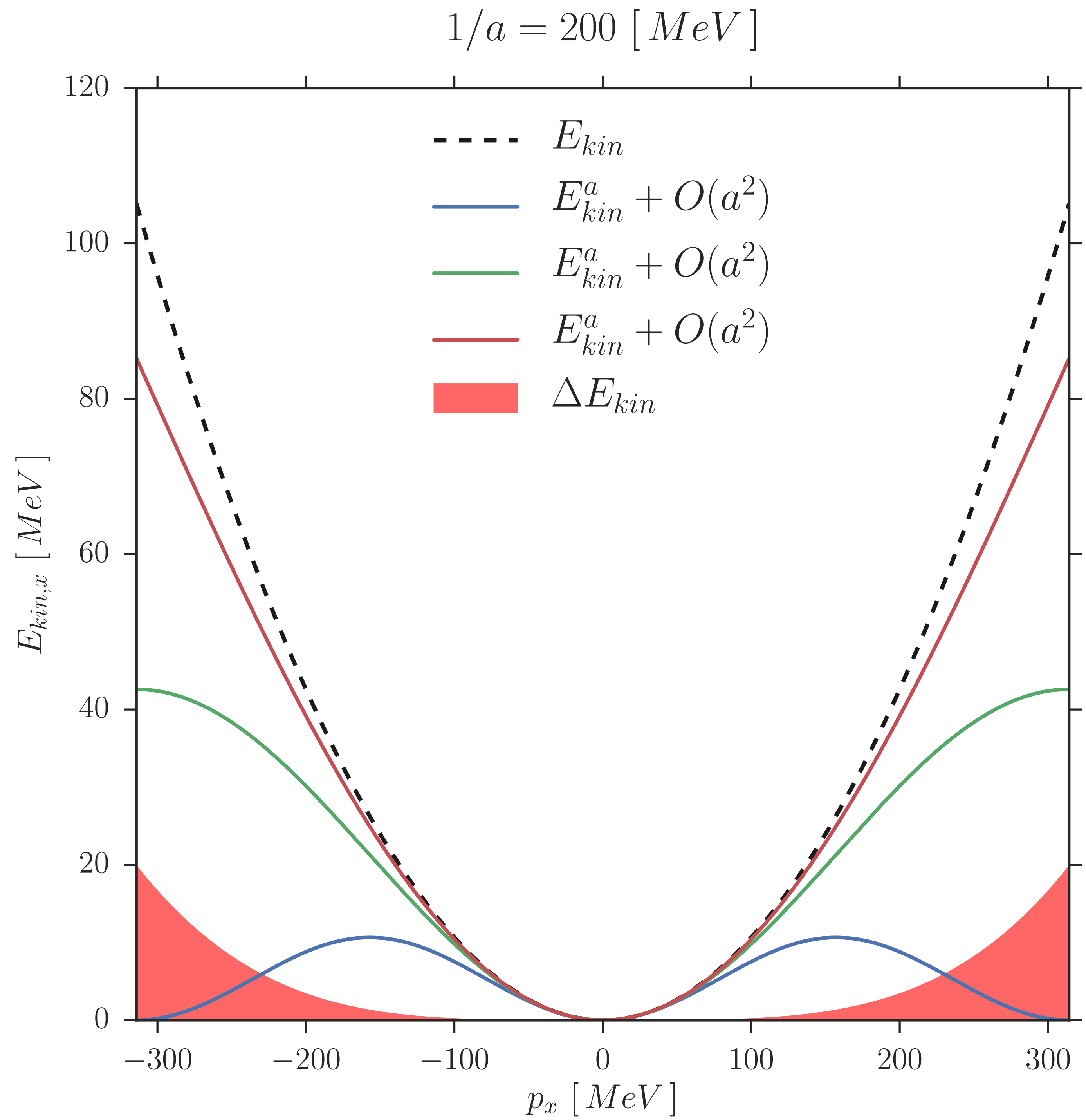
Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

- **Dispersion relations**



Mitglied der Helmholtz-Gemeinschaft

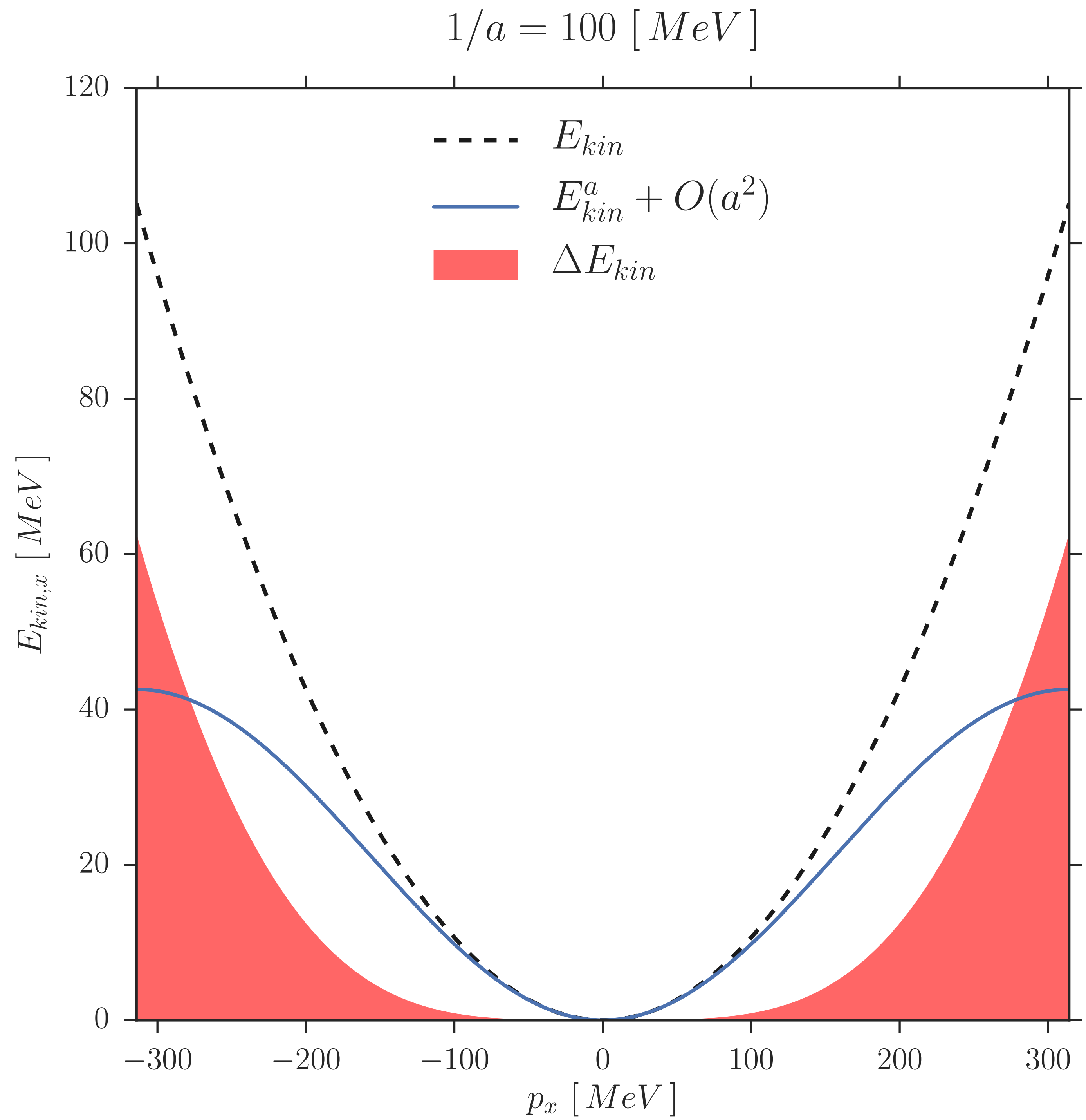
Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

- **Dispersion relations**



$$\partial_{x,a}^{(N)^2} f(\vec{r}) = \frac{1}{a^2} \sum_{n=0}^{N} (-1)^{n+1} \omega_n \left(f(\vec{r} + an\vec{e}_x) + f(\vec{r} - an\vec{e}_x) \right)$$

Mitglied der Helmholtz-Gemeinschaft

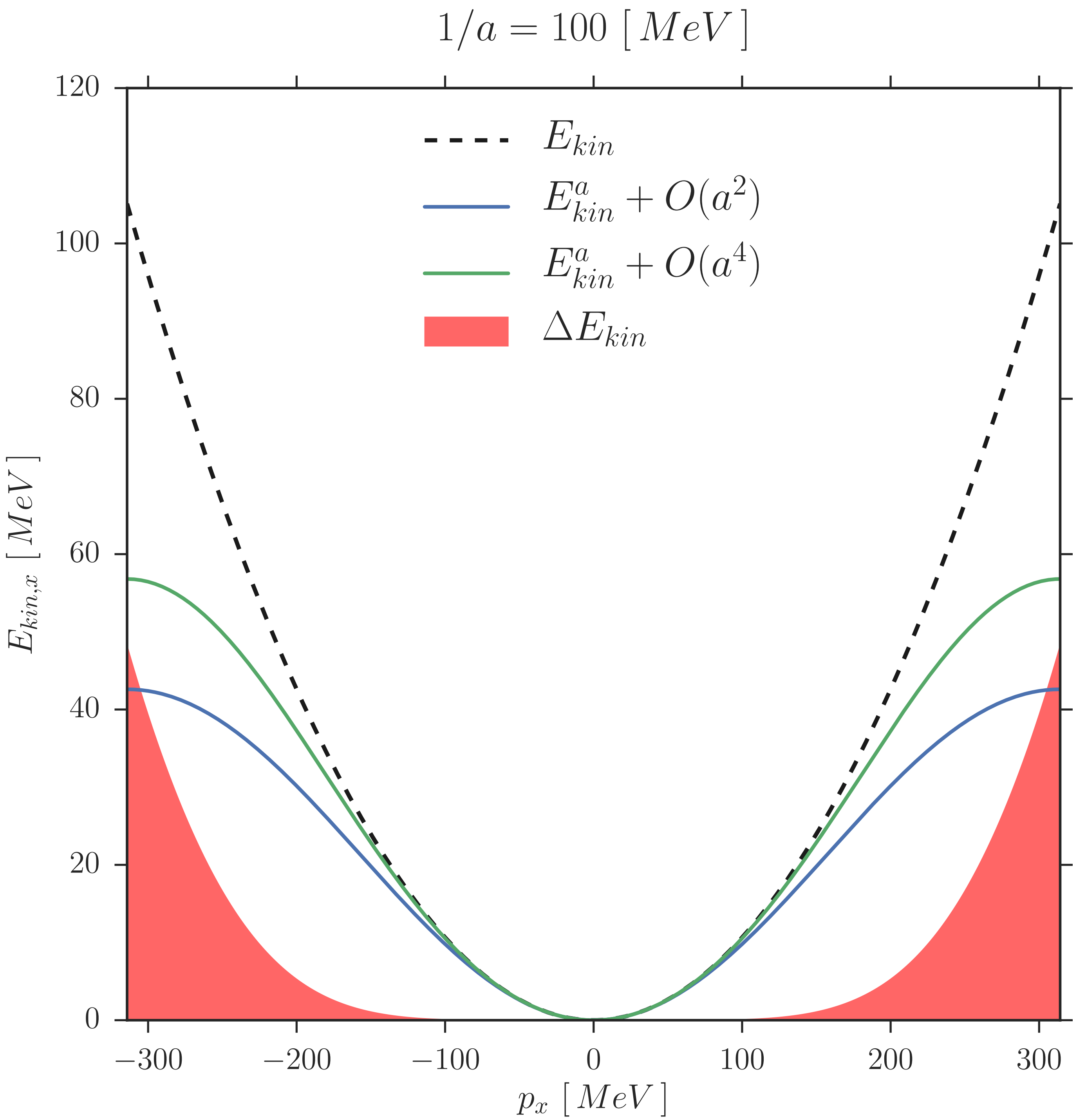
Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

- **Dispersion relations**



$$\partial_{x,a}^{(N)^2} f(\vec{r}) = \frac{1}{a^2} \sum_{n=0}^{N} (-1)^{n+1} \omega_n \left(f(\vec{r} + an\vec{e}_x) + f(\vec{r} - an\vec{e}_x) \right)$$

Mitglied der Helmholtz-Gemeinschaft

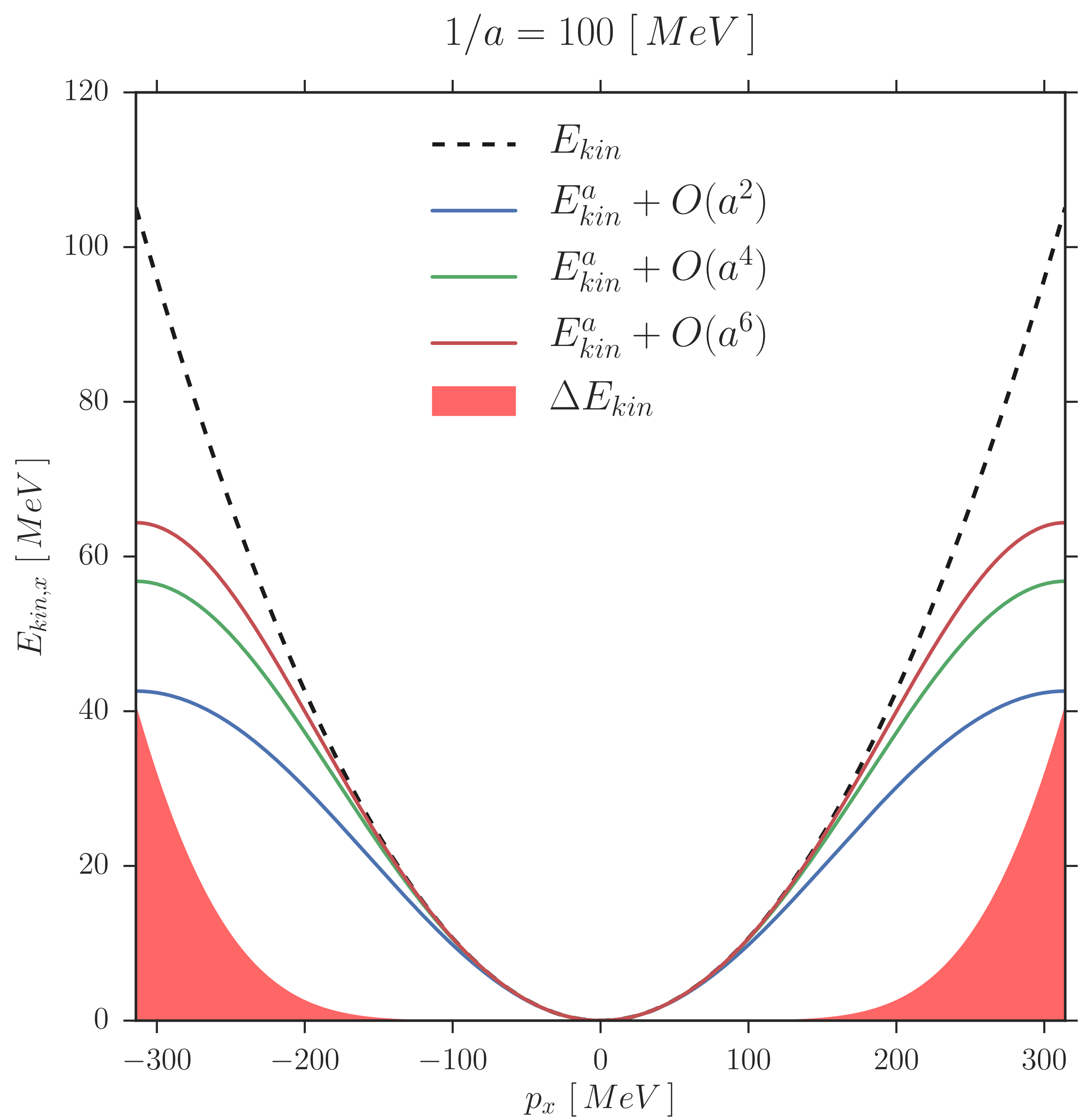
Dispersion relations

How does discretization affect momenta?

- ***Contact interactions***

  LECs are cutoff dependent (fitting)

- **Dispersion relations**



$$\partial^{(N)^2}_{x,a} f(\vec{r}) = \frac{1}{a^2} \sum_{n=0}^{N} (-1)^{n+1}\, \omega_n\, \left(f(\vec{r} + an\vec{e}_x) + f(\vec{r} - an\vec{e}_x)\right)$$

Mitglied der Helmholtz-Gemeinschaft

Twisted discrete dispersion: $N_L = 3$

$$a = 1.97\ fm$$

$$\vec{n}_p \sim \vec{n}'_p \quad \Leftrightarrow \quad \vec{n}_p = \vec{n}'_p + N_L \vec{e}$$

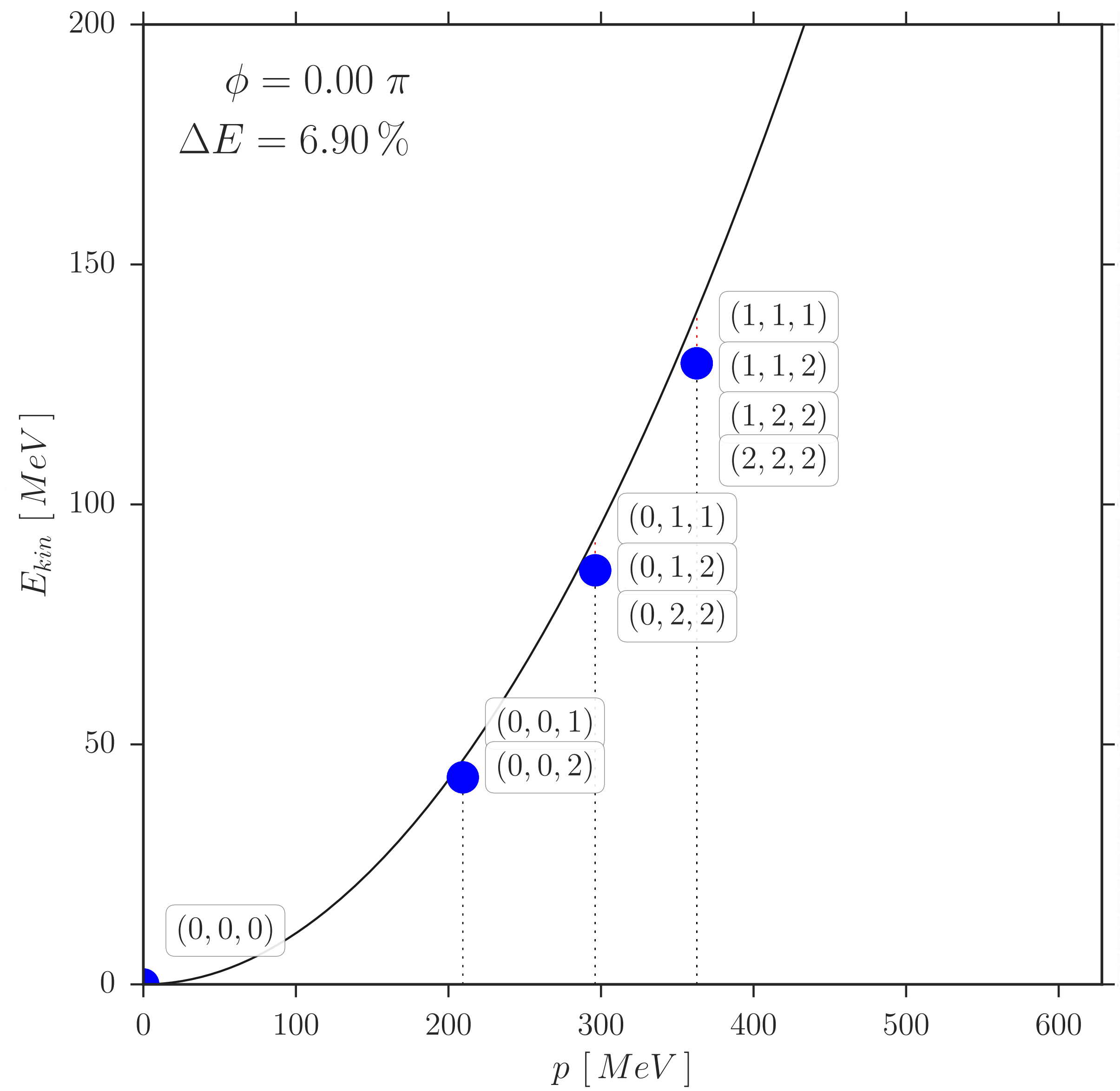
$$\vec{p}^{\vec{\phi}} = \frac{2\pi}{L}\vec{n}_p + \frac{\vec{\phi}}{L}$$

$$\Delta E := \text{mean}\left(\frac{E_{kin} - E_{kin}^{L,\vec{\phi},a}}{E_{kin}}\right)$$

Legend

Infinite volume continuum dispersion

Finite volume discrete dispersion



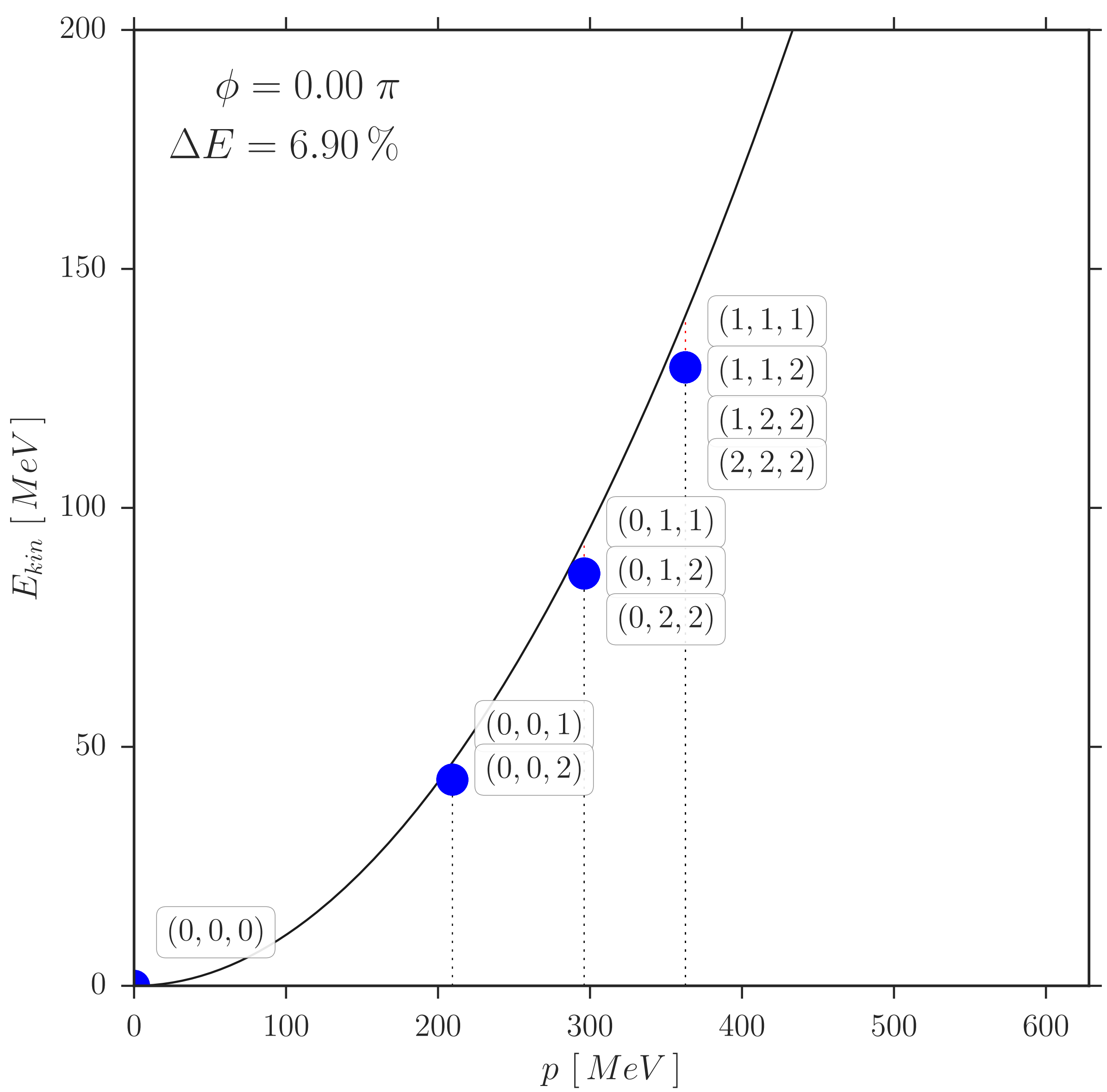
Mitglied der Helmholtz-Gemeinschaft

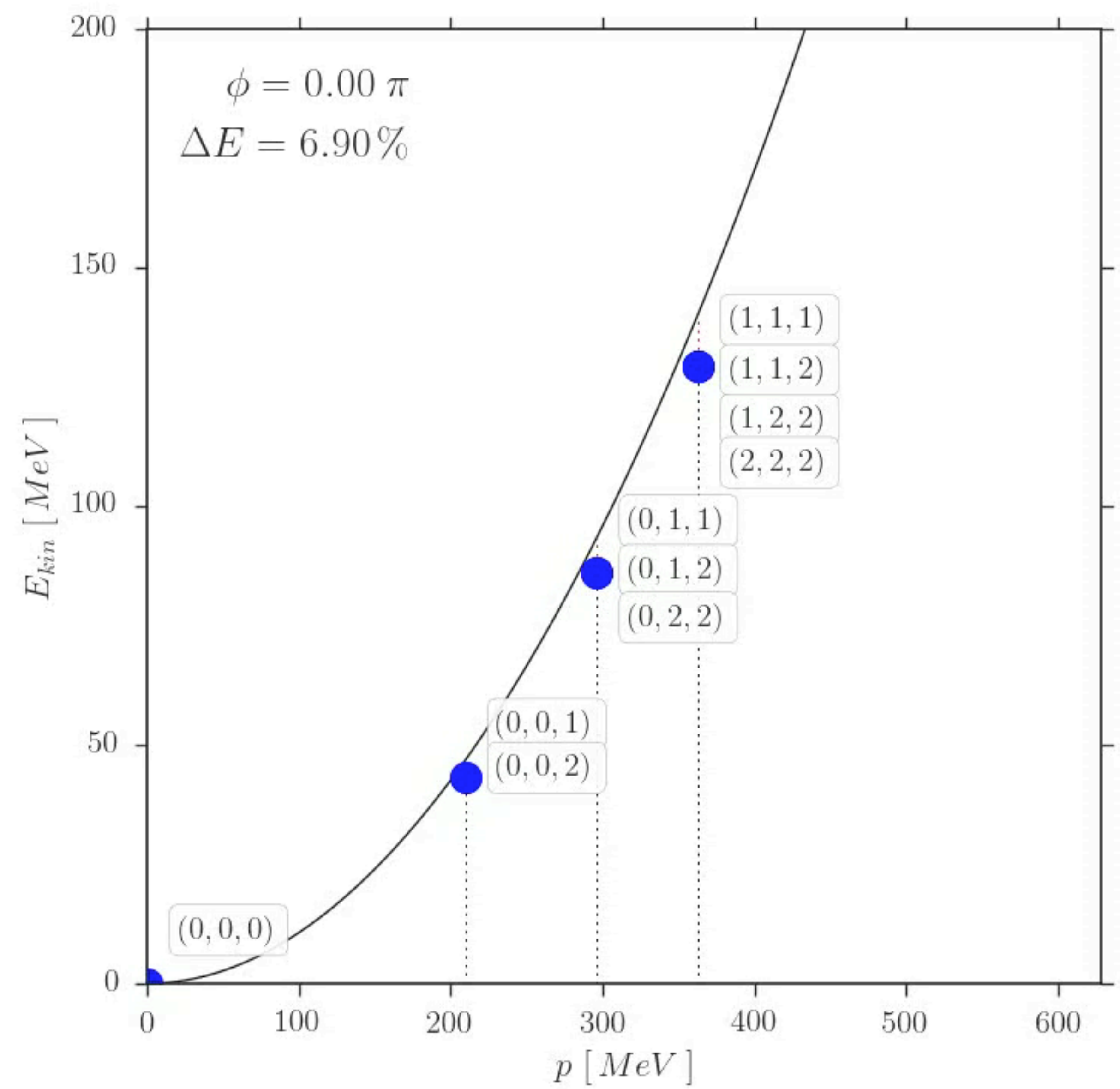
Twisted discrete dispersion: $N_L = 3$

$a = 1.97\ fm$

$$\vec{n}_p \sim \vec{n}'_p \iff \vec{n}_p = \vec{n}'_p + N_L \vec{e}$$

$$p^{\vec{\phi}} = \frac{2\pi}{L}\vec{n}_p + \frac{\vec{\phi}}{L}$$





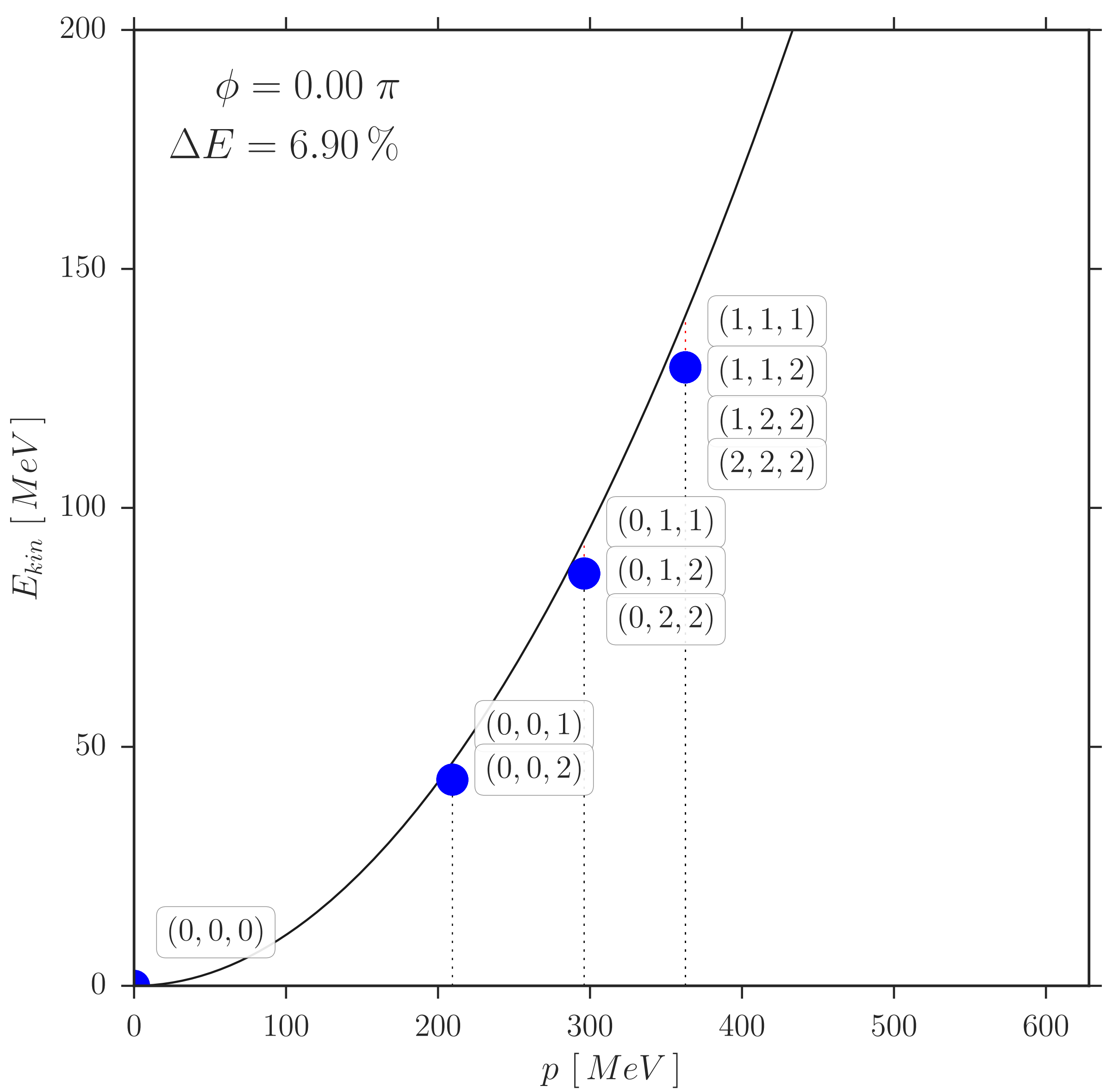
Mitglied der Helmholtz-Gemeinschaft

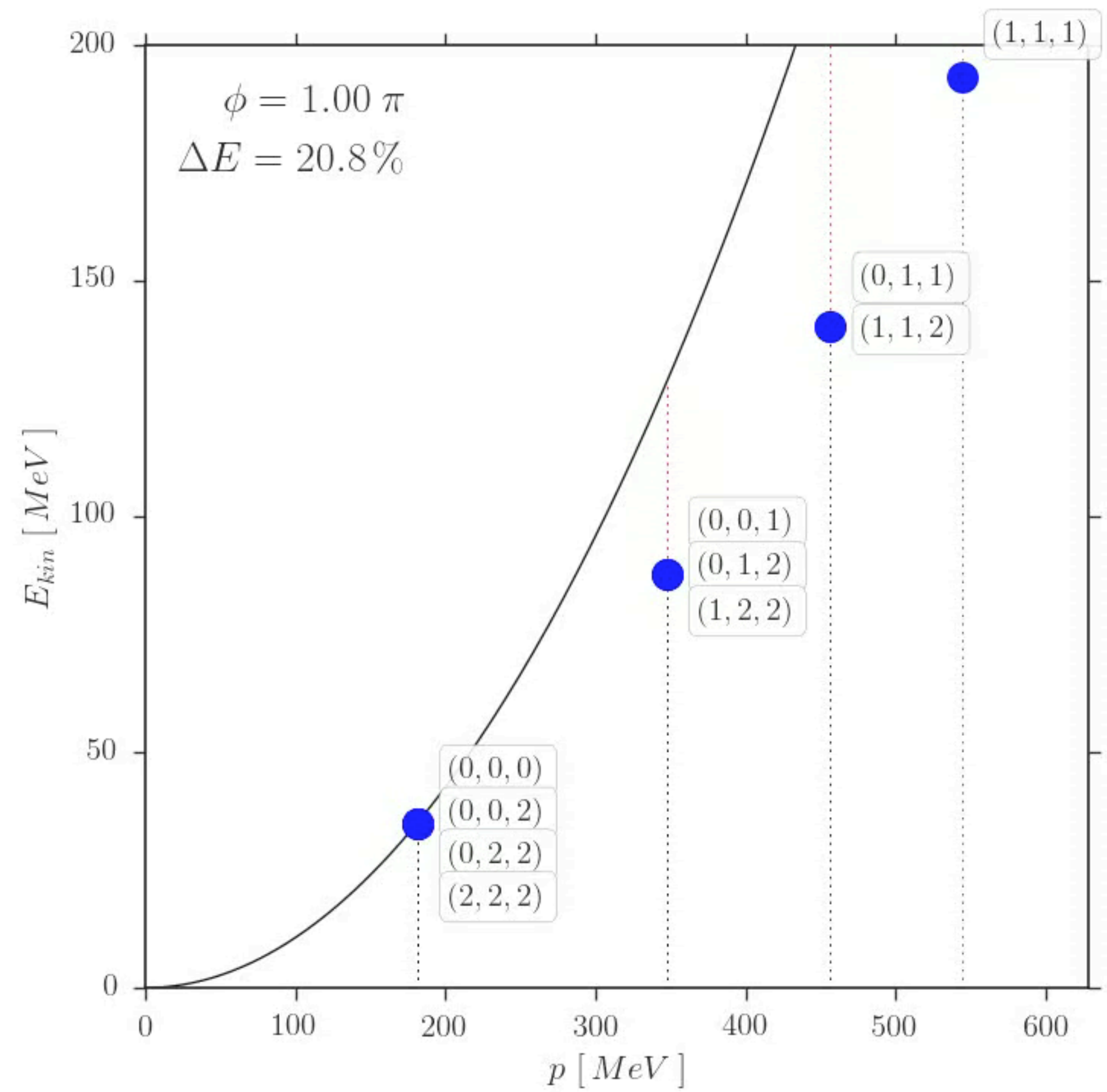
Twisted discrete dispersion: $N_L = 3$

$a = 1.97\ fm$

$$\vec{n}_p \sim \vec{n}'_p \;\Leftrightarrow\; \vec{n}_p = \vec{n}'_p + N_L \vec{e}$$

$$\vec{p}^{\vec{\phi}} = \frac{2\pi}{L}\vec{n}_p + \frac{\vec{\phi}}{L}$$





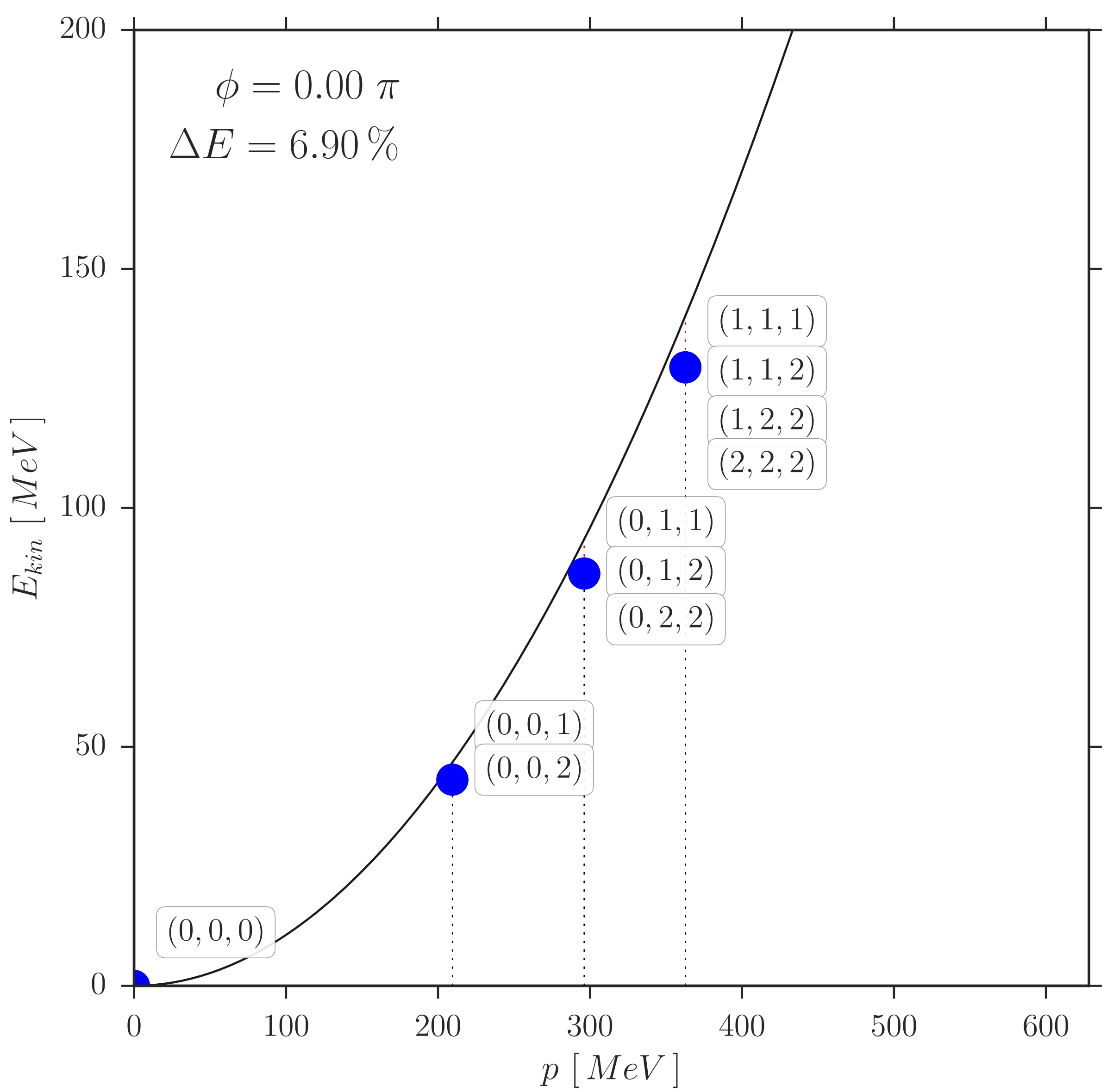
Mitglied der Helmholtz-Gemeinschaft

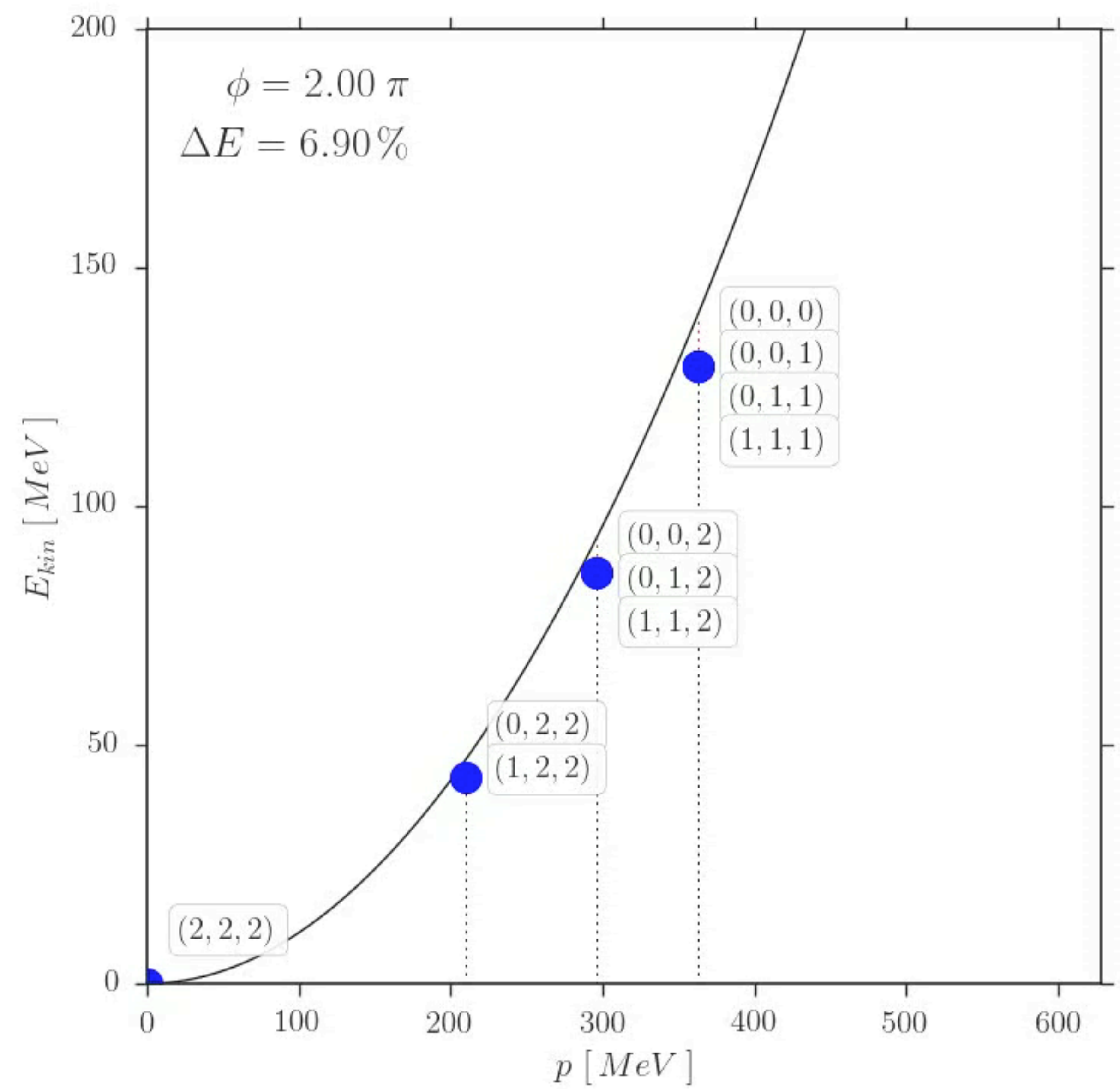
Twisted discrete dispersion: $N_L = 3$

$$a = 1.97\ fm$$

$$\vec{n}_p \sim \vec{n}'_p \ \Leftrightarrow\ \vec{n}_p = \vec{n}'_p + N_L \vec{e}$$

$$p^{\vec{\phi}} = \frac{2\pi}{L}\vec{n}_p + \frac{\vec{\phi}}{L}$$





Mitglied der Helmholtz-Gemeinschaft

Formalism & Error Analysis

$$\boxed{\hat{H}_L \left|\psi\right\rangle = E_L \left|\psi\right\rangle \ , \quad V_L(\vec{n}) = \frac{c}{a^3}\delta_{\vec{n},\vec{0}}}$$

Sources of errors

(Numerical deviation from theoretical prediction)

- ~~**Contact interaction estimate**~~
  (Fitting on Lattice)
- **Solving procedure**
  (Lanczos like iteration)
- **Resolution not sufficient**
  (Discretization errors)
- **Box too small**
  (Finite Volume)

Uncertainty of solving procedure

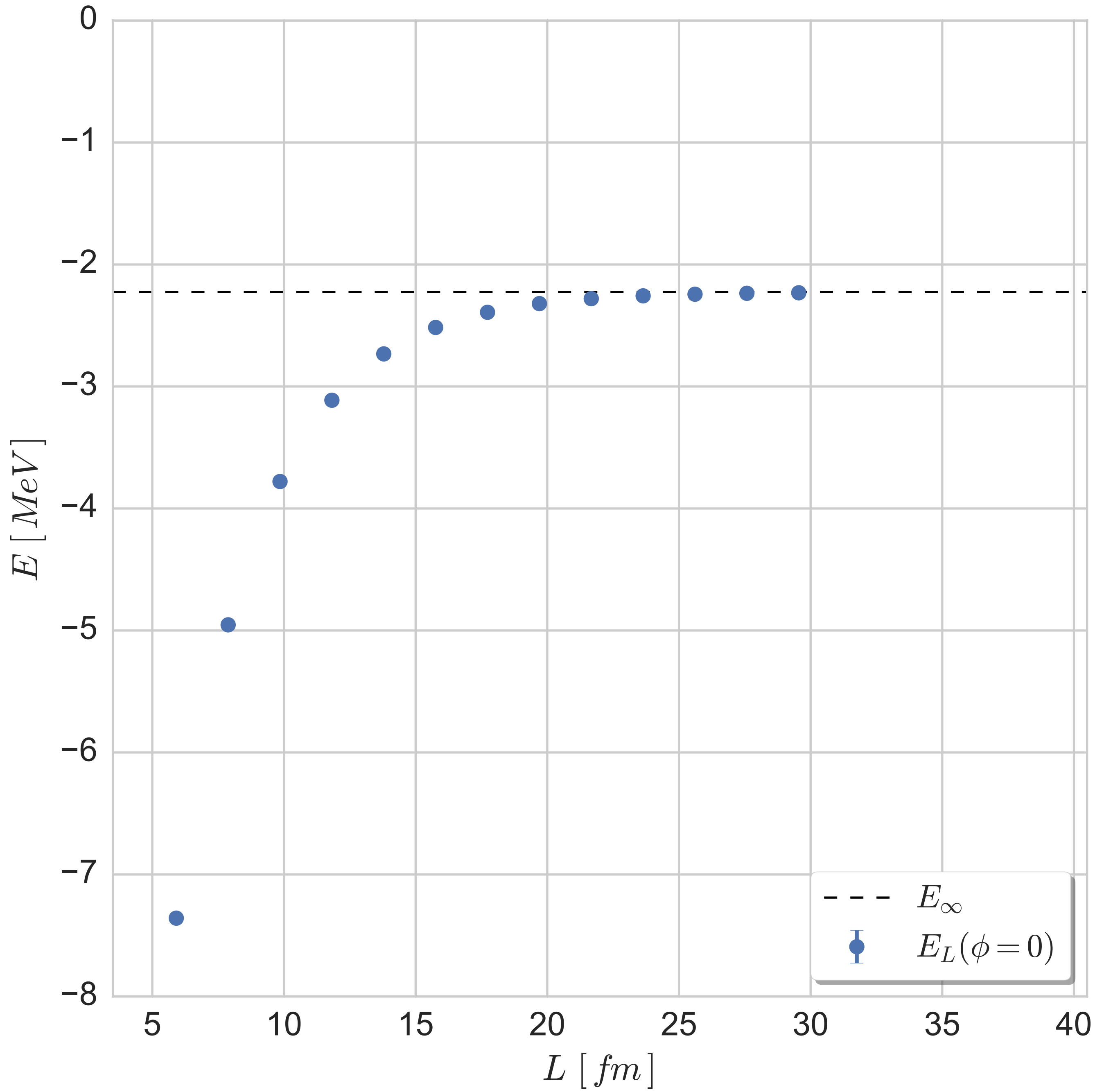
$$\boxed{=: \delta E_S \simeq 10^{-4} [\, MeV \,]}$$

Same spacing for all computations (?)

Size of NLO errors?

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

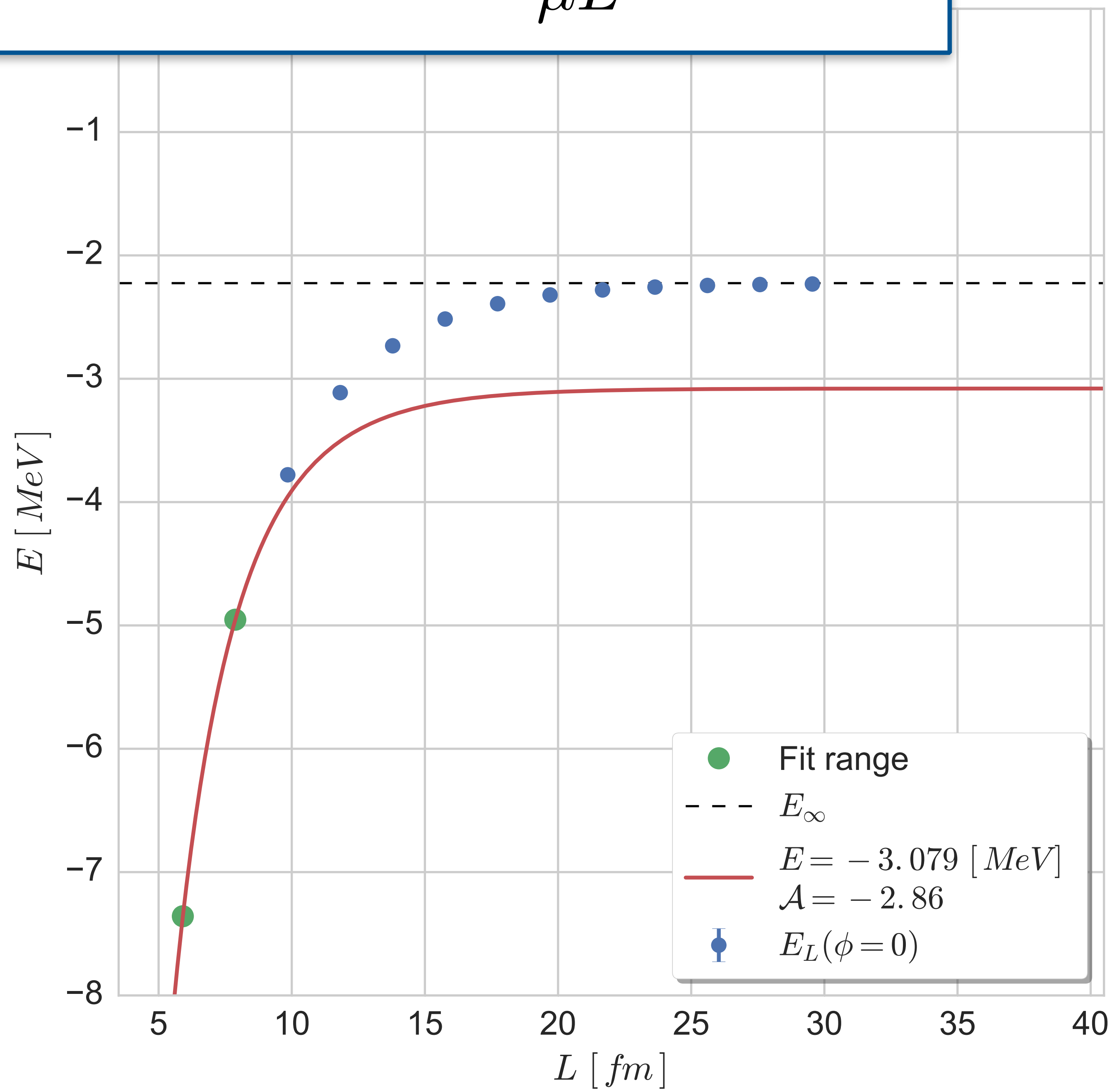


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

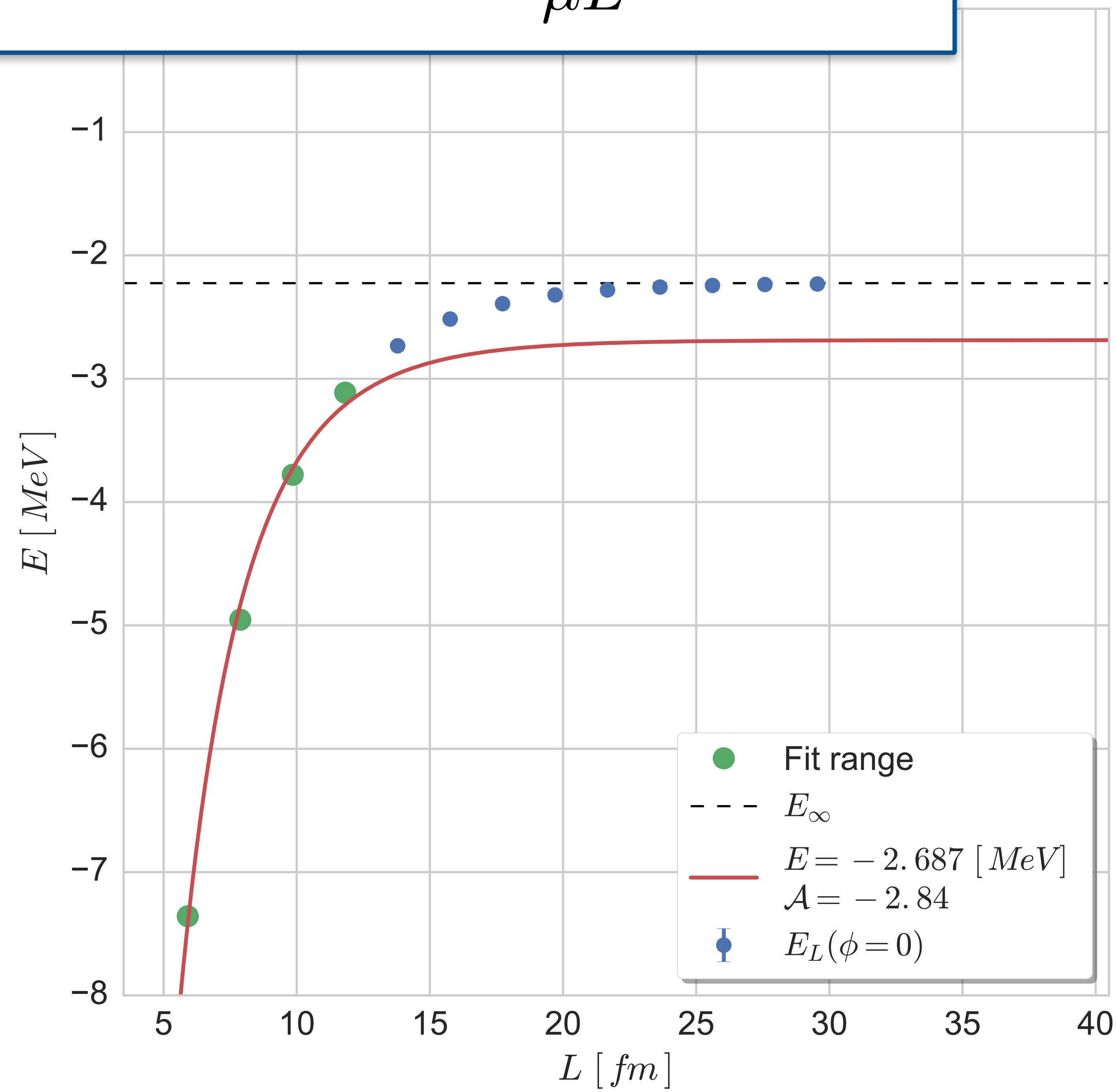


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

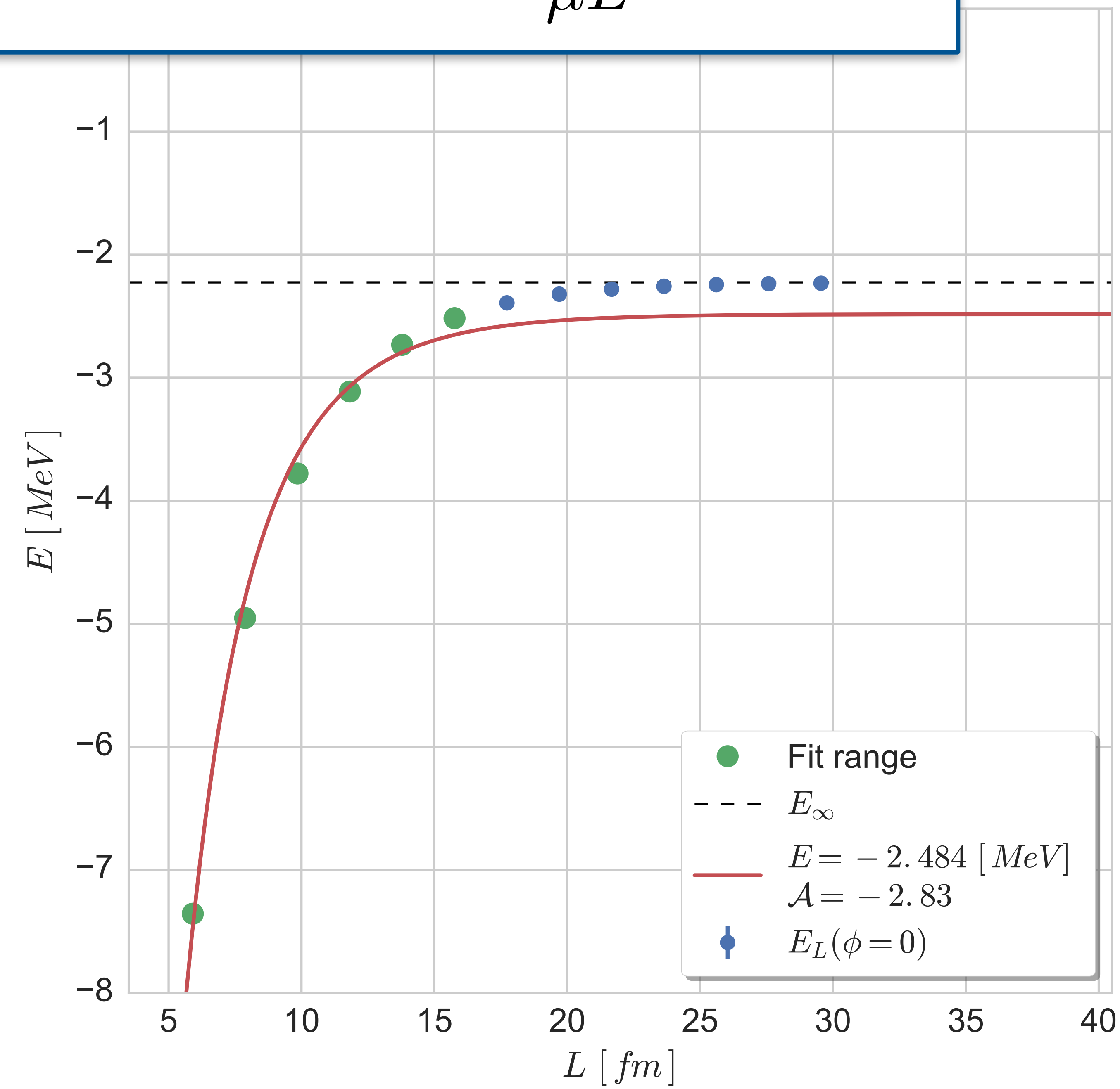


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties**
  Errors:
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

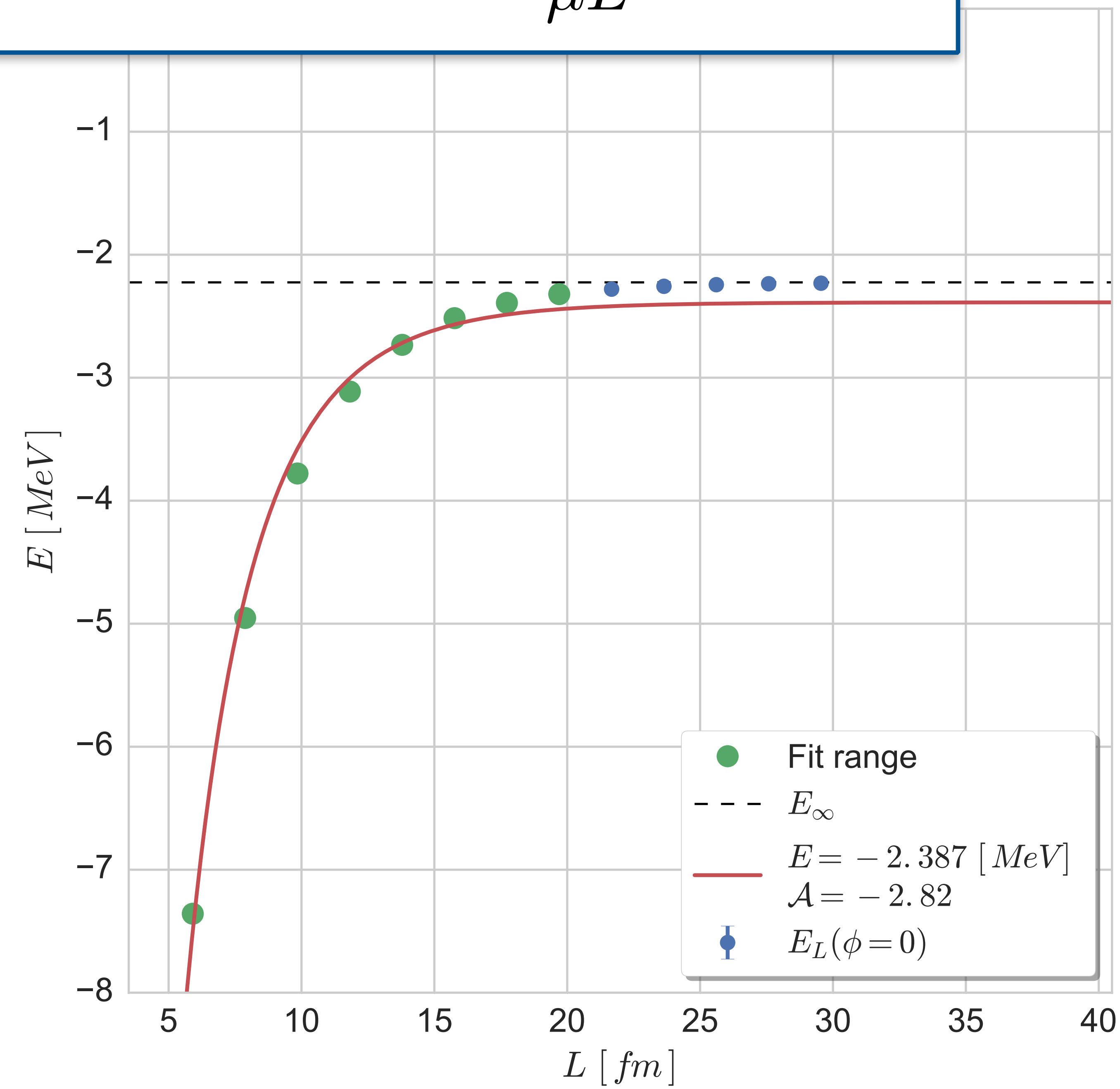


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

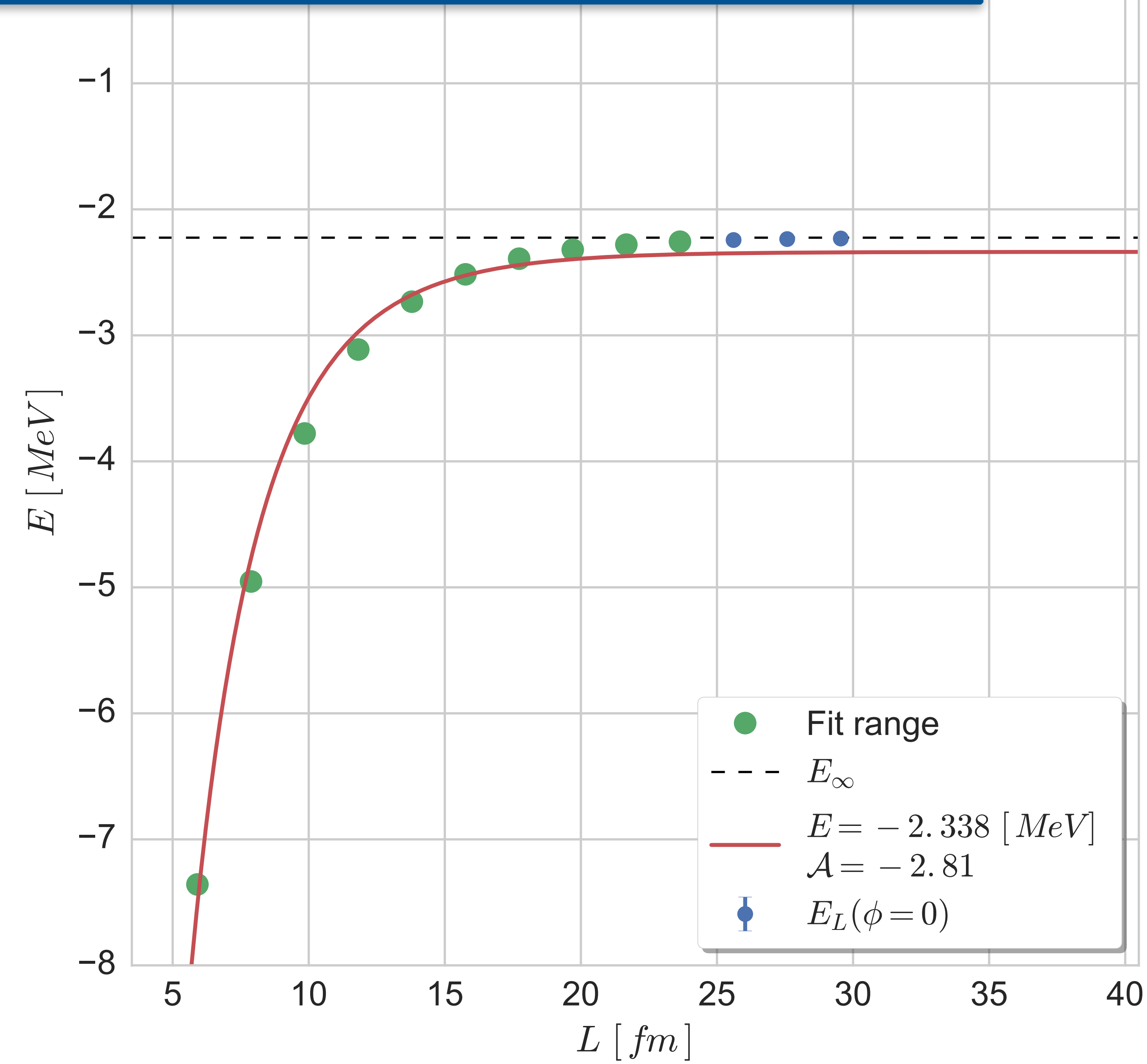


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \overset{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

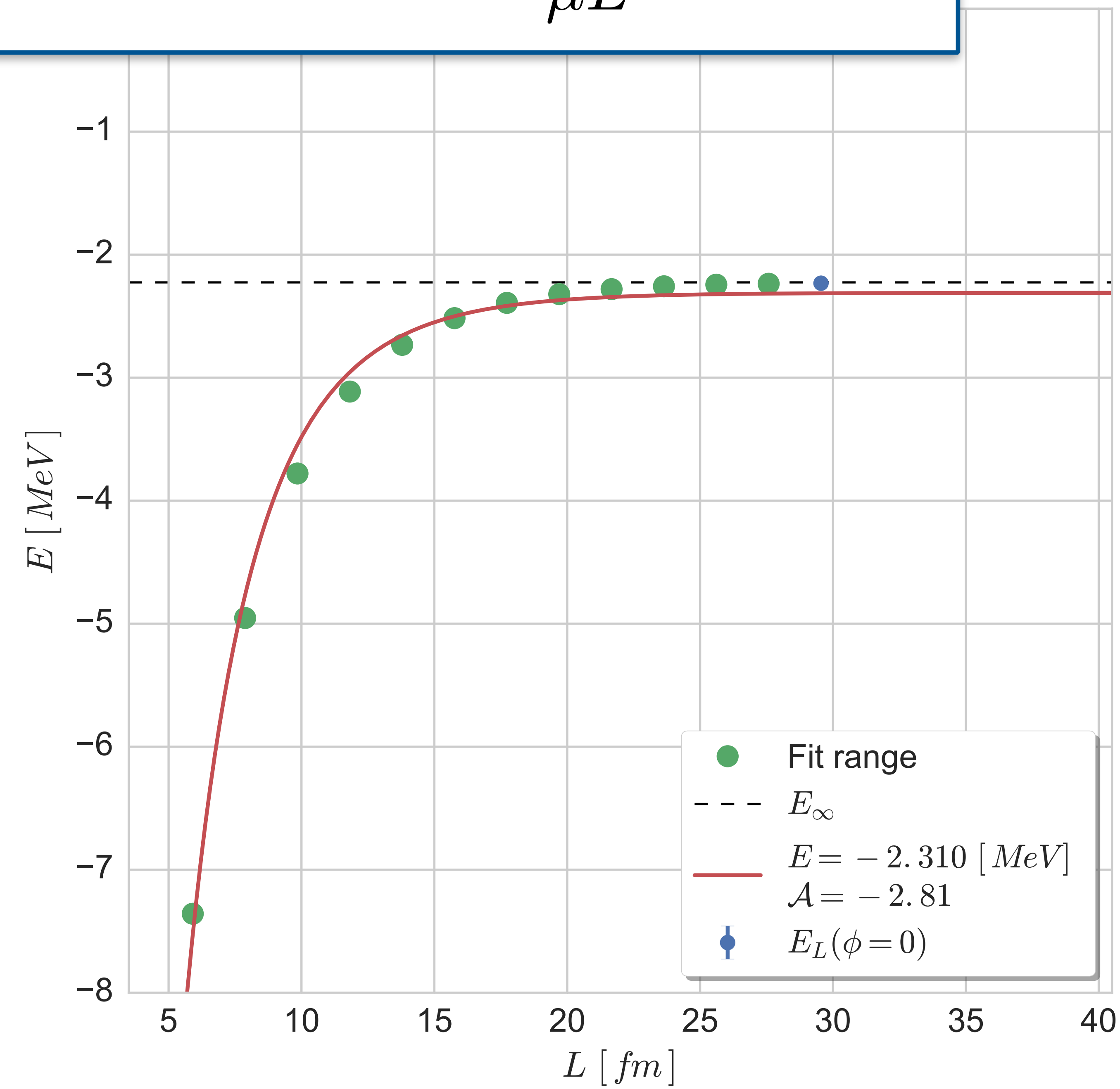


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties**
  Errors:
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

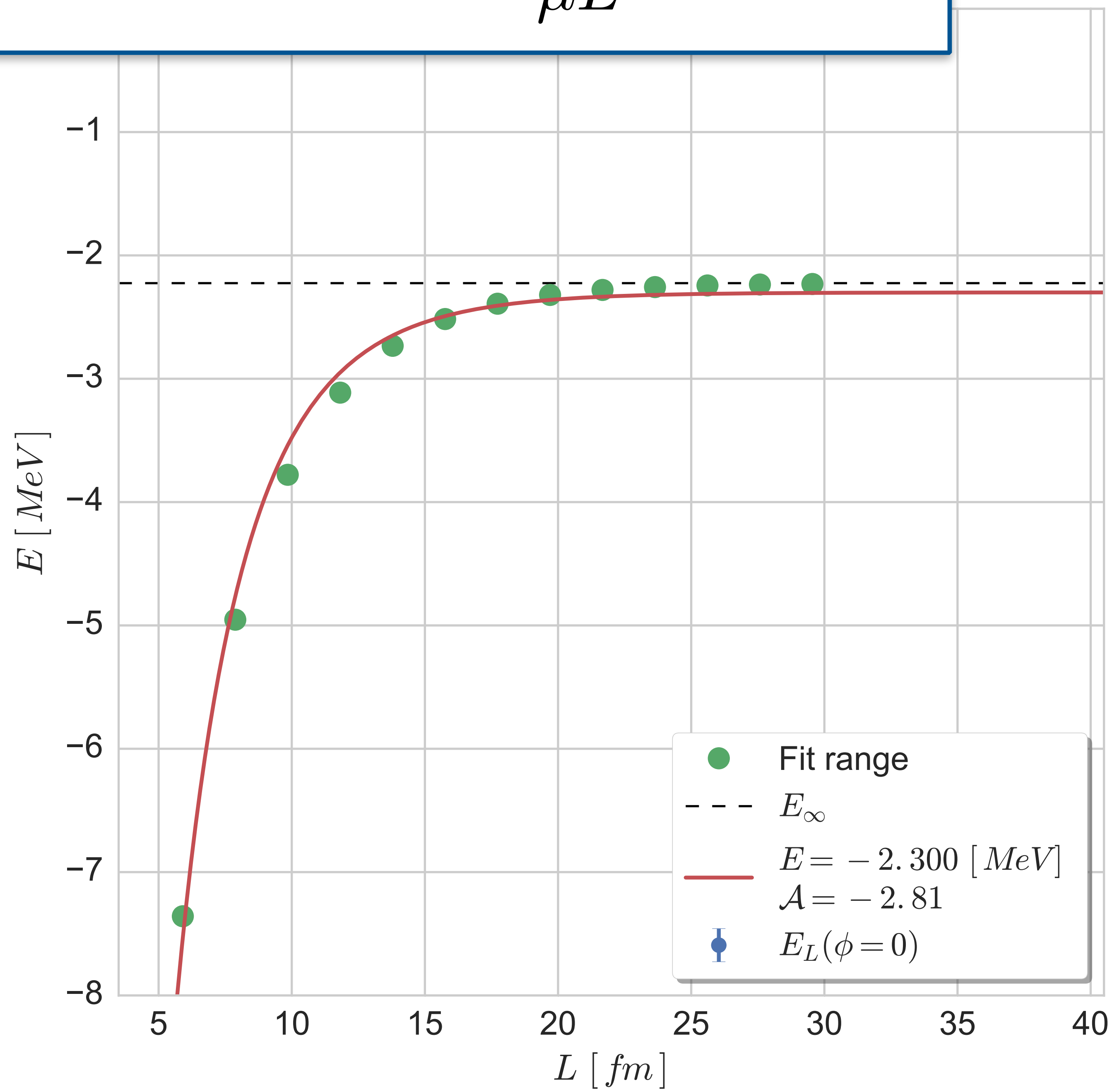


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

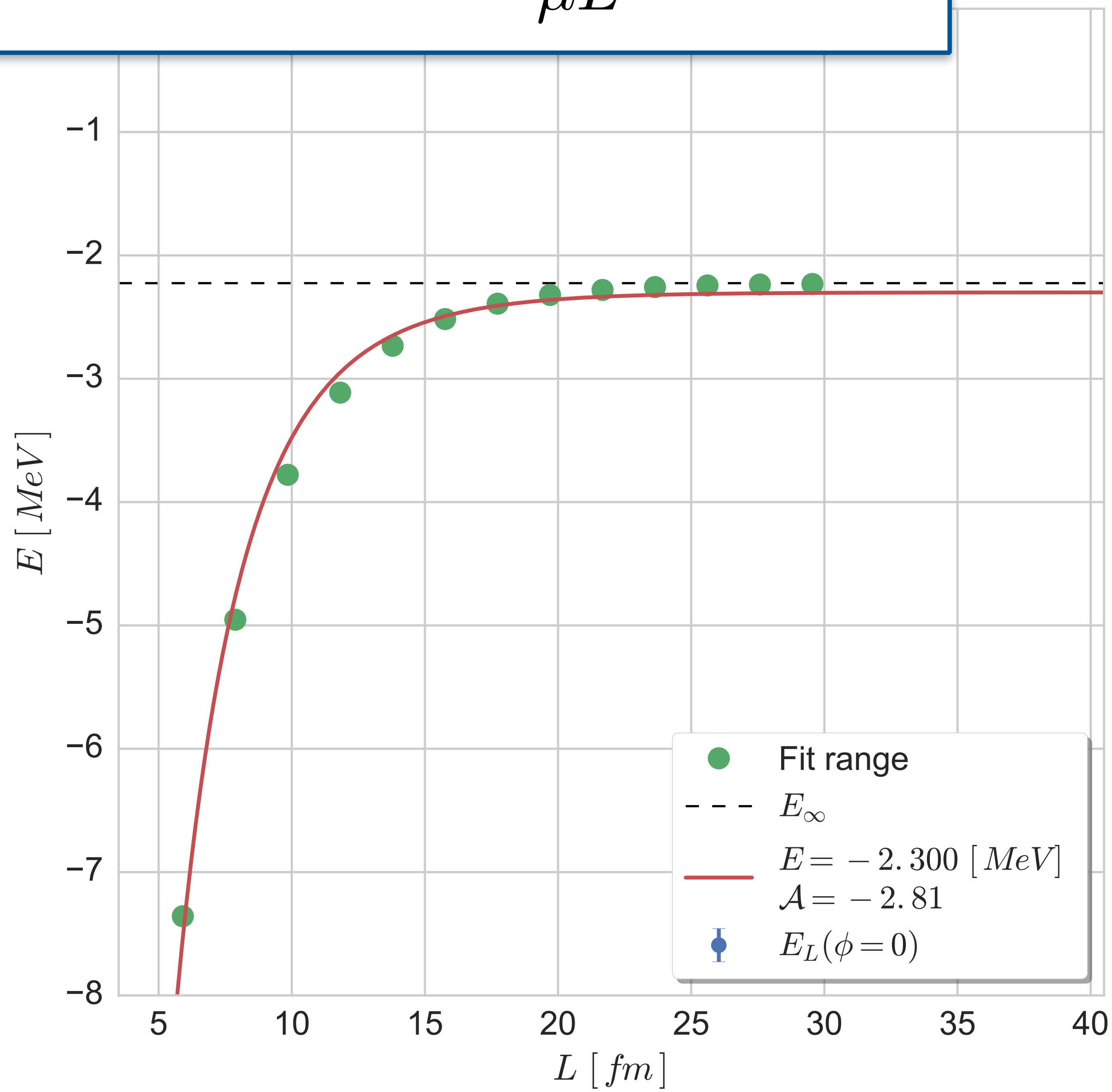


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

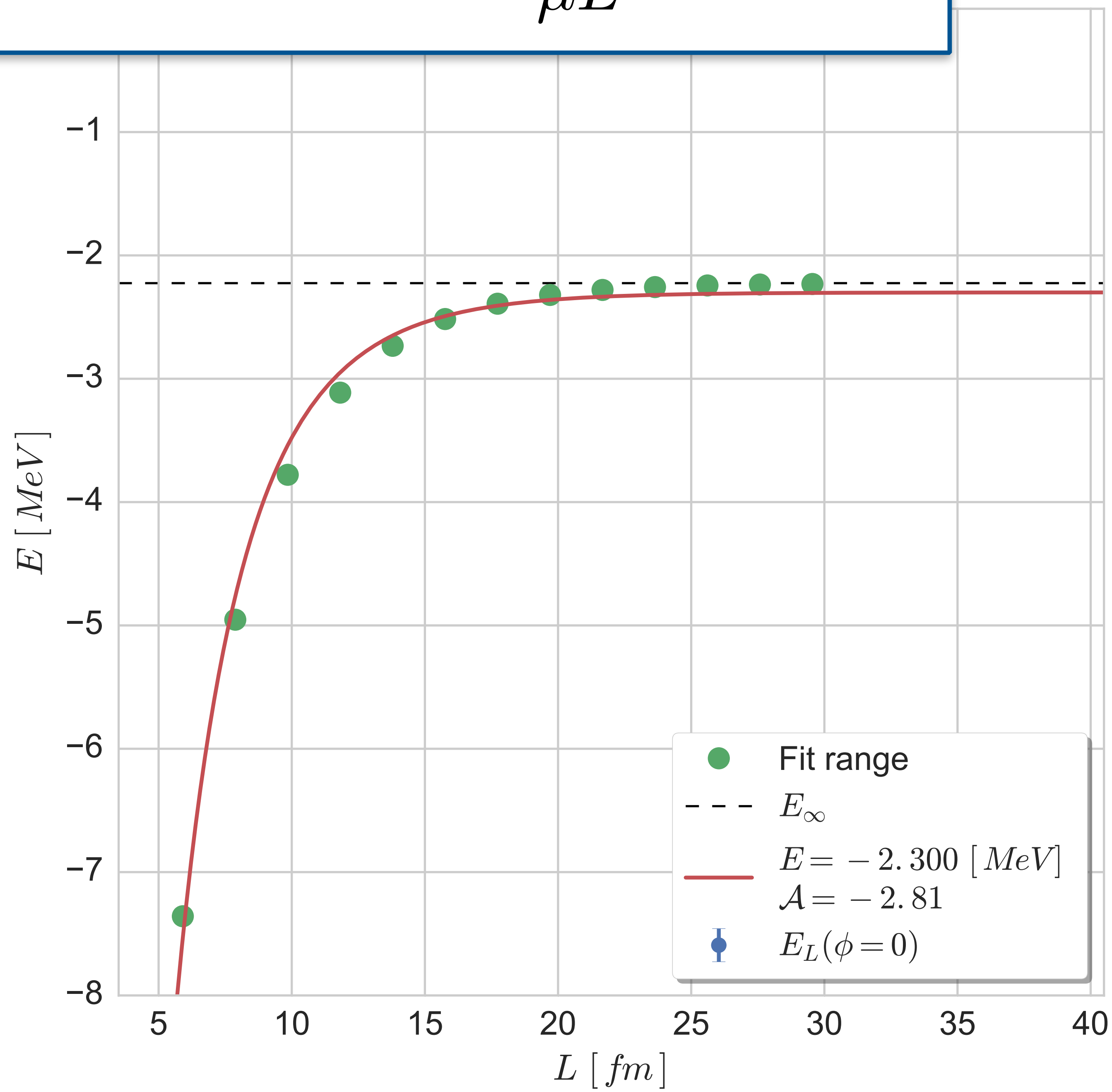
$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E) L}}{\mu L} \mathcal{A} + E$$



- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Convergence?

Error Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

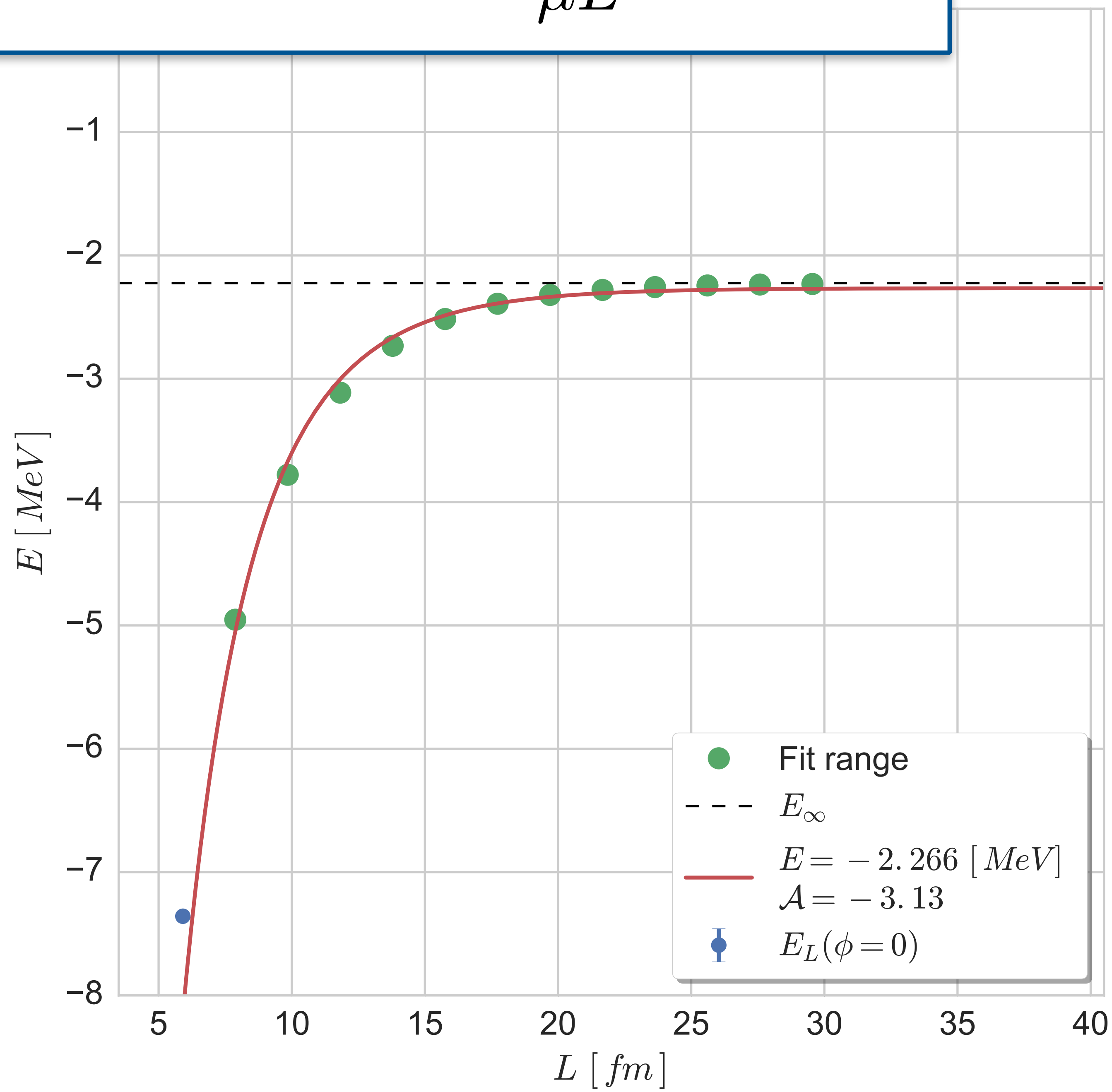


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

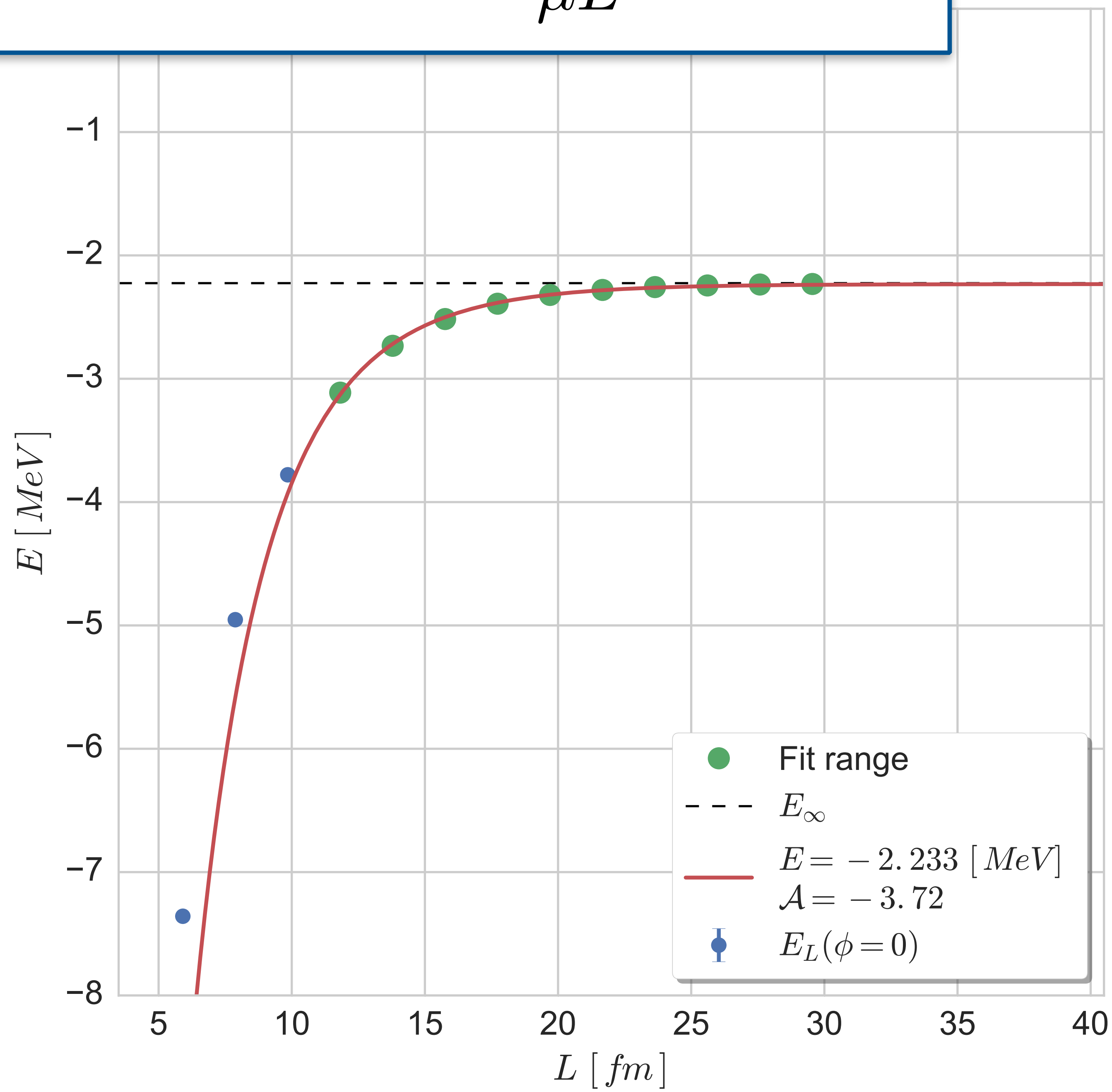


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

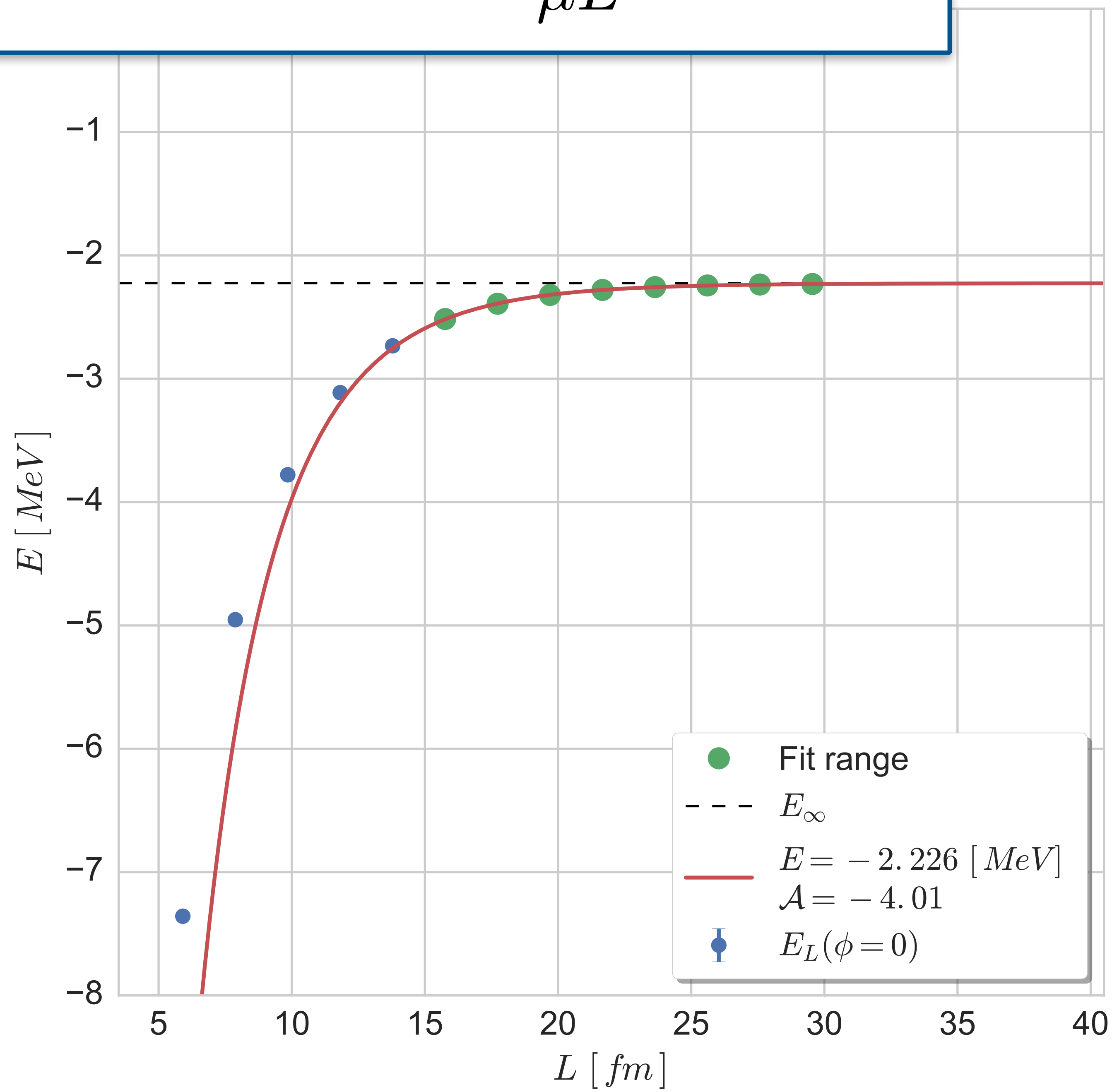


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

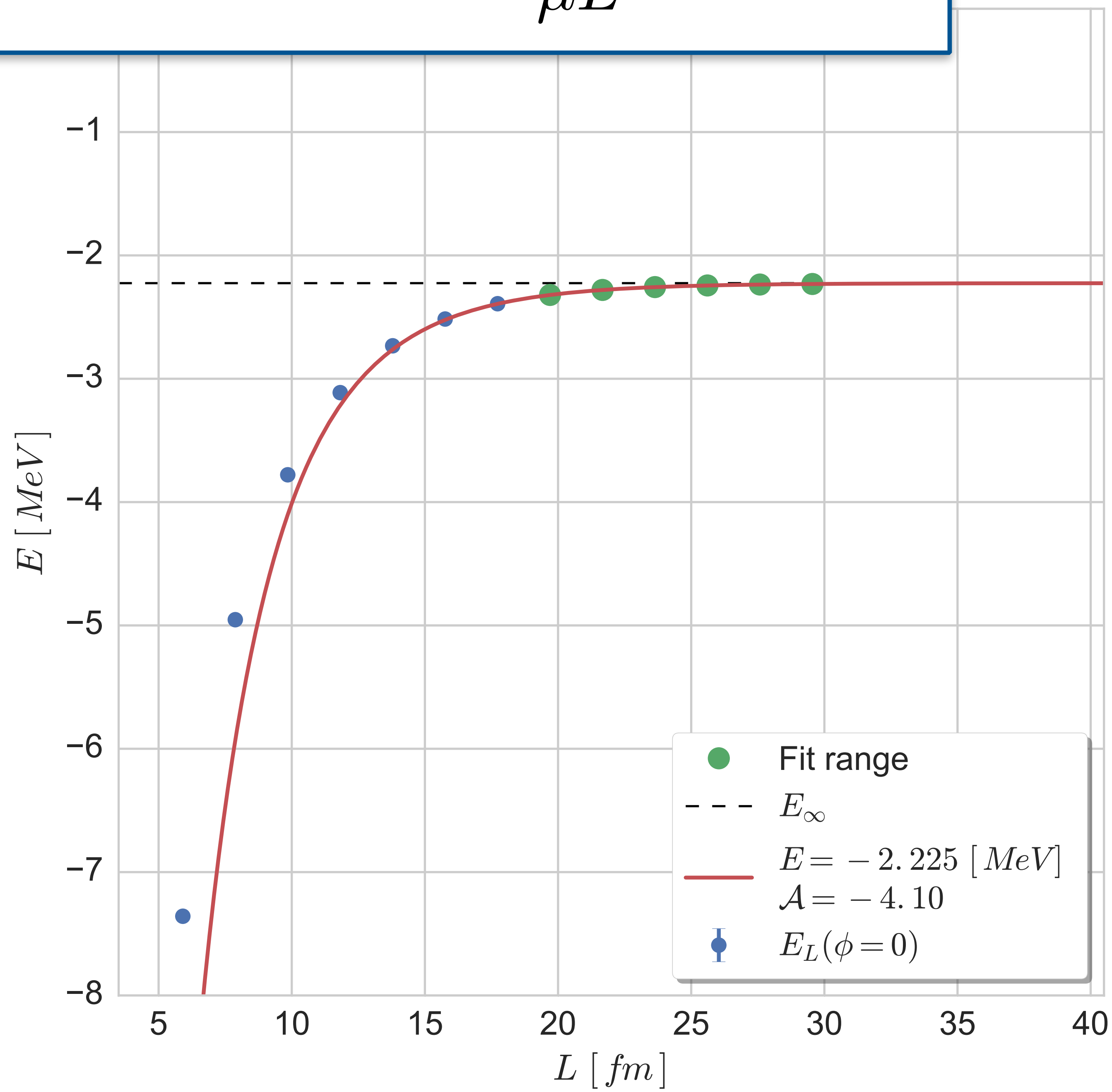


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \overset{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

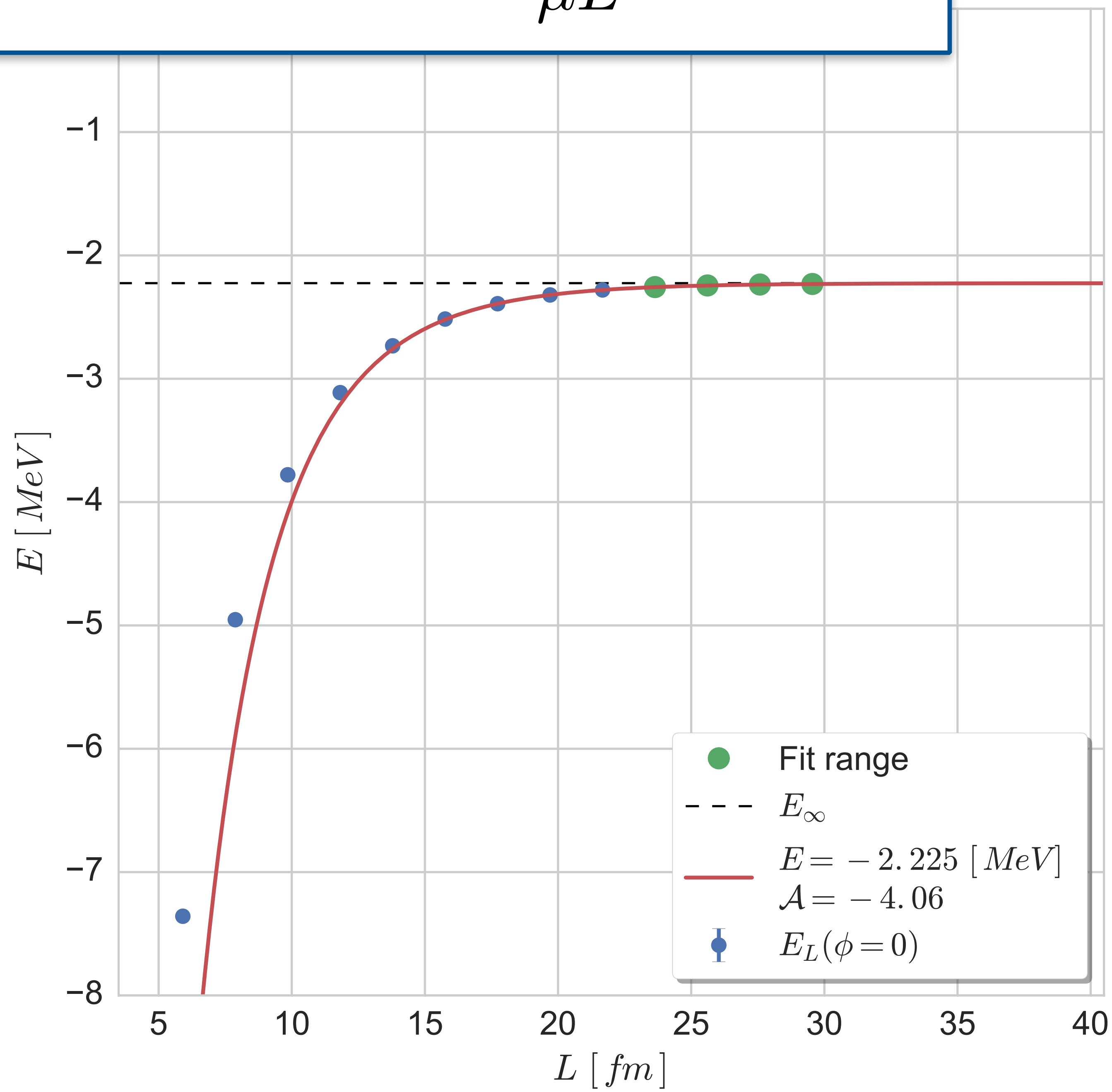


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \overset{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$

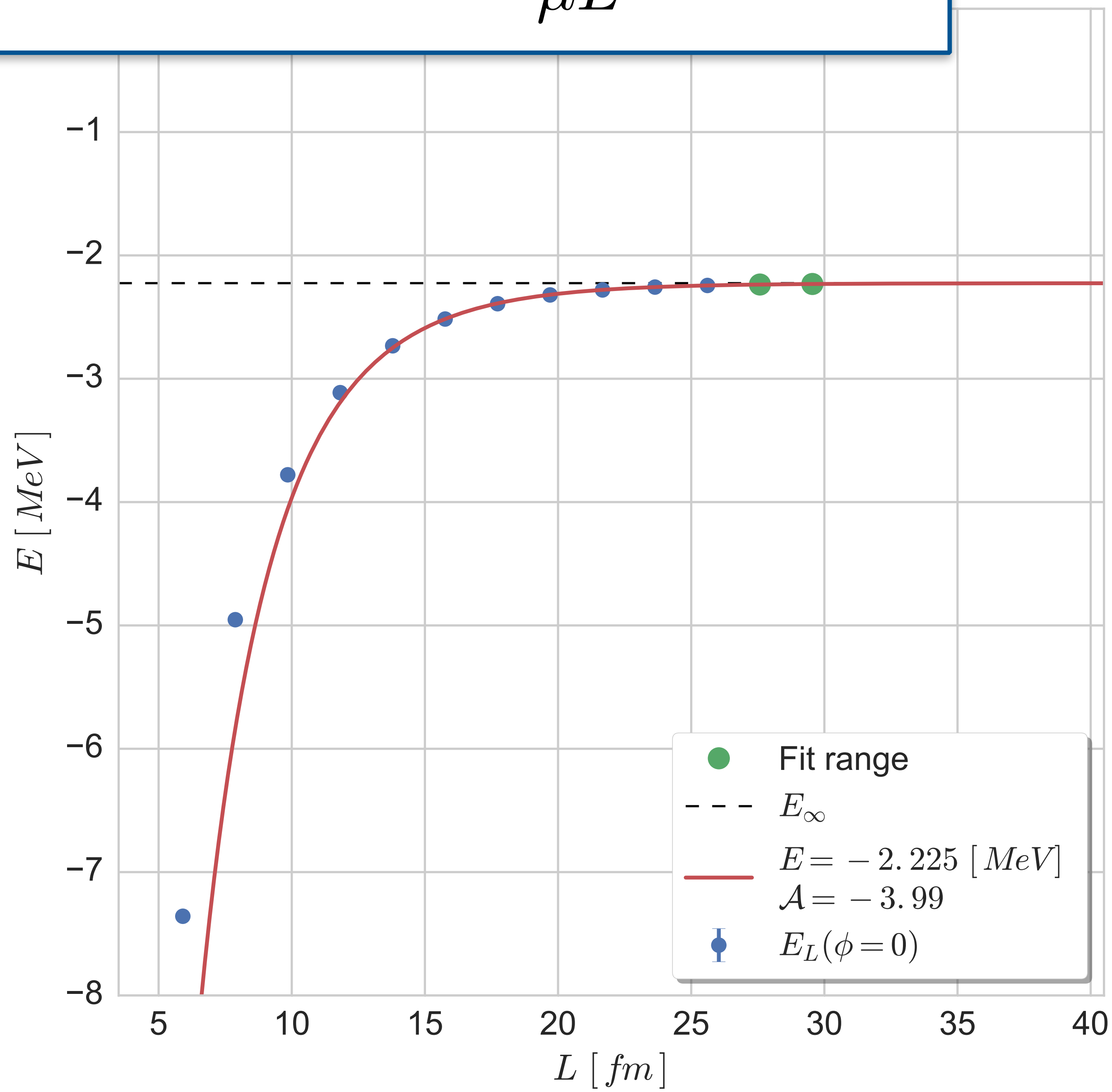


- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting

Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$E_L(E,\mathcal{A}) \overset{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L}\mathcal{A} + E$$



$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$

- **Goal:**
  Reliable results for small boxes
- **Data uncertainties Errors:**
  Numerical errors
- **Problem:**
  Results for small boxes affect fitting
- **Solution:**
  'Re-weight' data points

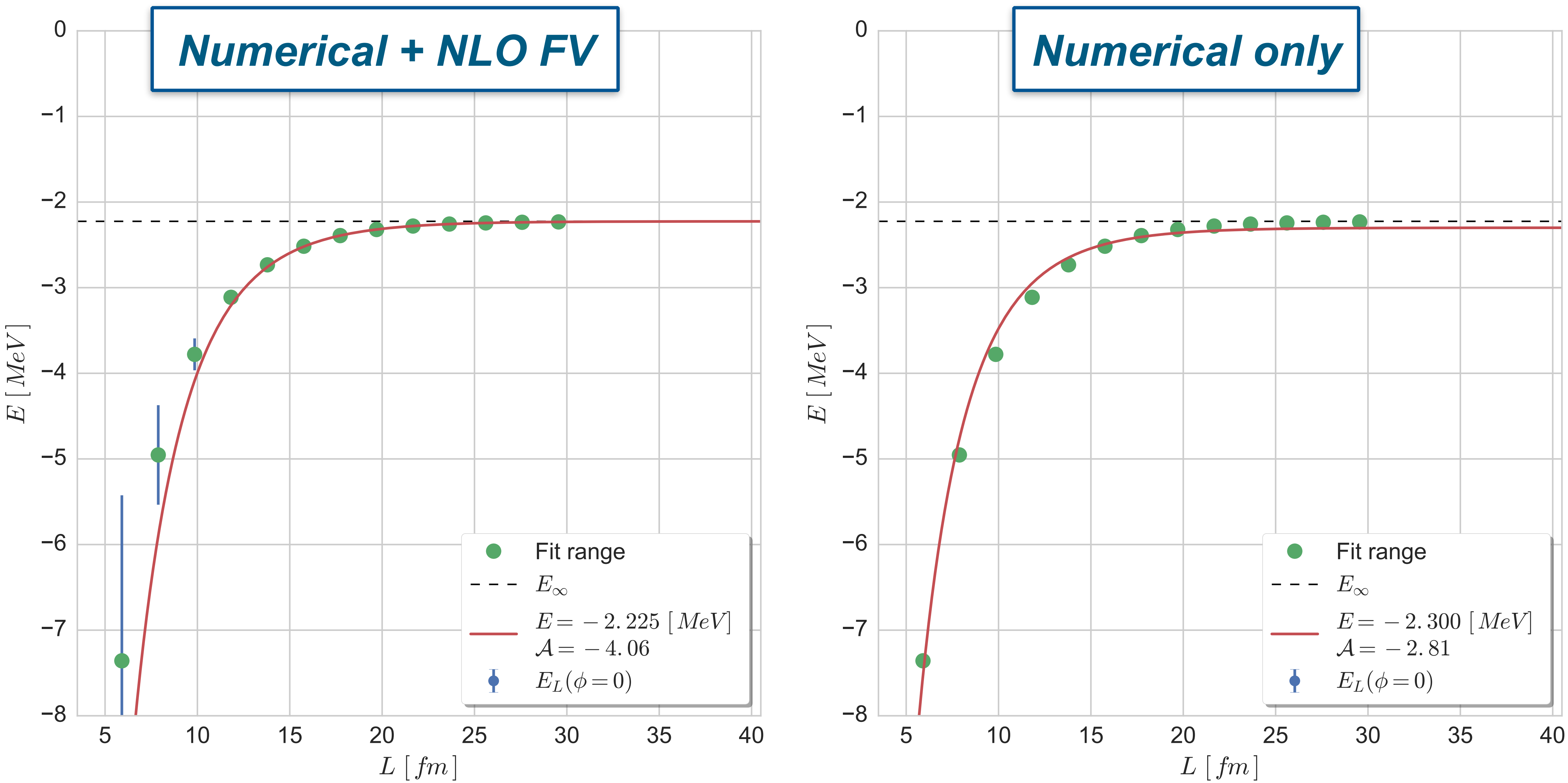
Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$\Delta E_L^{(NLO)} \simeq A_0 \frac{e^{-\sqrt{2}\kappa L}}{\mu L}$$

$$E_L(L,\phi) - E_\infty \simeq \Delta E_L^{(LO)}(L,\phi) + \Delta E_L^{(NLO)}(L,\phi) =: \Delta E_L^{(LO)}(L,\phi) + \delta(\Delta E_L^{(LO)}(L,\phi))$$

$E = -2.225\ [MeV]$
$\mathcal{A} = -3.99$



Mitglied der Helmholtz-Gemeinschaft

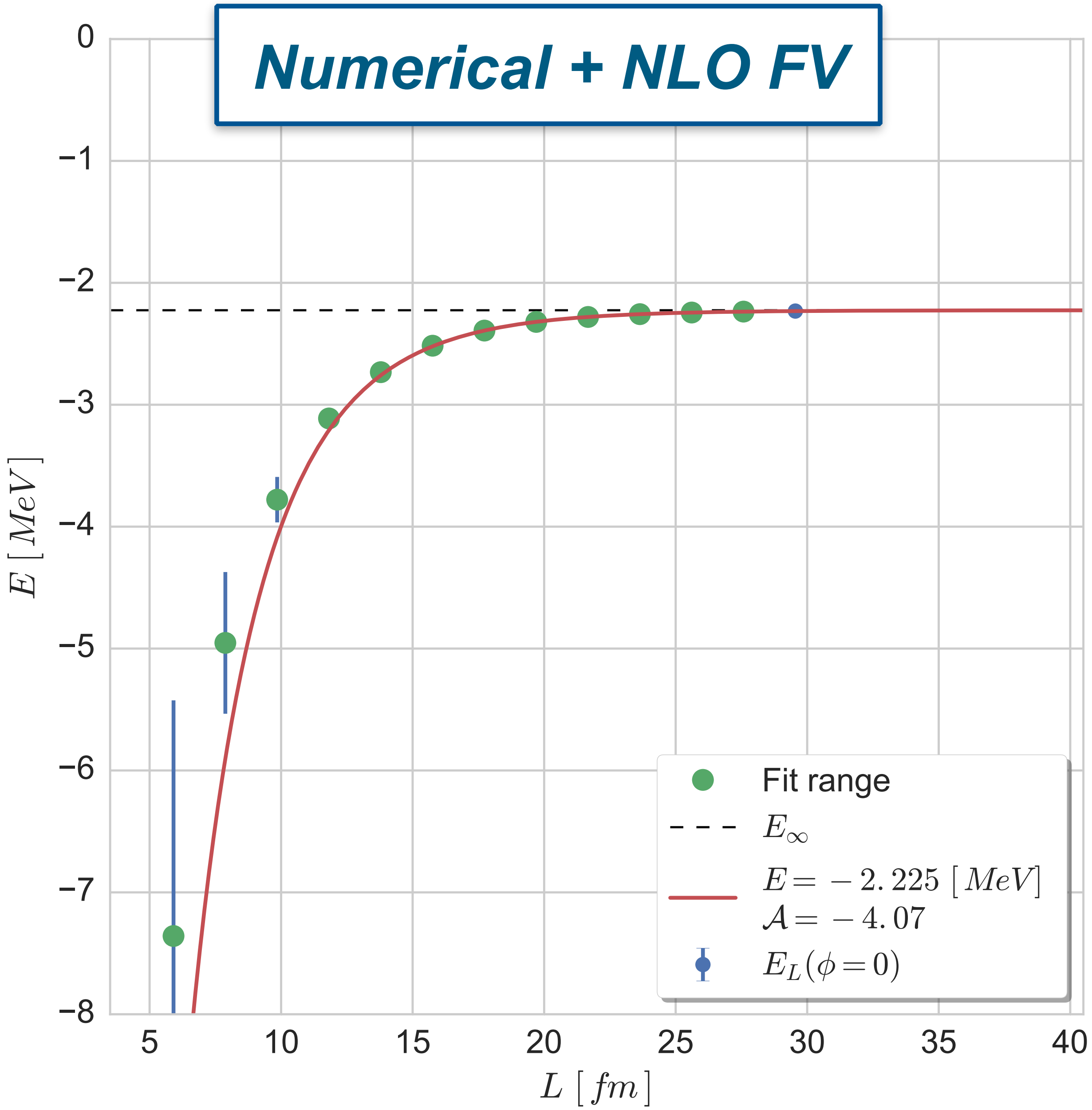
Error Analysis

$$\Delta E_L^{(NLO)} \simeq A_0 \frac{e^{-\sqrt{2}\kappa L}}{\mu L}$$

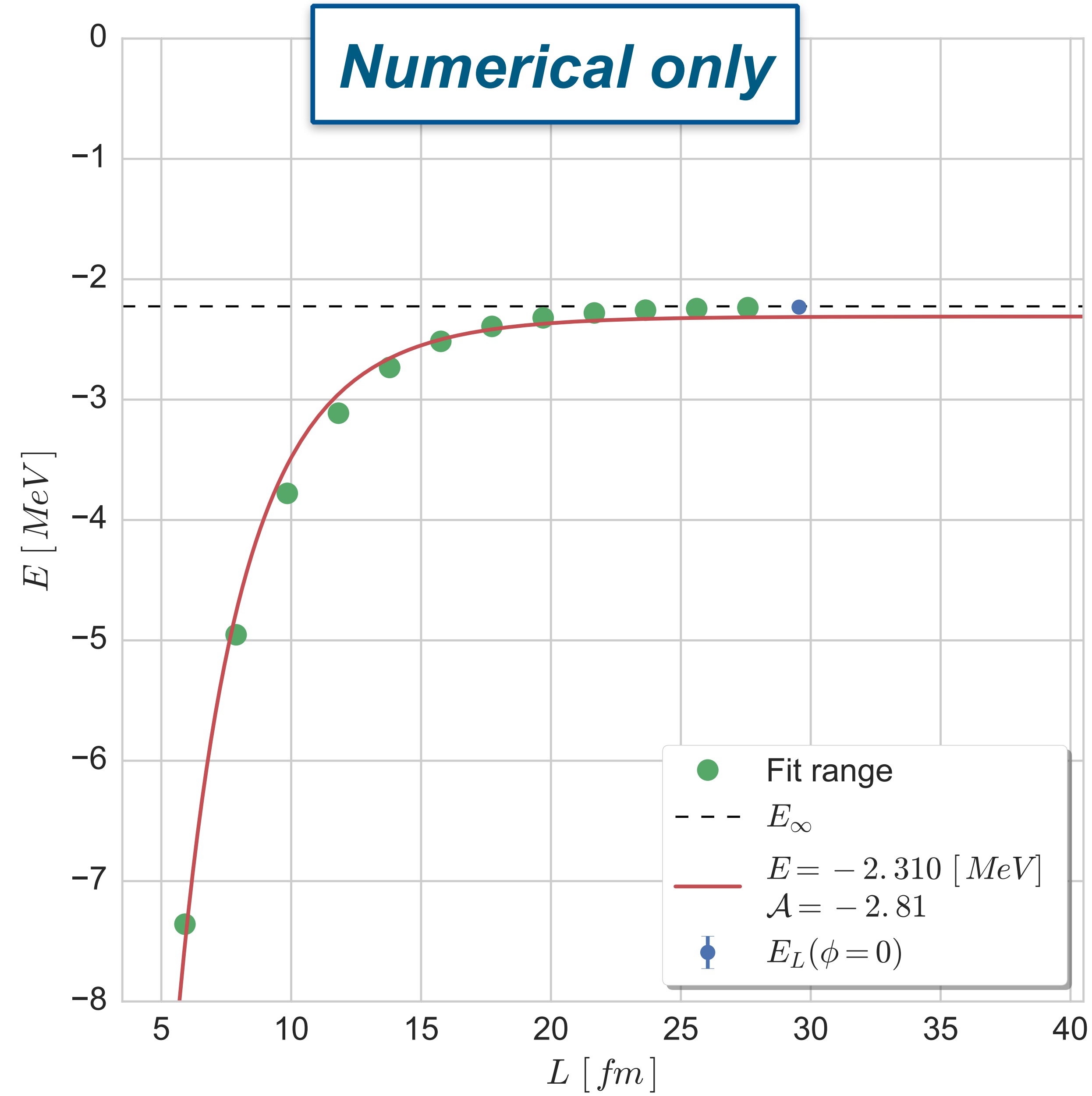
$$E_L(L,\phi) - E_\infty \simeq \Delta E_L^{(LO)}(L,\phi) + \Delta E_L^{(NLO)}(L,\phi)$$
$$=: \Delta E_L^{(LO)}(L,\phi) + \delta(\Delta E_L^{(LO)}(L,\phi))$$

$E = -2.225\ [MeV]$
$\mathcal{A} = -3.99$

Numerical + NLO FV



Numerical only

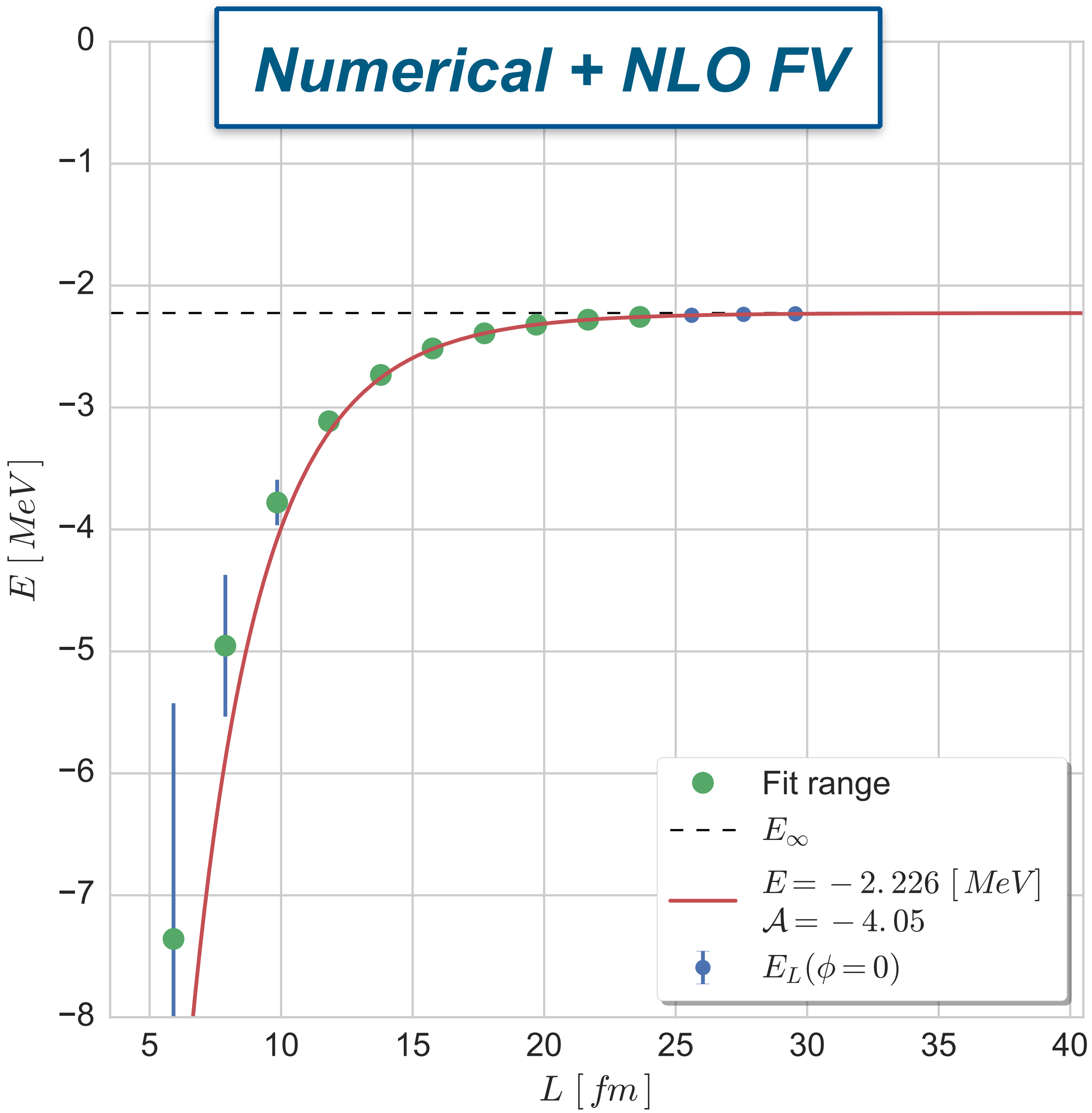


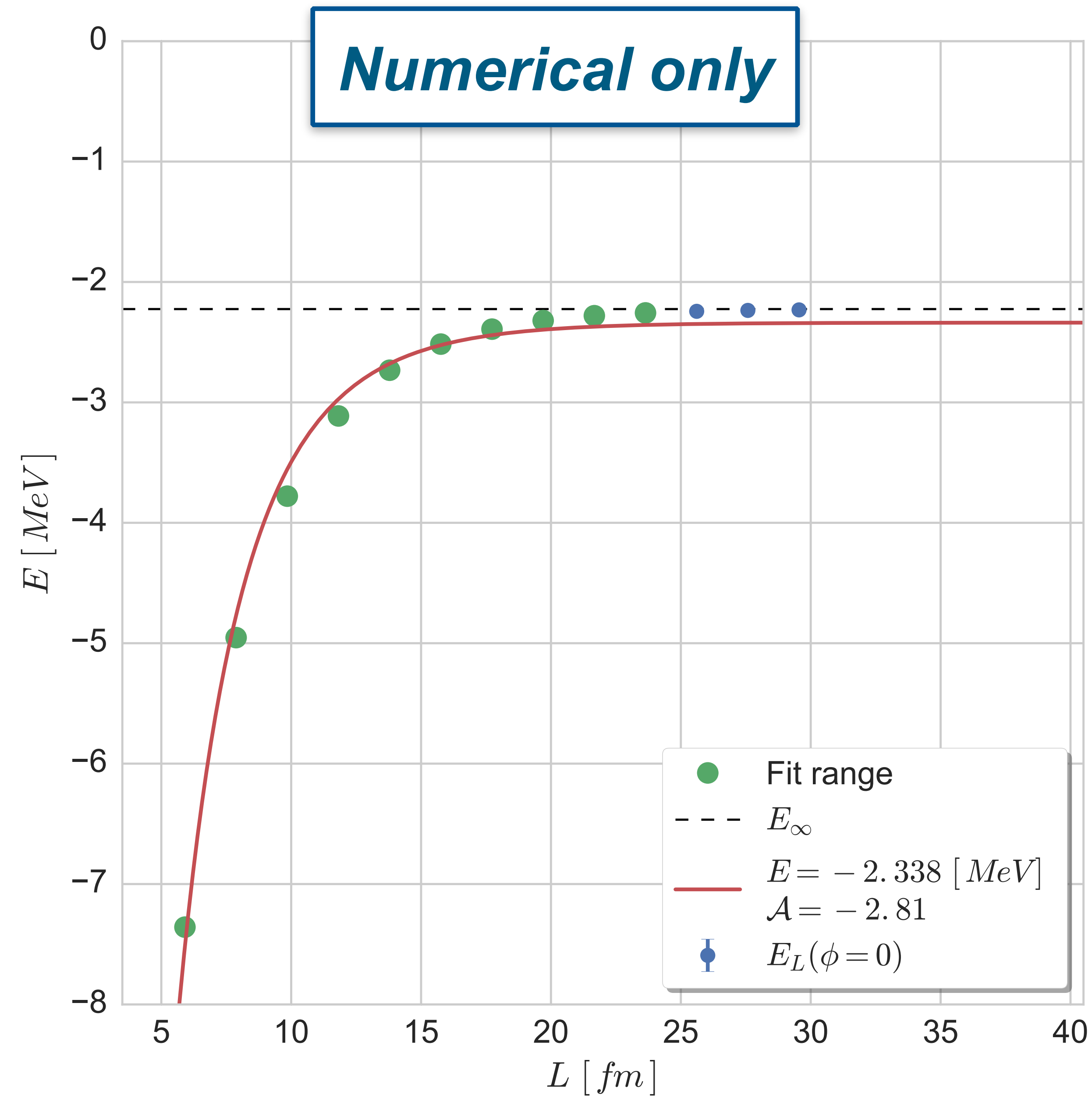
Error Analysis

$$\Delta E_L^{(NLO)} \simeq A_0 \frac{e^{-\sqrt{2}\kappa L}}{\mu L}$$

$$E_L(L,\phi) - E_\infty \simeq \Delta E_L^{(LO)}(L,\phi) + \Delta E_L^{(NLO)}(L,\phi)$$
$$=: \Delta E_L^{(LO)}(L,\phi) + \delta(\Delta E_L^{(LO)}(L,\phi))$$

$E = -2.225\ [MeV]$
$\mathcal{A} = -3.99$





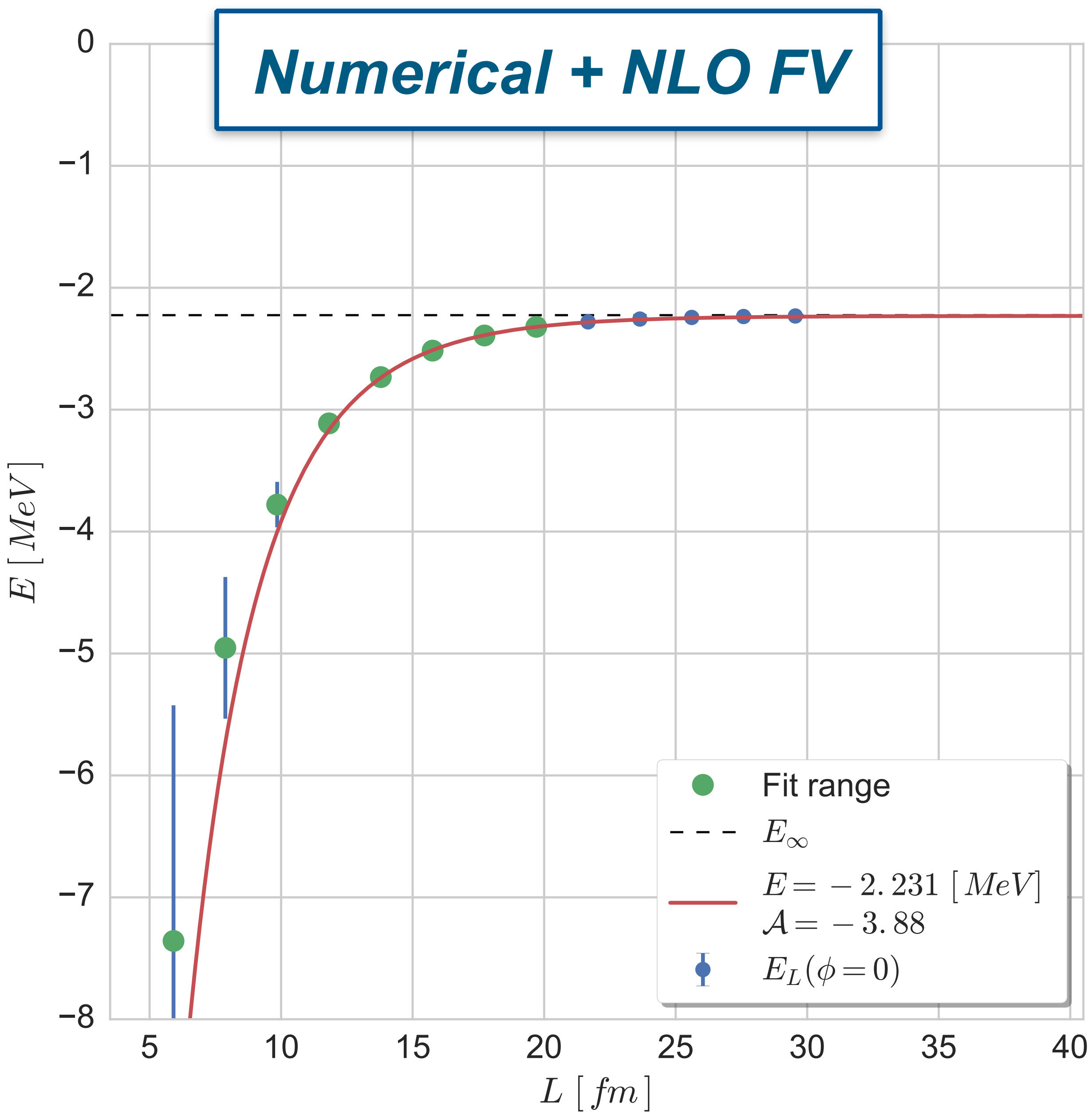
Mitglied der Helmholtz-Gemeinschaft

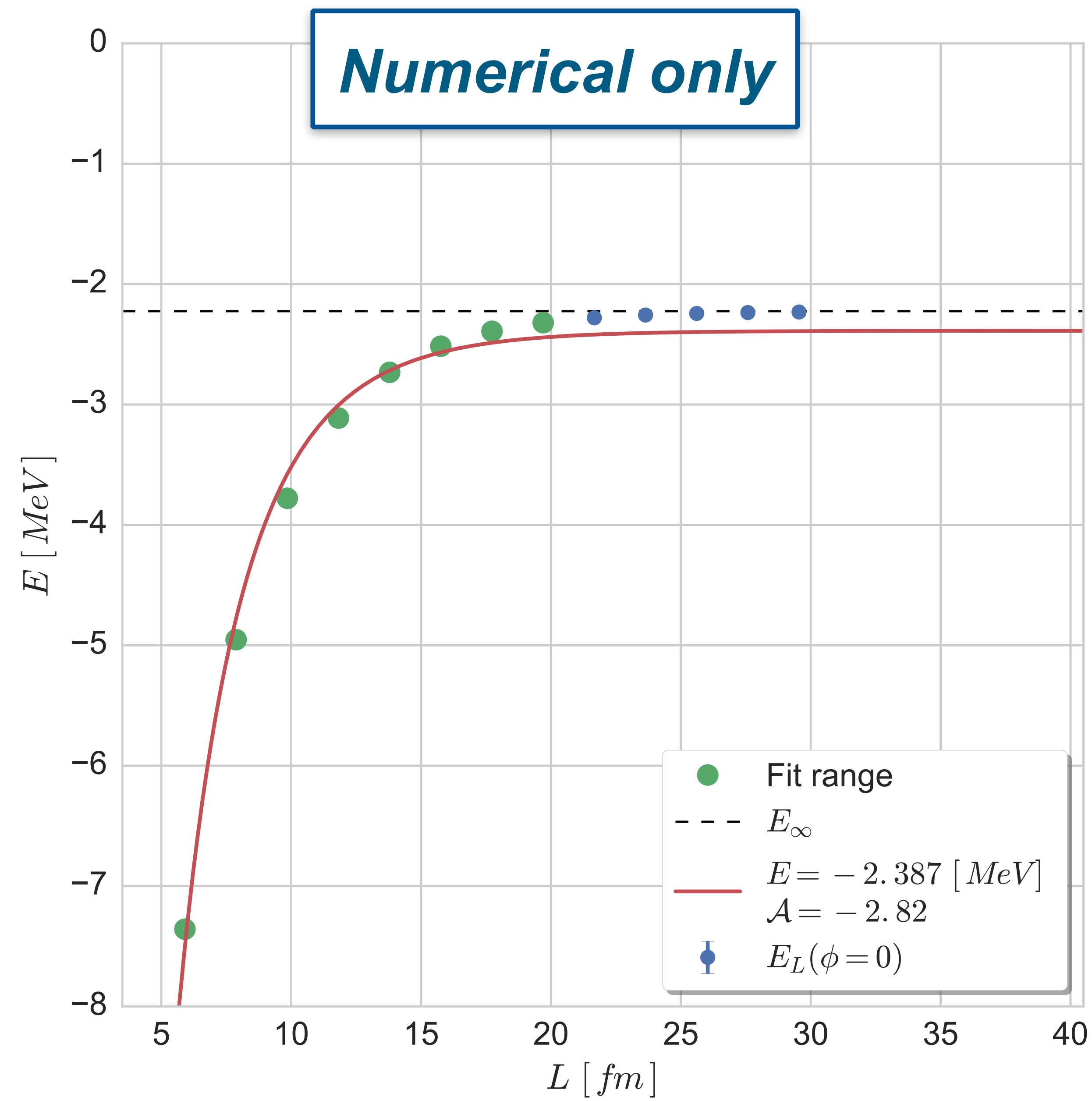
Error Analysis

$$\Delta E_L^{(NLO)} \simeq A_0 \frac{e^{-\sqrt{2}\kappa L}}{\mu L}$$

$$\begin{aligned} E_L(L,\phi) - E_\infty &\simeq \Delta E_L^{(LO)}(L,\phi) + \Delta E_L^{(NLO)}(L,\phi) \\ &=: \Delta E_L^{(LO)}(L,\phi) + \delta(\Delta E_L^{(LO)}(L,\phi)) \end{aligned}$$

$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$





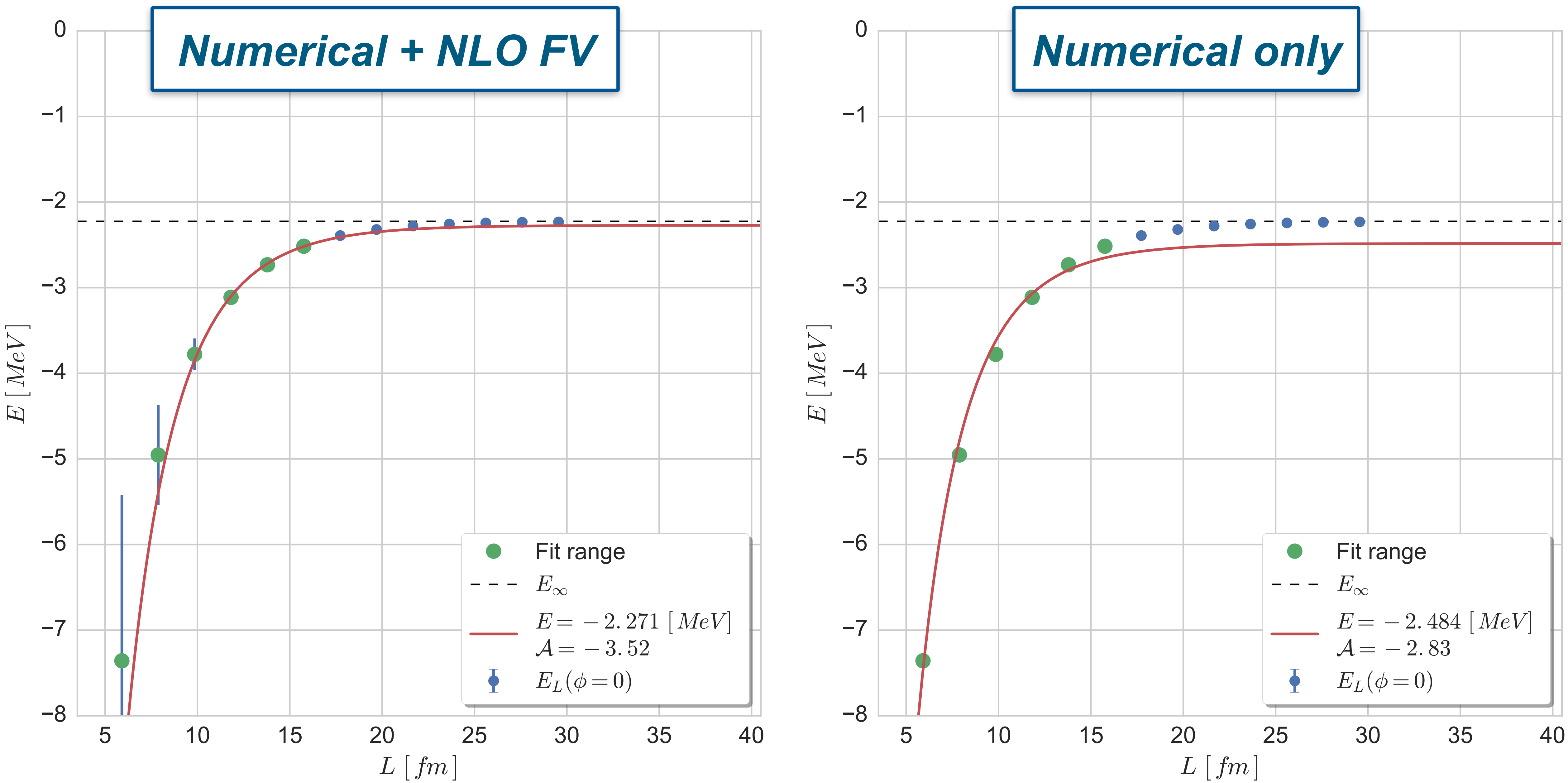
Mitglied der Helmholtz-Gemeinschaft

Error Analysis

$$\Delta E_L^{(NLO)} \simeq A_0 \frac{e^{-\sqrt{2}\kappa L}}{\mu L}$$

$$E_L(L,\phi) - E_\infty \simeq \Delta E_L^{(LO)}(L,\phi) + \Delta E_L^{(NLO)}(L,\phi)$$
$$=: \Delta E_L^{(LO)}(L,\phi) + \delta(\Delta E_L^{(LO)}(L,\phi))$$

$E = -2.225\ [MeV]$
$\mathcal{A} = -3.99$



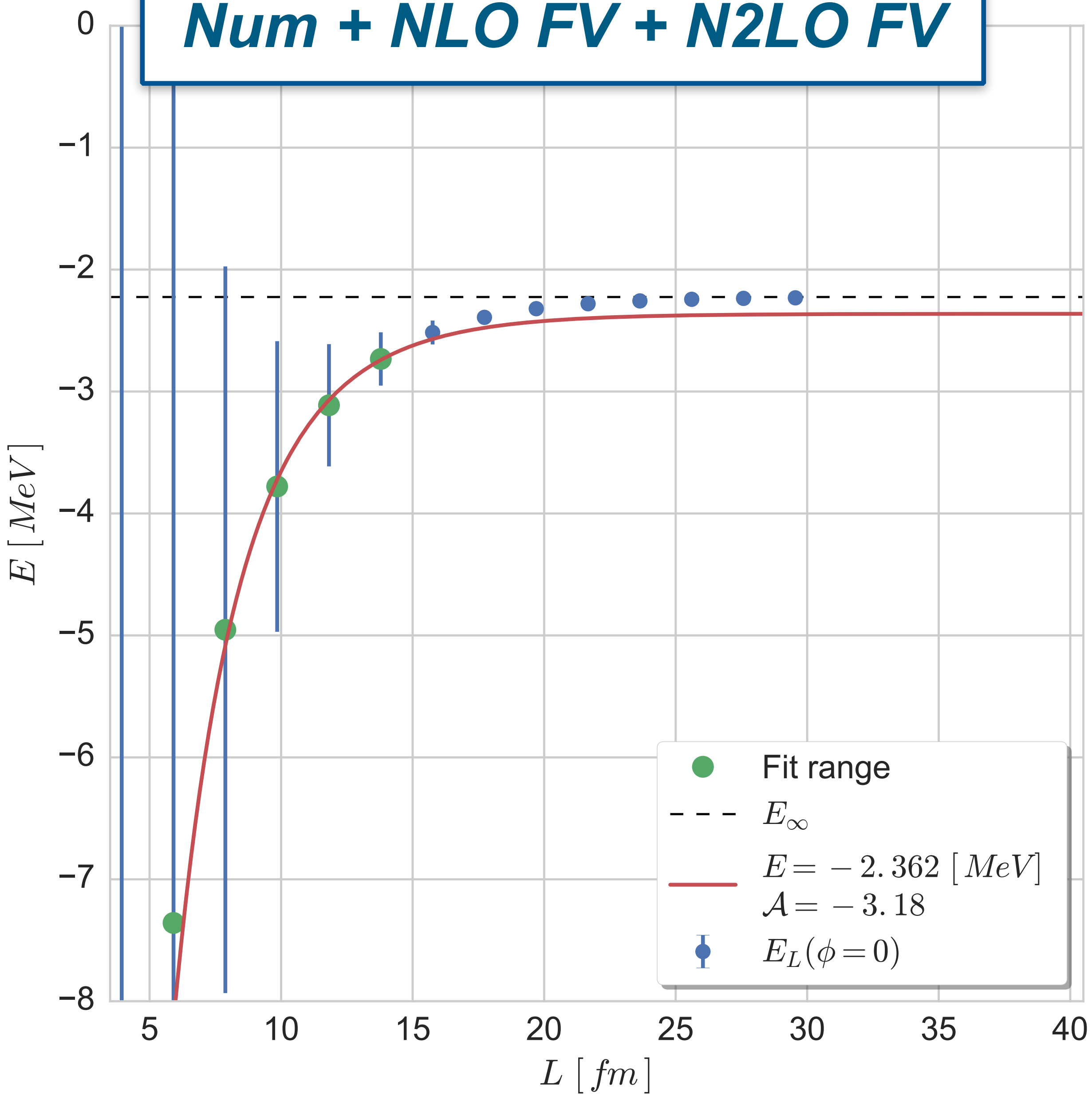
Mitglied der Helmholtz-Gemeinschaft

Error Analysis

- **Estimate uncertainty:**
  compute new correlated distributions within error bars for propagation

$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$

Num + NLO FV + N2LO FV

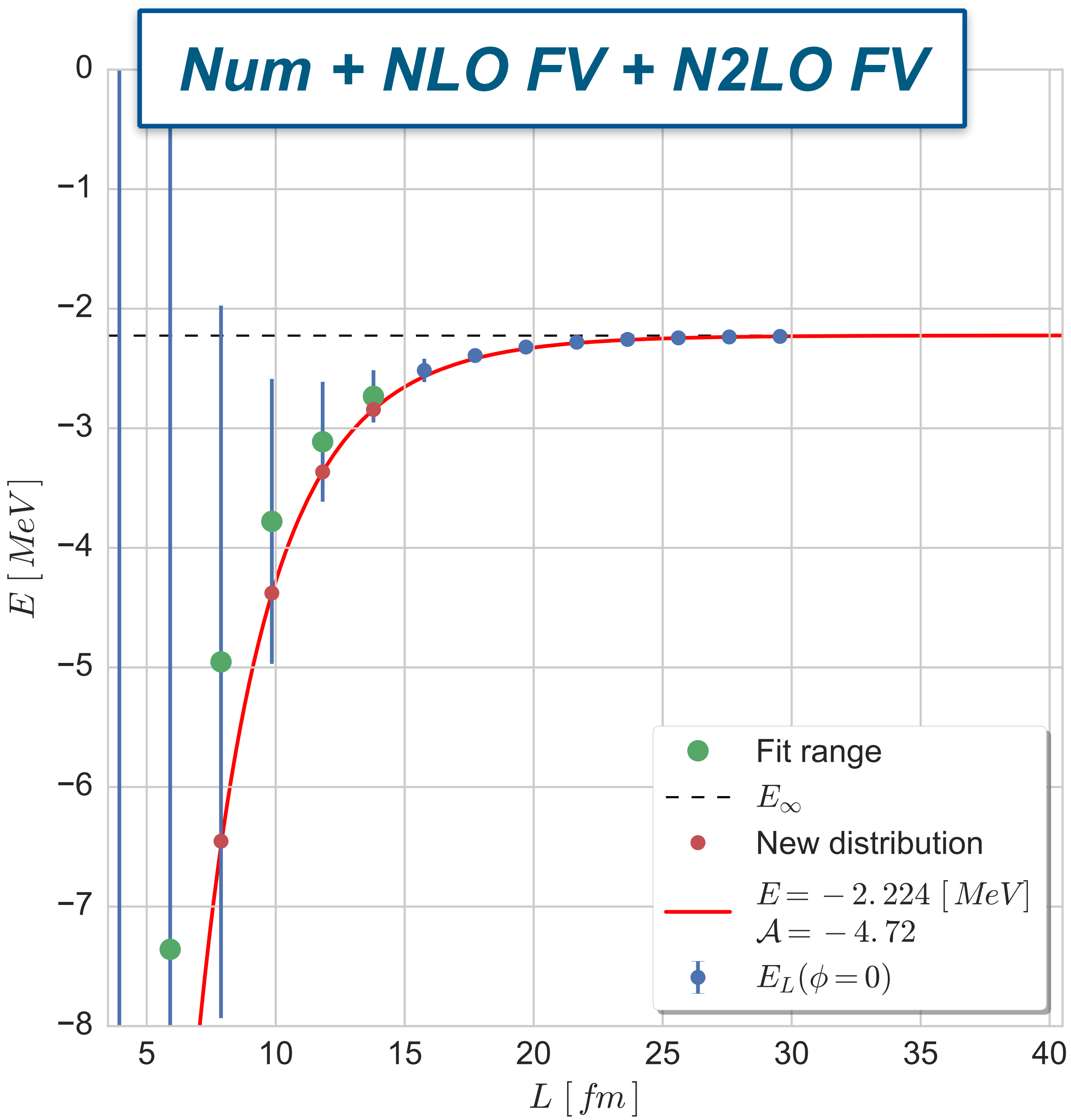


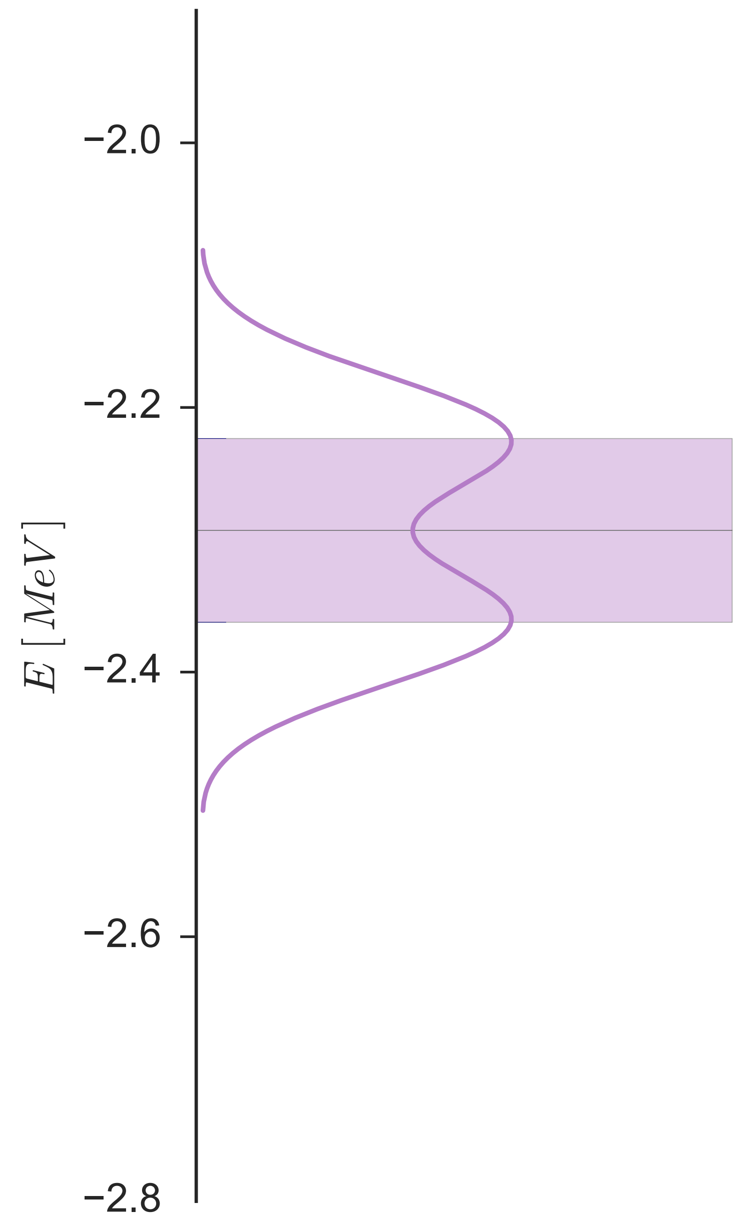
Mitglied der Helmholtz-Gemeinschaft

Error Analysis

- **Estimate uncertainty:**
  compute new correlated distributions within error bars for propagation

$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$

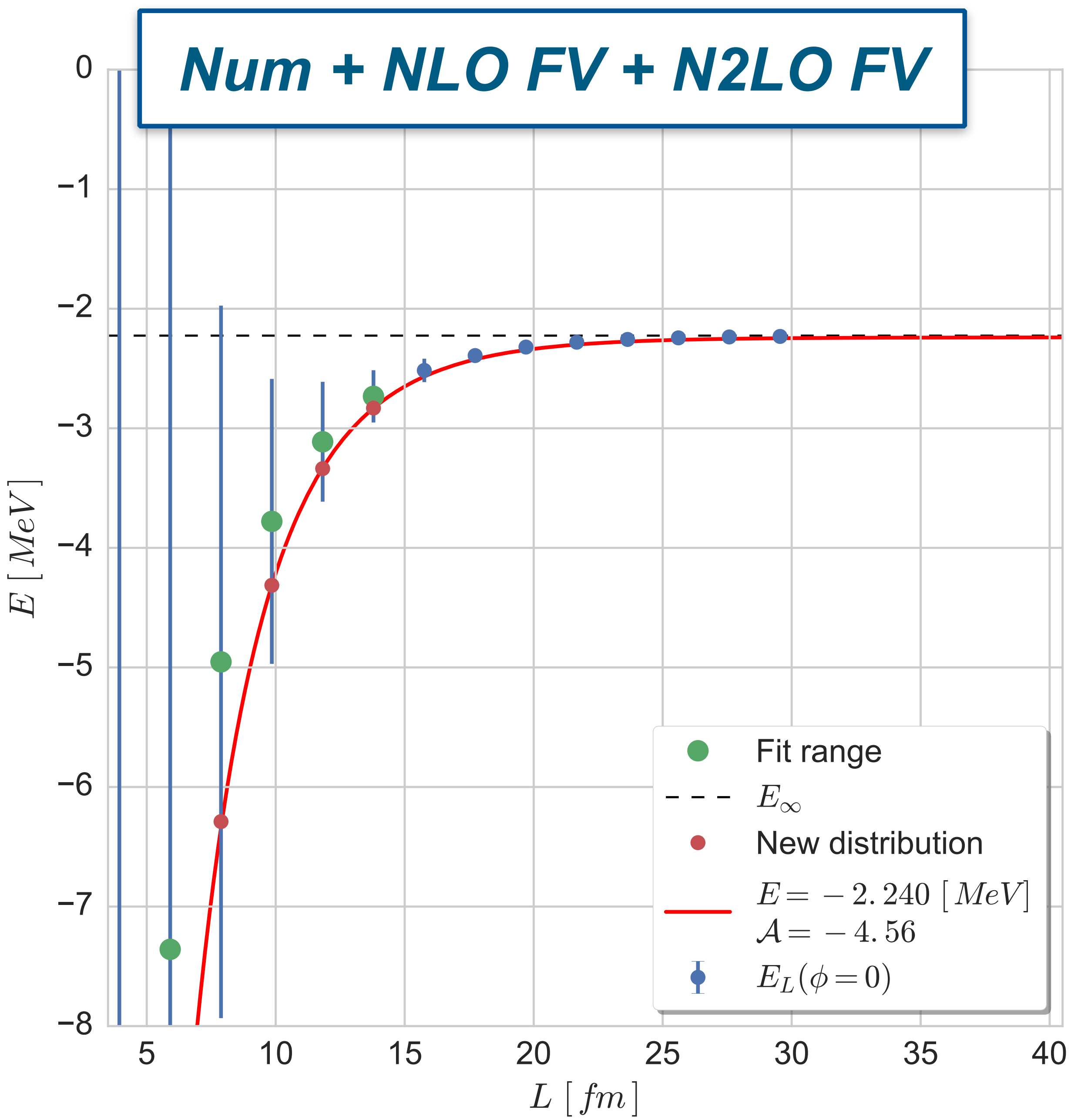


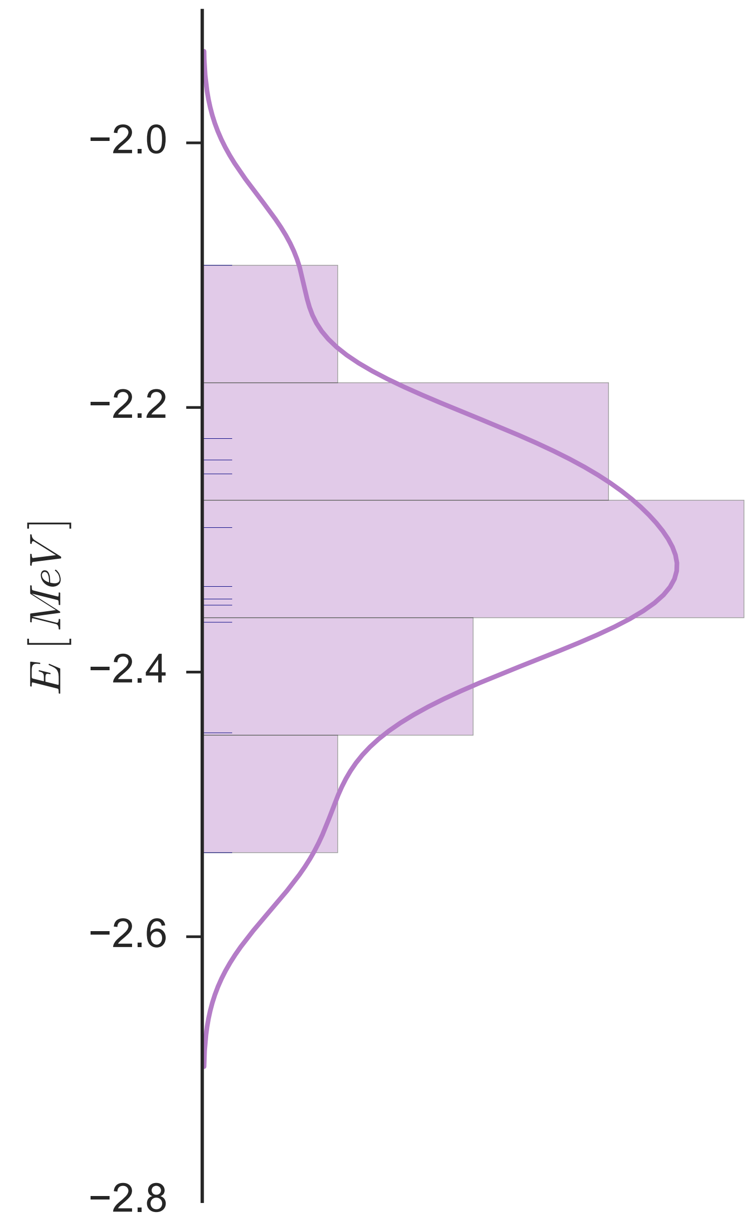


Error Analysis

- **Estimate uncertainty:**
  compute new correlated distributions within error bars for propagation

$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$





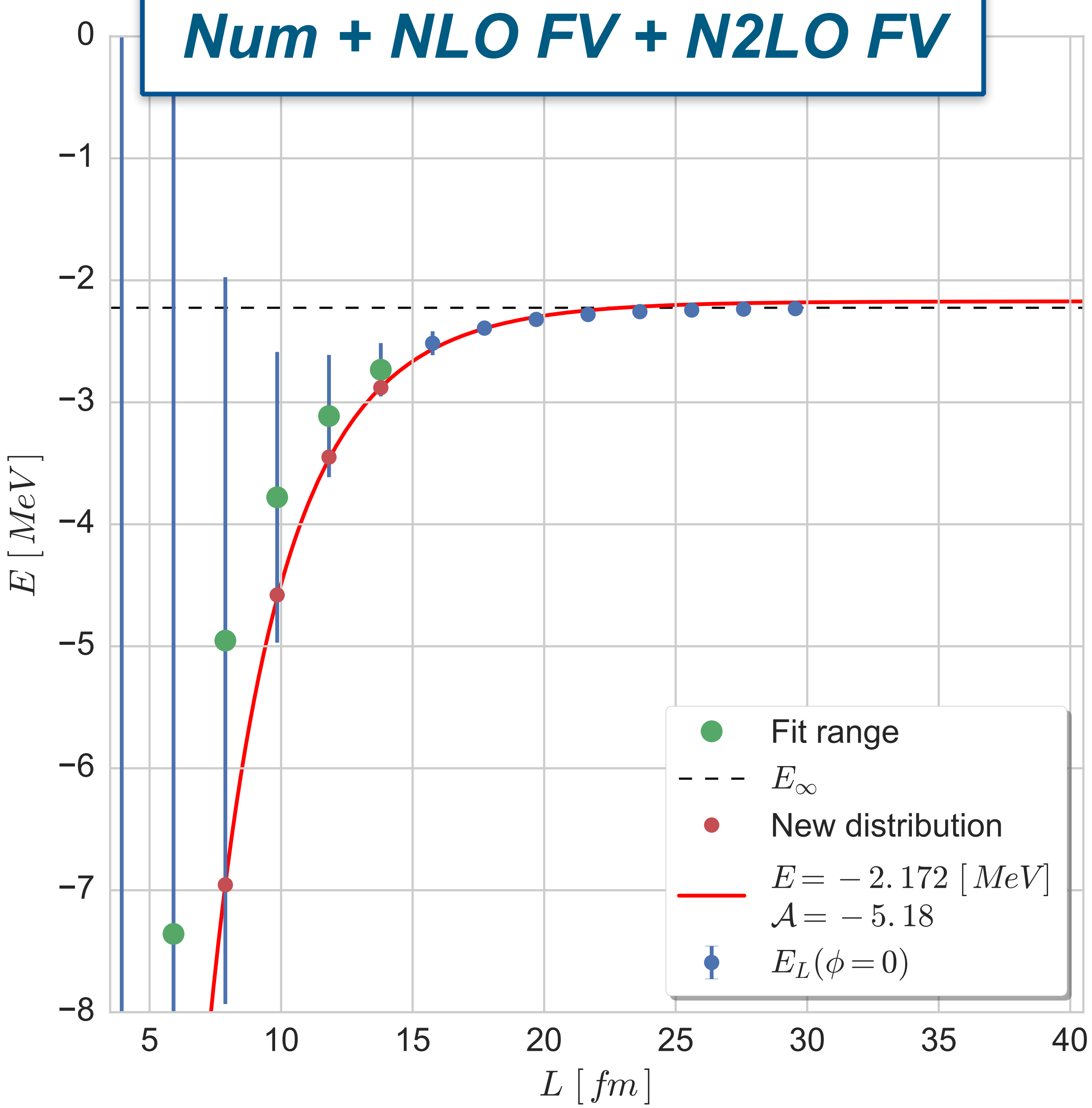
Mitglied der Helmholtz-Gemeinschaft

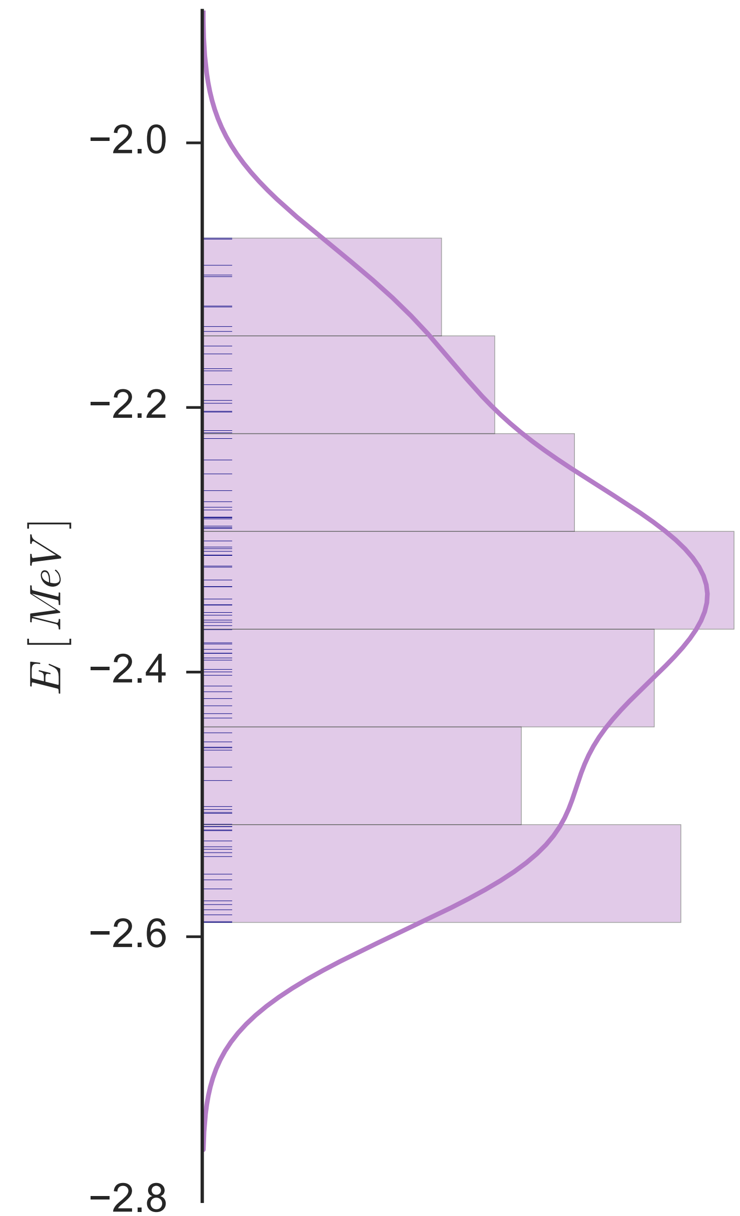
Error Analysis

- **Estimate uncertainty:**
  compute new correlated distributions within error bars for propagation

$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$

Num + NLO FV + N2LO FV



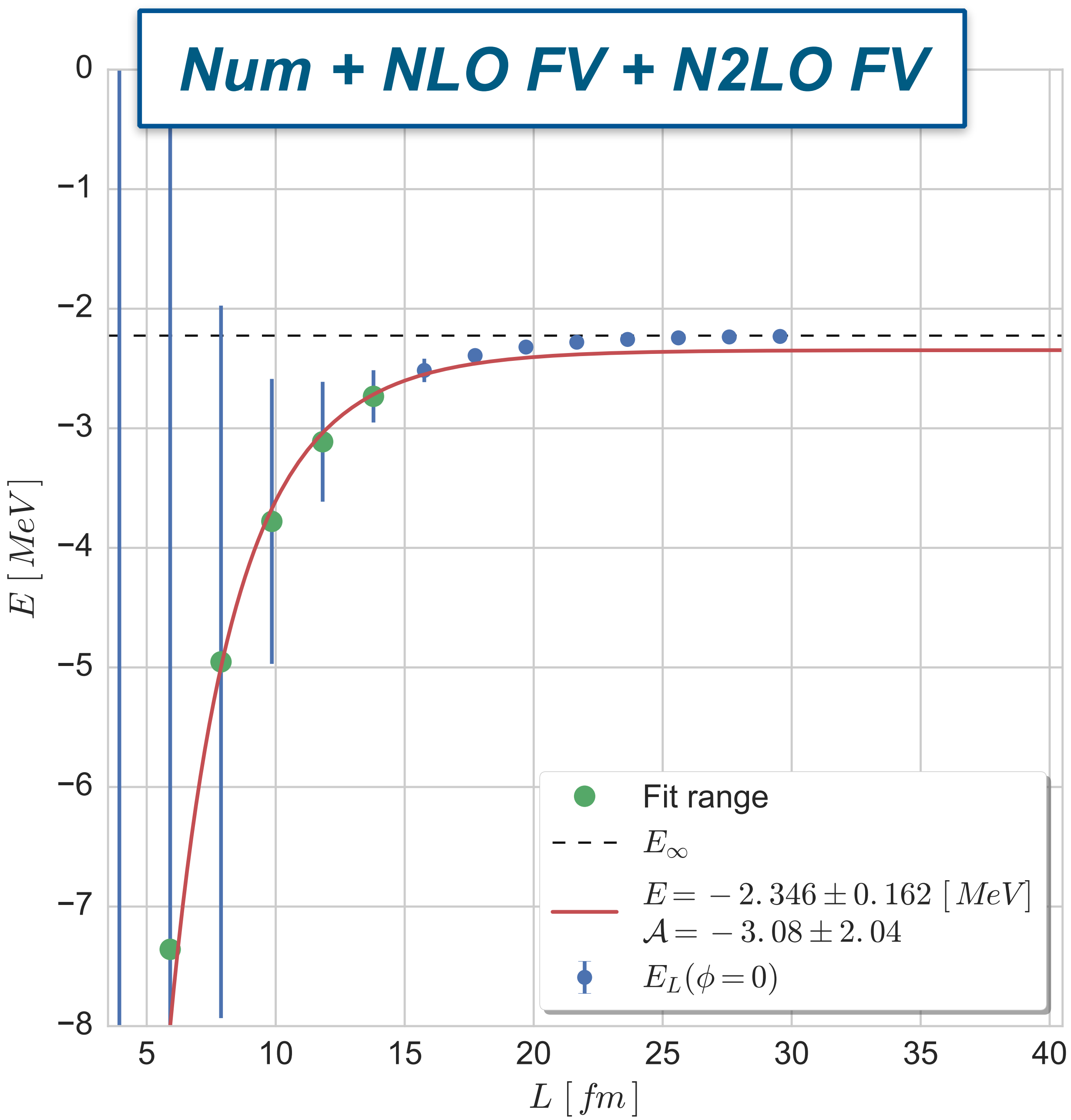


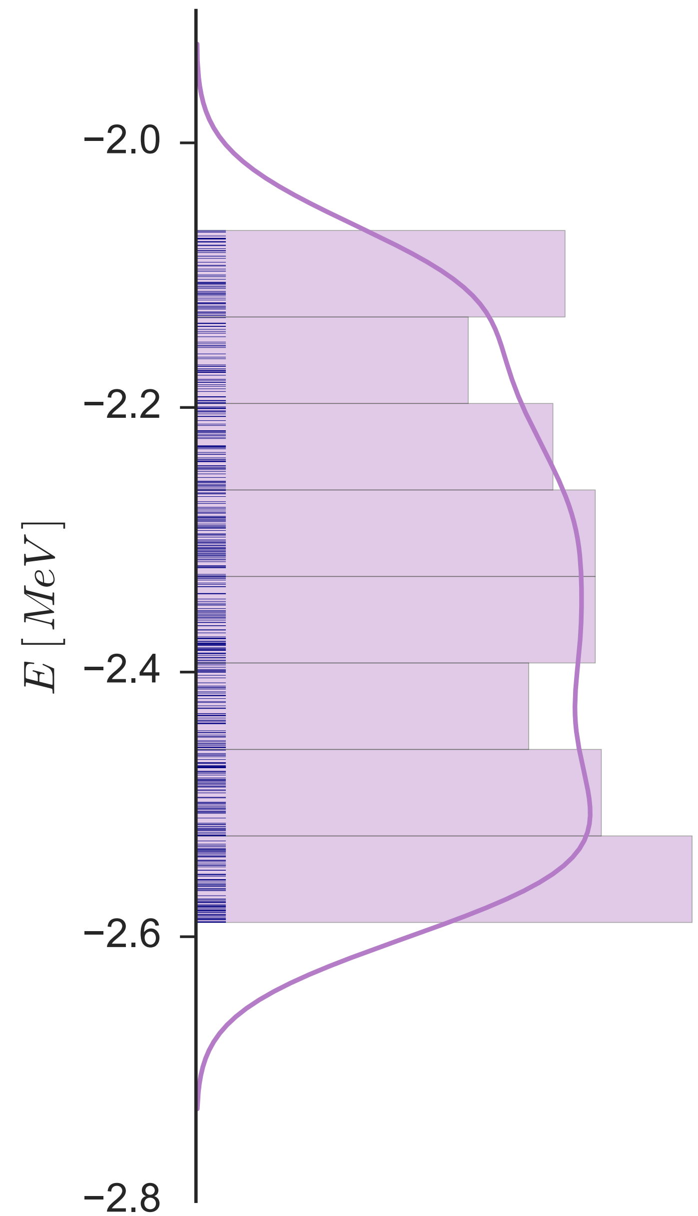
Mitglied der Helmholtz-Gemeinschaft

Error Analysis

- **Estimate uncertainty:**
  compute new correlated distributions within error bars for propagation

$$E = -2.225\ [MeV]$$
$$\mathcal{A} = -3.99$$





Mitglied der Helmholtz-Gemeinschaft

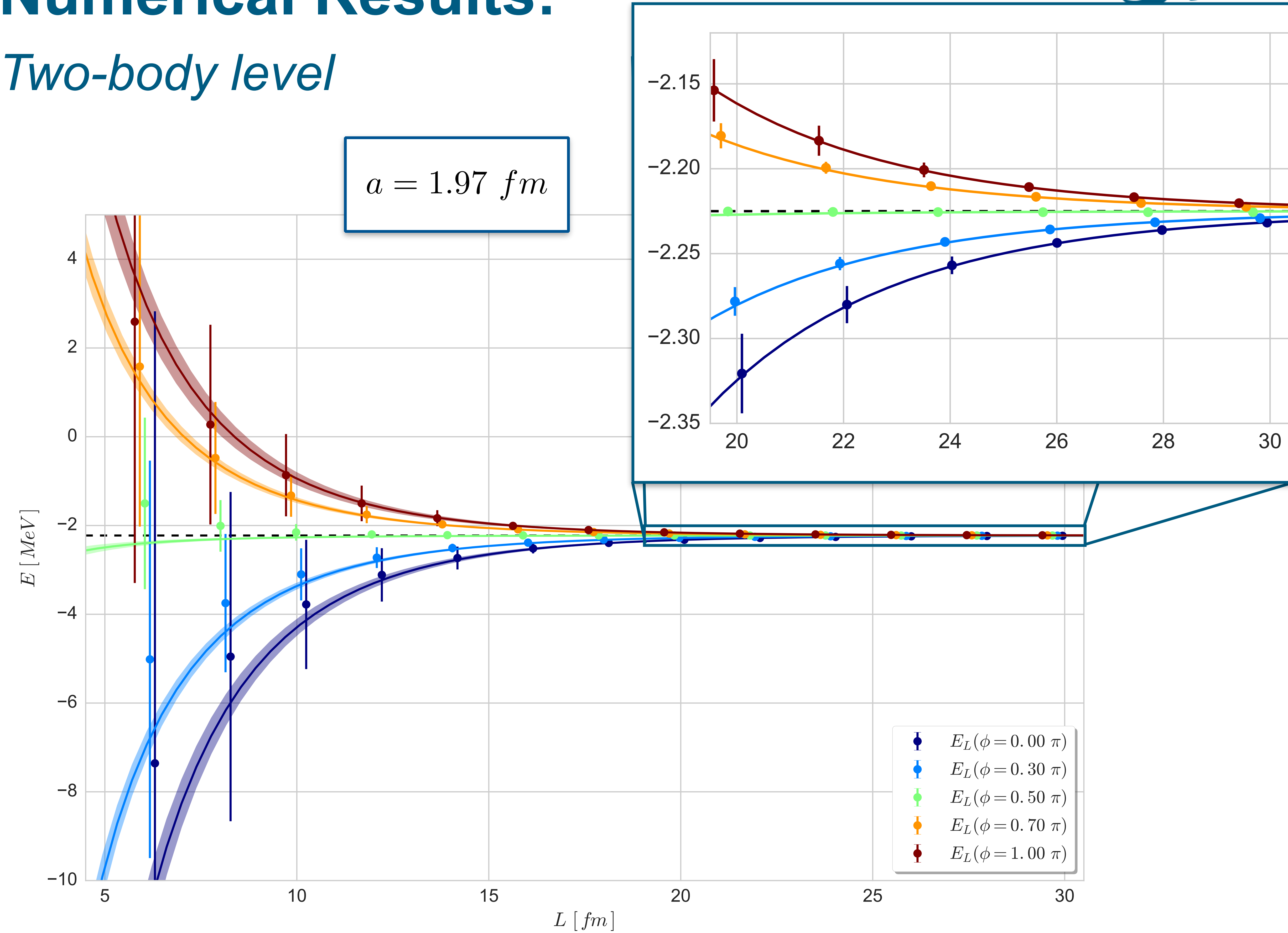
Two-Body Results

Mitglied der Helmholtz-Gemeinschaft

Numerical Results:

Two-body level

$a = 1.97\ fm$

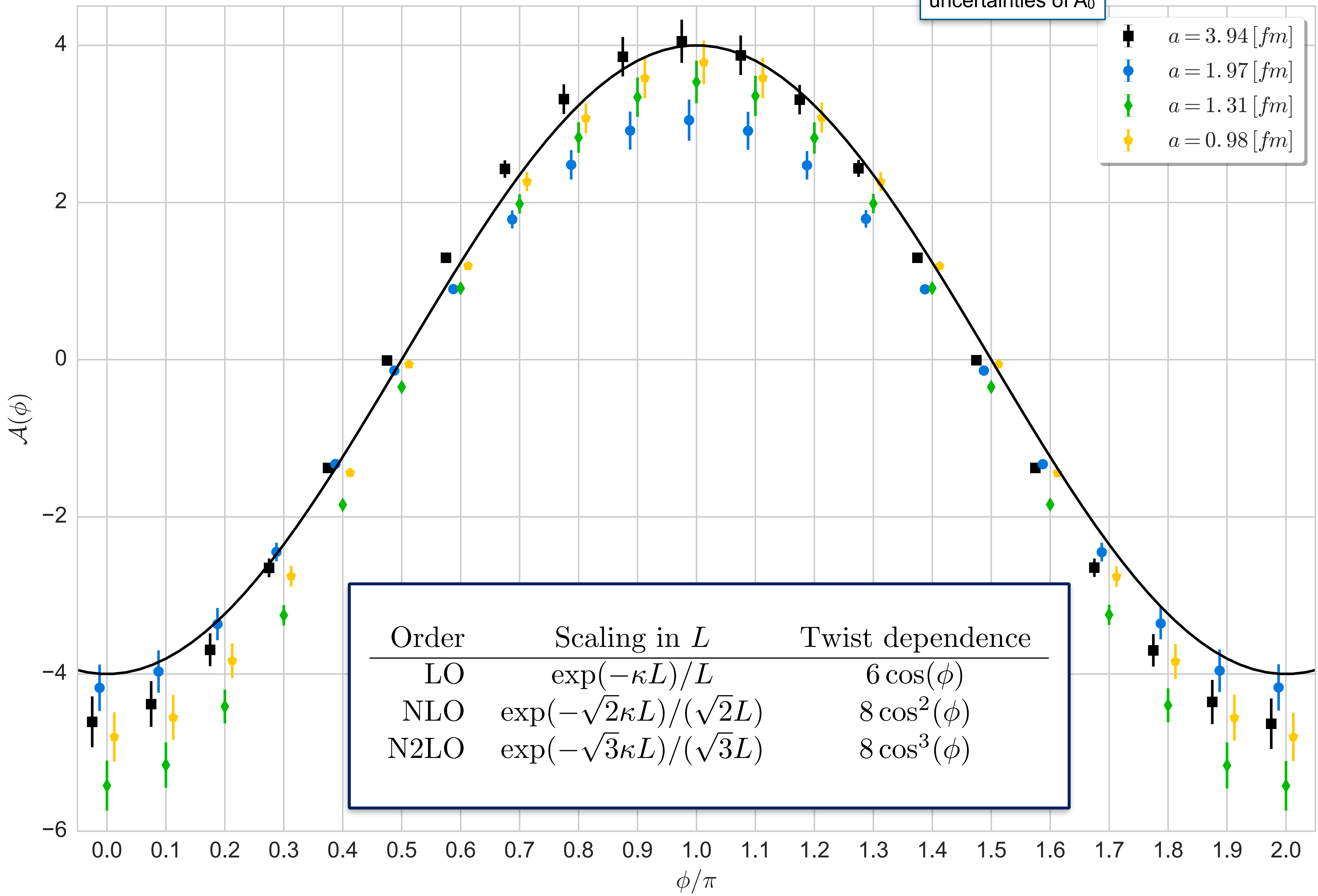


Mitglied der Helmholtz-Gemeinschaft

Numerical Analysis

$$E_L(E, \mathcal{A}) \stackrel{!}{=} A_0 \frac{e^{-\kappa(E)L}}{\mu L} \mathcal{A} + E$$

Not including uncertainties of A_0



Order	Scaling in L	Twist dependence
LO	$\exp(-\kappa L)/L$	$6\cos(\phi)$
NLO	$\exp(-\sqrt{2}\kappa L)/(\sqrt{2}L)$	$8\cos^2(\phi)$
N2LO	$\exp(-\sqrt{3}\kappa L)/(\sqrt{3}L)$	$8\cos^3(\phi)$

Mitglied der Helmholtz-Gemeinschaft

Mitglied der Helmholtz-Gemeinschaft

The Three-Body Case

3-Body — What are the twists?

“*Spectrum of three-body bound states in a finite volume*”,
U. G. Meißner, G. Ríos,
A. Rusetsky
[arXiv:1412.4969],
Phys.Rev.Lett. **114**

$$\Delta E_L^{(LO)}(L, \{\vec{\phi}_i = \vec{0}\}) = \sum_{i=1}^{3} \sum_{(\vec{n}_i, \vec{n}_j, \vec{n}_k) \in M_i} v(\vec{n}_i, \vec{n}_j, \vec{n}_k)$$

Set which minimizes relative hyper radius

$$v(\vec{n}_i, \vec{n}_j, \vec{n}_k) := \int \mathrm{d}^3\vec{x}_i\, \mathrm{d}^3\vec{y}_i\; \psi^*_\infty(\vec{x}_i, \vec{y}_i) V_i(x_i) \psi_\infty(\vec{x}_i - (\vec{n}_j + \vec{n}_k)L, \vec{y}_i + \frac{1}{\sqrt{3}}(\vec{n}_j + \vec{n}_k - 2\vec{n}_i)L)$$

Jacobi coordinate shift expressed in one particle coordinates

For twisted boundaries

$$\Delta E_L^{(LO)}(L, \{\vec{\phi}_i\}) = \sum_{i=1}^{3} \sum_{(\vec{n}_i, \vec{n}_j, \vec{n}_k) \in M_i} v(\vec{n}_i, \vec{n}_j, \vec{n}_k)\; e^{-i \sum_{l=1}^{3} \vec{\phi}_l \cdot \vec{n}_l}$$

Result at unitary limit

$$\Delta E_L^{(LO)}(L, \{\vec{\phi}_i\}) = \frac{\mathcal{N}_{PB}^{(LO)}}{9} \frac{\exp\left(-\frac{2}{\sqrt{3}}\kappa L\right)}{(\kappa L)^{3/2}} \sum_{i,j=1}^{3} \cos(\vec{e}_j \cdot \vec{\phi}_i)$$

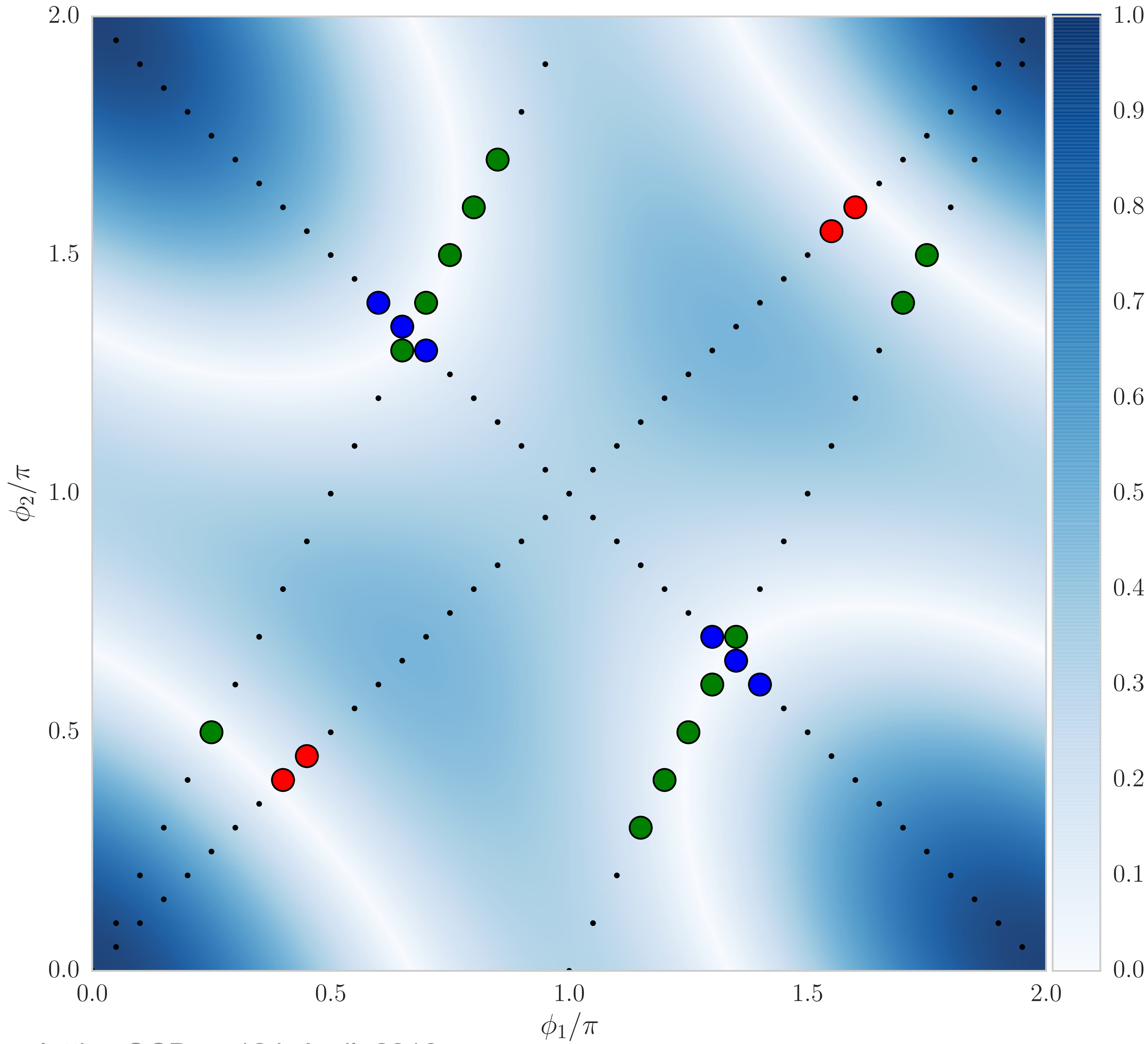
Mitglied der Helmholtz-Gemeinschaft

3-Body — What are the twists?

Relative LO Error Amplitude

CMS constraint

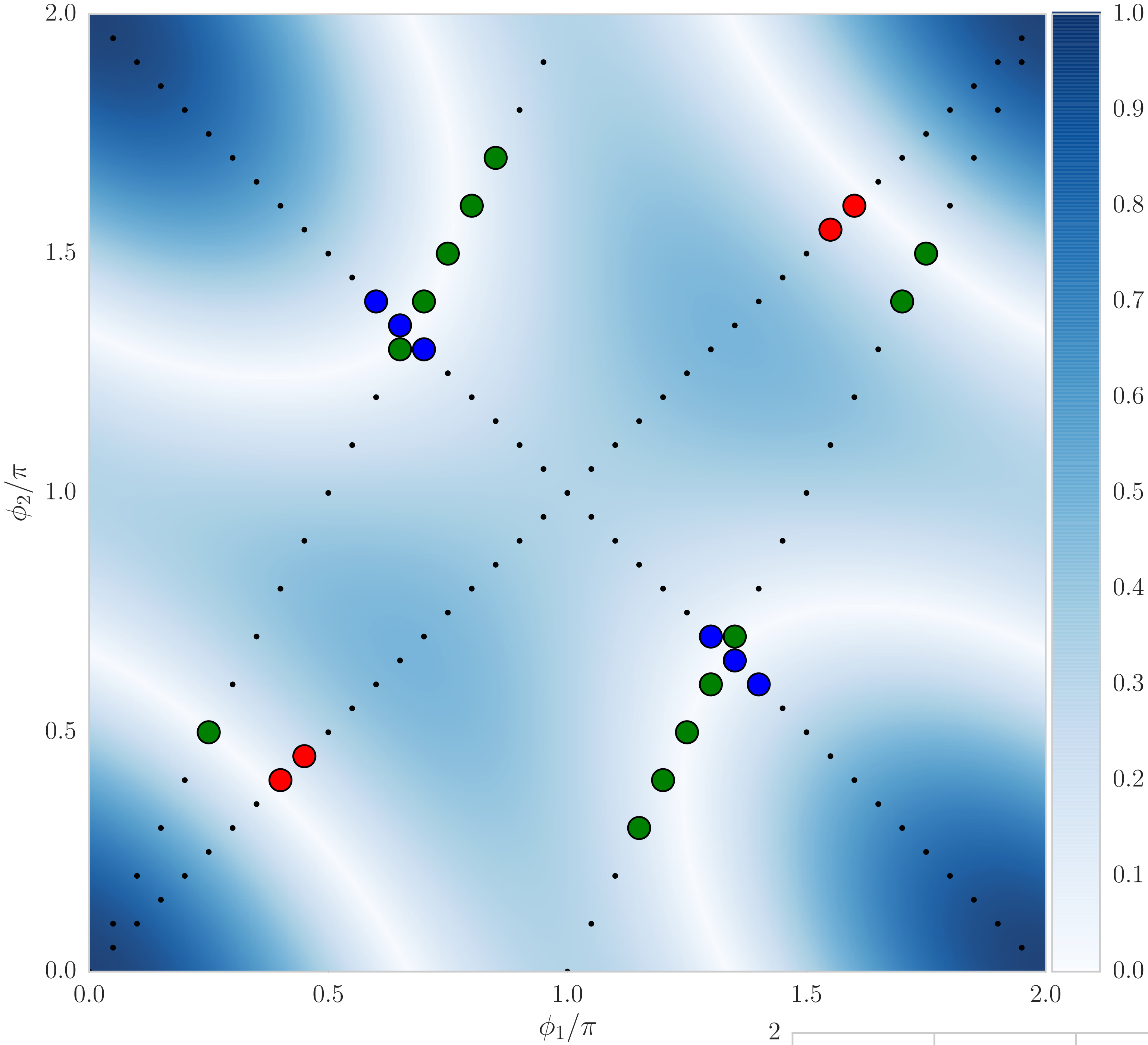
$$\mathcal{A}(\phi_1, \phi_2) = \cos(\phi_1) + \cos(\phi_2) + \underline{\cos(\phi_1 + \phi_2)}$$



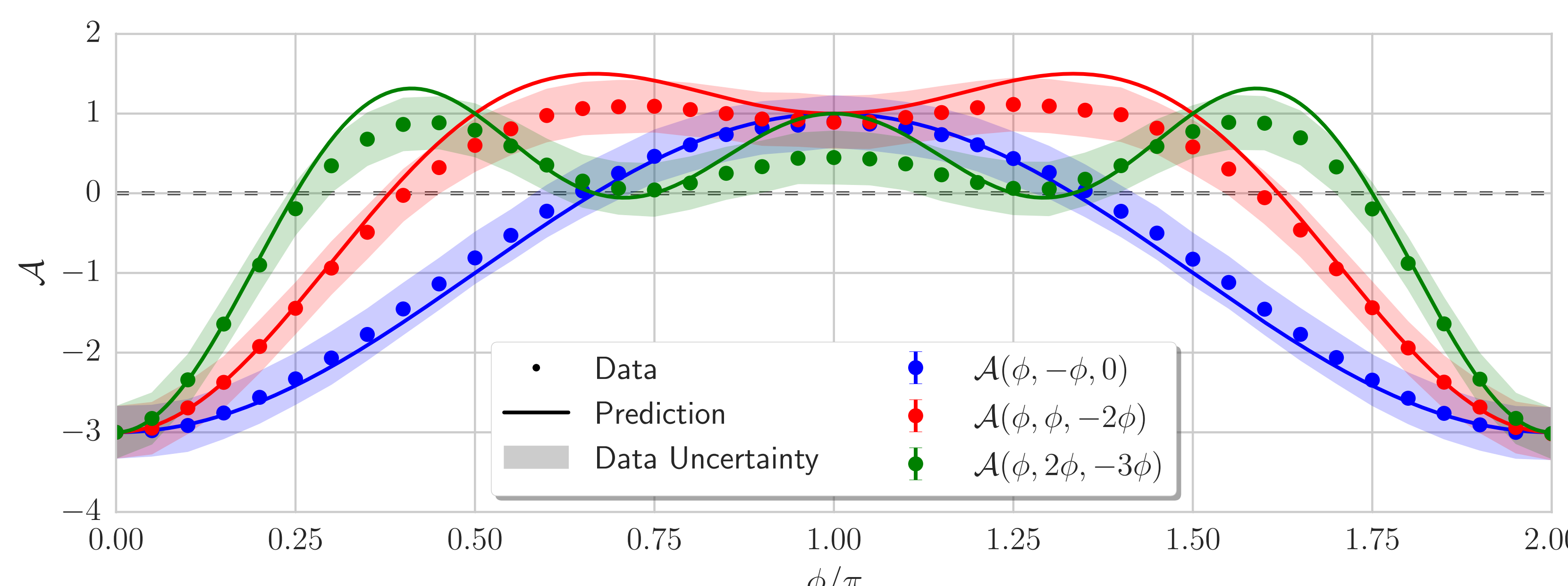
Numerical Findings

- *Probed twists*
- *'iPB' consistent twists*

Mitglied der Helmholtz-Gemeinschaft



ϕ_2/π
ϕ_1/π

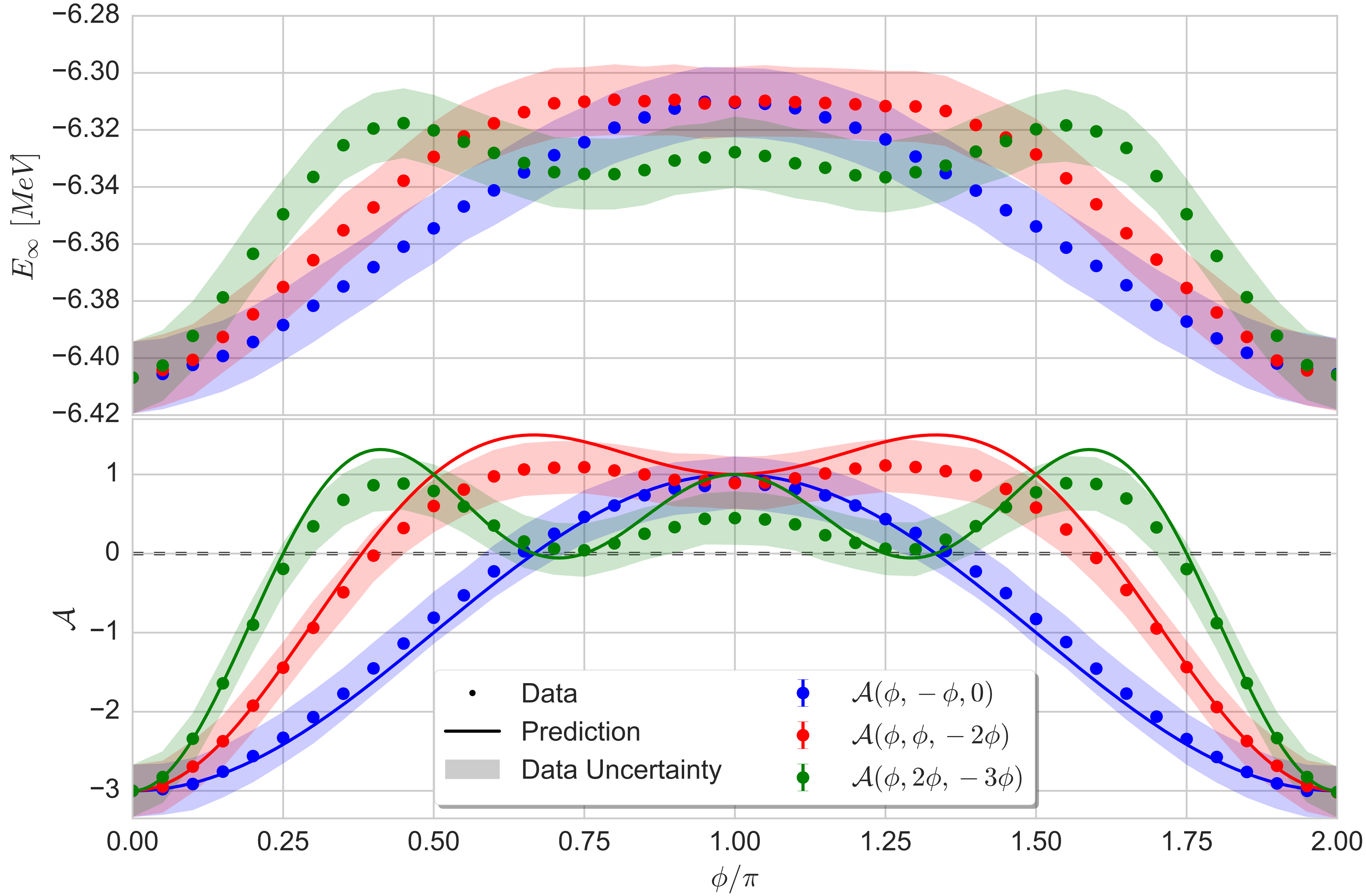


$\mathcal{A}$
ϕ/π
Data
Prediction
Data Uncertainty
$\mathcal{A}(\phi, -\phi, 0)$
$\mathcal{A}(\phi, \phi, -2\phi)$
$\mathcal{A}(\phi, 2\phi, -3\phi)$

3-Body results

$$\Delta E_L^{(LO)}(L,\phi_i) = A(\phi_i)\frac{e^{-\frac{2}{\sqrt{3}}\kappa L}}{(\kappa L)^{3/2}}$$

$$\mathcal{A}(\phi_i) := 3\,\frac{A(\phi_i)}{A_{\max}} = \sum_{i=1}^{3}\cos(\phi_i)$$

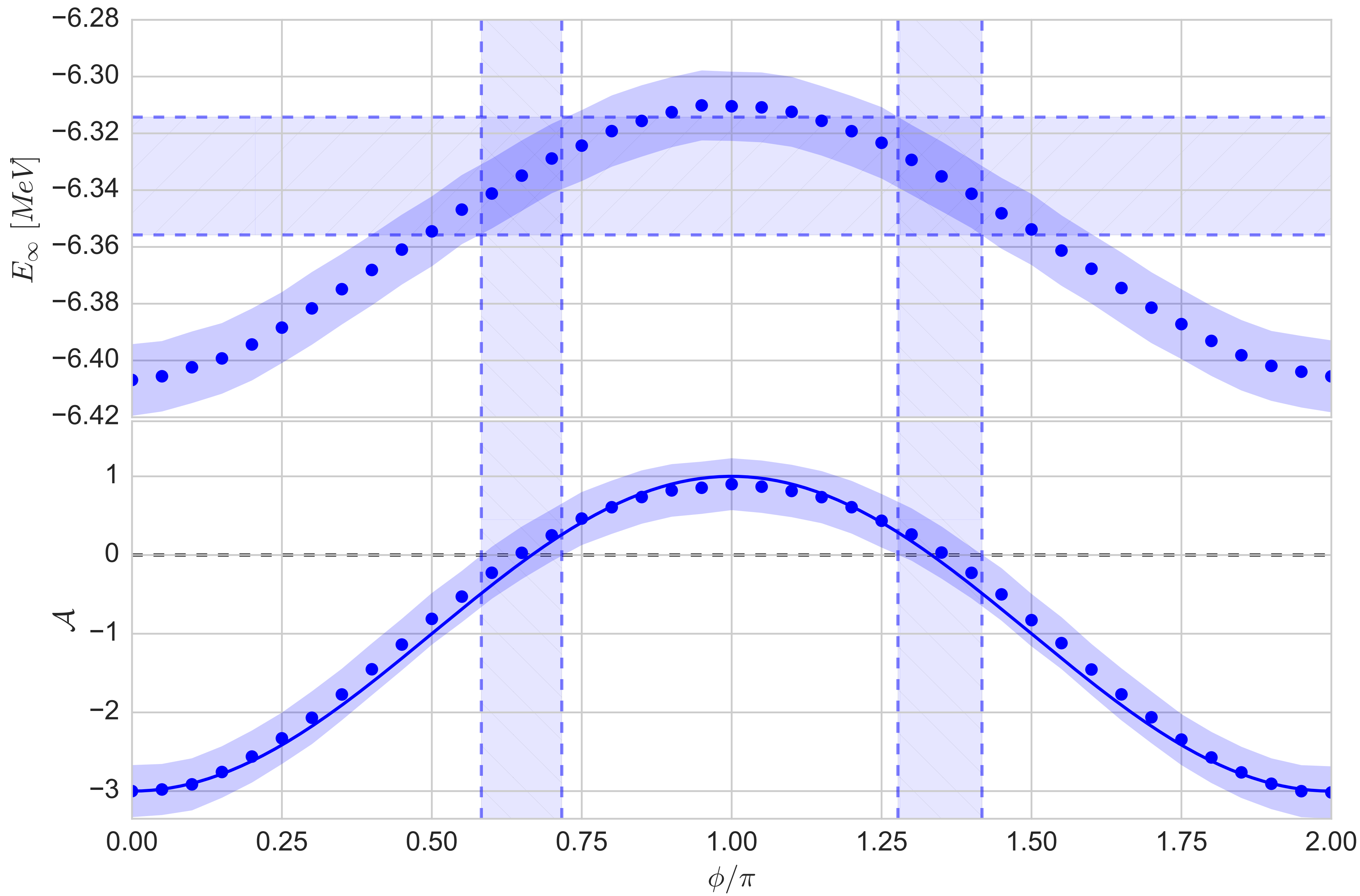


Mitglied der Helmholtz-Gemeinschaft

3-Body results

$$\Delta E_L^{(LO)}(L, \phi_i) = A(\phi_i) \frac{e^{-\frac{2}{\sqrt{3}}\kappa L}}{(\kappa L)^{3/2}}$$

$$\mathcal{A}(\phi_i) := 3\,\frac{A(\phi_i)}{A_{\max}} = \sum_{i=1}^{3} \cos(\phi_i)$$

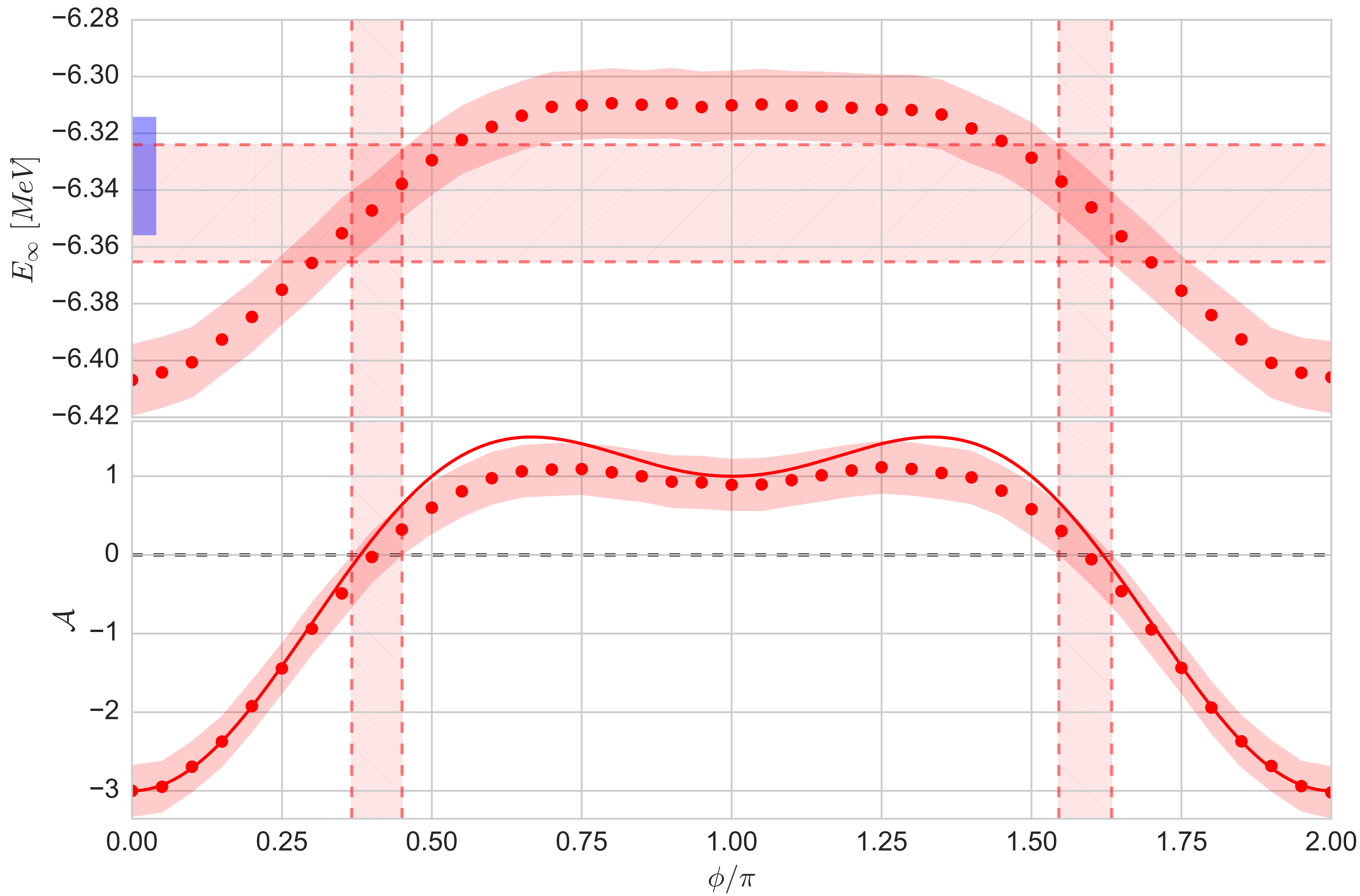


Mitglied der Helmholtz-Gemeinschaft

3-Body results

$$\Delta E_L^{(LO)}(L, \phi_i) = A(\phi_i) \frac{e^{-\frac{2}{\sqrt{3}}\kappa L}}{(\kappa L)^{3/2}}$$

$$\mathcal{A}(\phi_i) := 3\,\frac{A(\phi_i)}{A_{\max}} = \sum_{i=1}^{3} \cos(\phi_i)$$

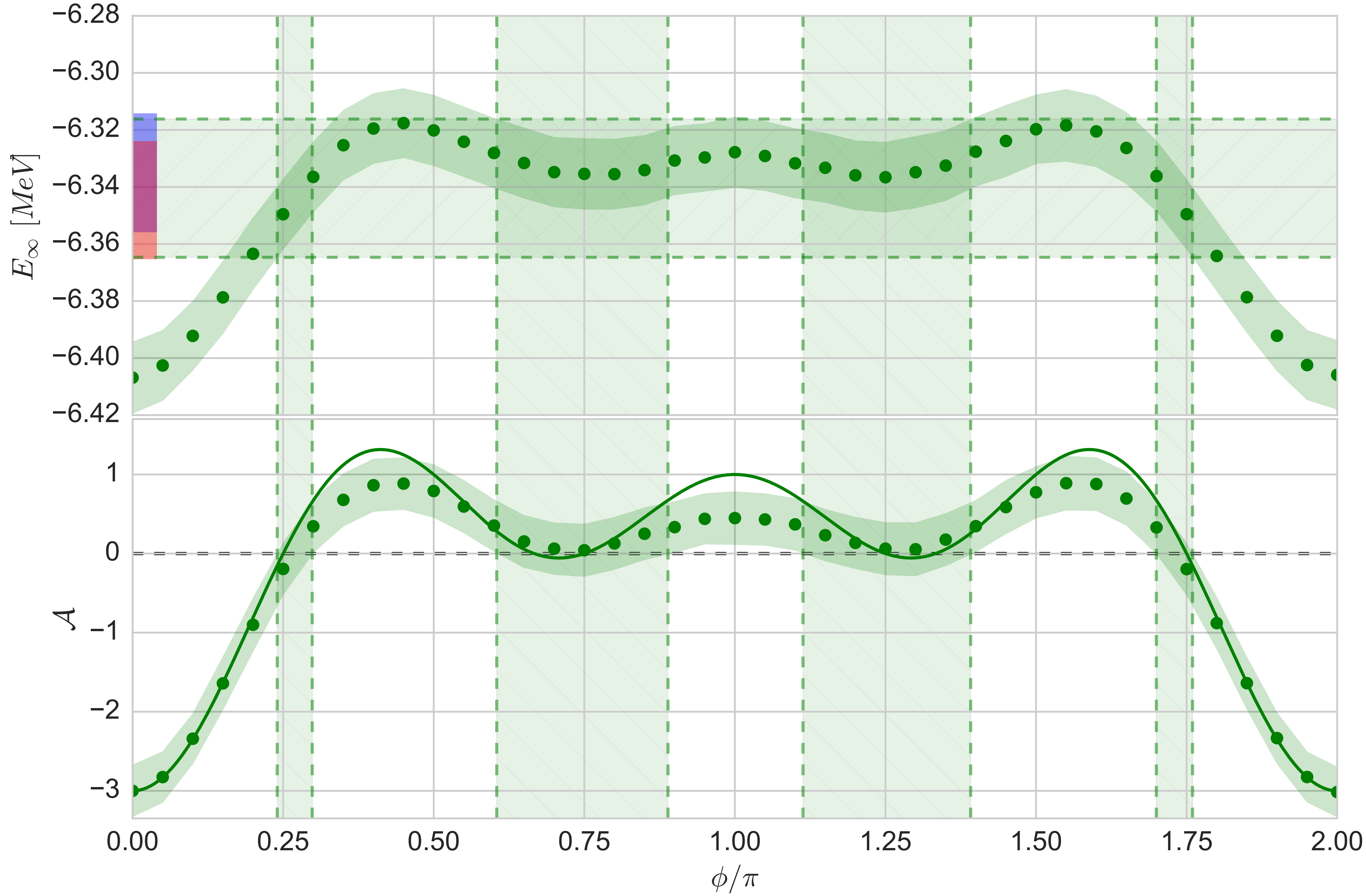


Mitglied der Helmholtz-Gemeinschaft

3-Body results

$$\Delta E_L^{(LO)}(L,\phi_i) = A(\phi_i)\frac{e^{-\frac{2}{\sqrt{3}}\kappa L}}{(\kappa L)^{3/2}}$$

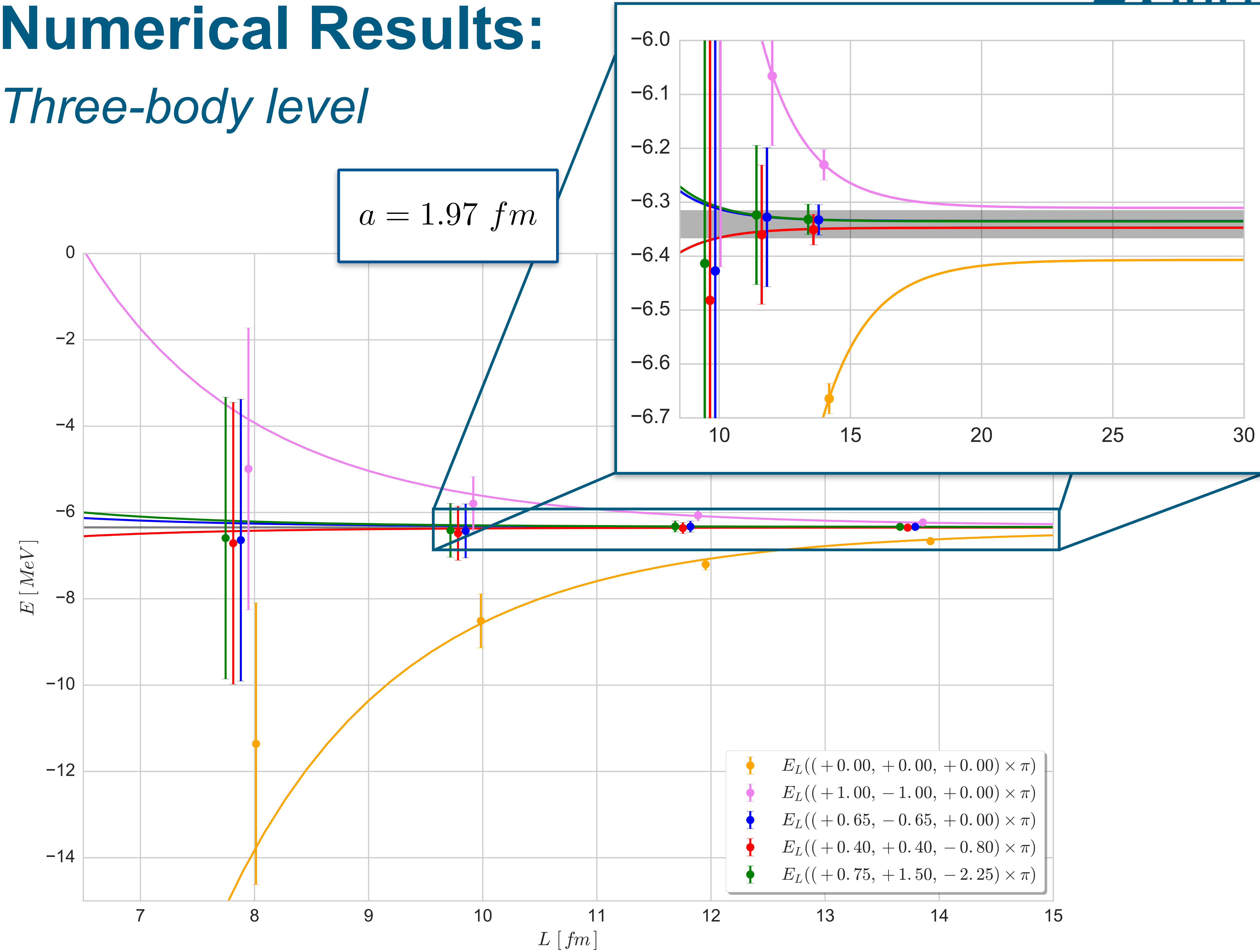
$$\mathcal{A}(\phi_i) := 3\,\frac{A(\phi_i)}{A_{\max}} = \sum_{i=1}^{3}\cos(\phi_i)$$



Mitglied der Helmholtz-Gemeinschaft

Numerical Results:

Three-body level



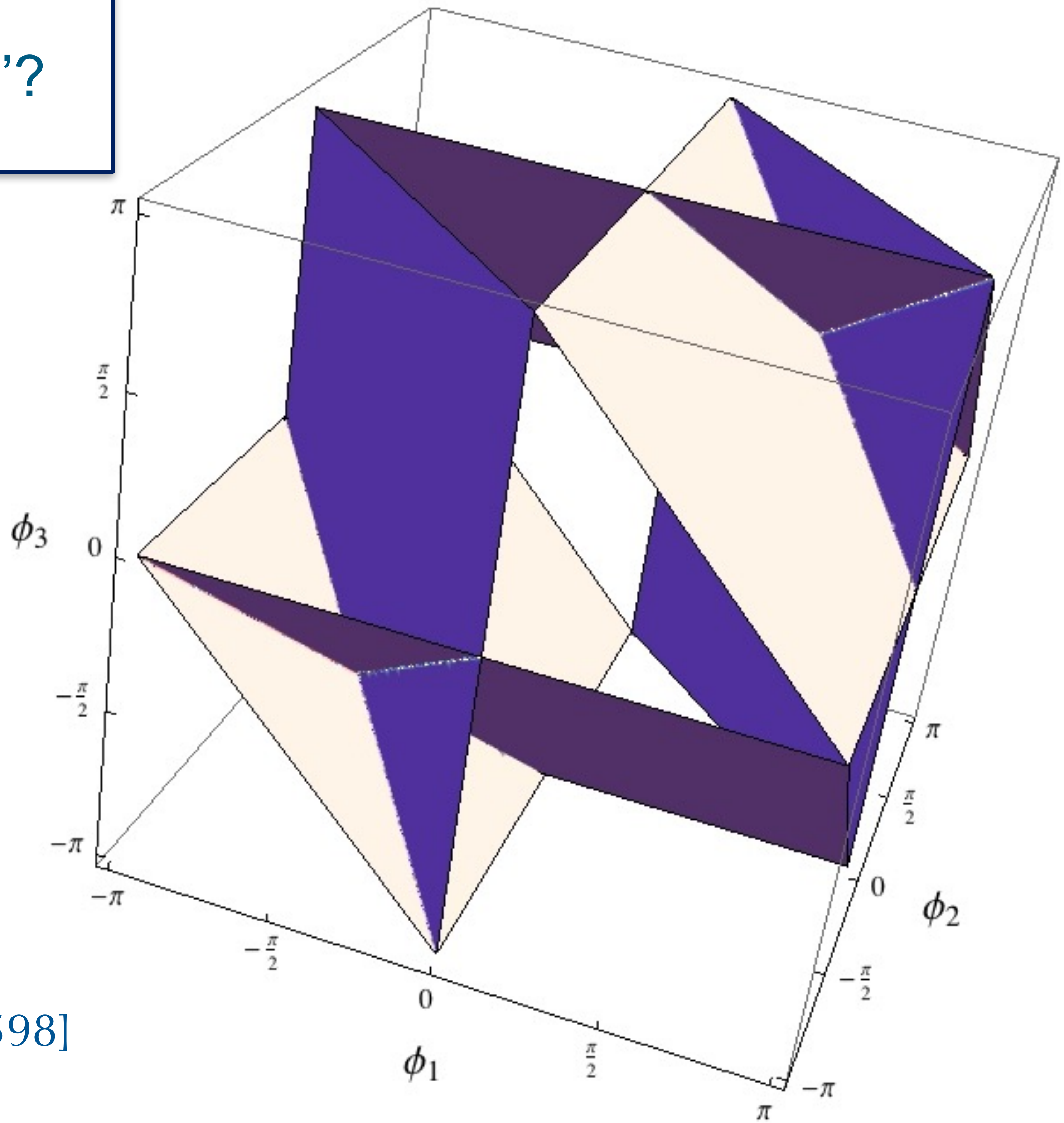
Summary

- **Twists are easy to implement**
  - *Multiply off diagonal terms by phase*
  - *Claim: Twist do not increase sign oscillations (Future)*
- **Twisted boundaries for reduced FV effects**
  - *Twist averaging vs iPBs*
  - *One can extract infinite volume results without knowing the functional dependence*
- **Effects of twists on non-bound states?**
  - *Mapping out the phase shifts?*
- **iPBs for larger systems (more Nuclei)?** *(Future)*
  - *Can one find the twist dependence for larger systems? (Seems like yes)*
- **iPBs for other partial waves?** *(Future)*
  - *Two-body results already known*
- **Can one relate this to relativistic systems?**

- **Are there time like twists?**
  - *Reduce the lattice in time direction and simultaneously increase precision*

Mitglied der Helmholtz-Gemeinschaft

4-Body ‘iPBs’?



[arXiv:1511.06598]

Thank you for your attention