Effective theory for lattice nuclei

(using Monte Carlo methods)

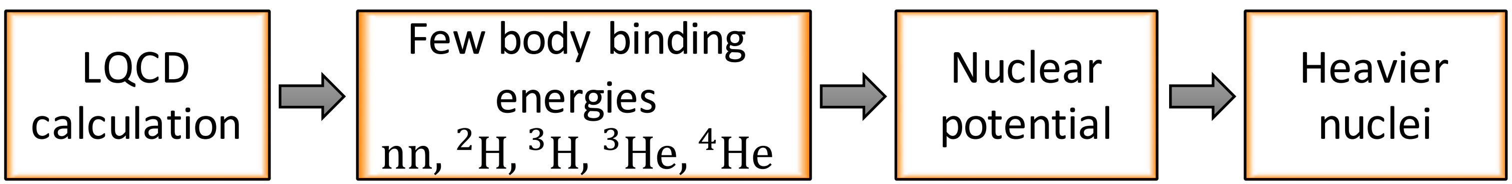
Lorenzo Contessi

(TIFPA, Università degli studi di Trento)

Overview:

- Motivations for pionless EFT and procedure
- Monte Carlo Method
- More about Effective Theories
- Some results
- Conclusions

Connect nuclear physics with QCD



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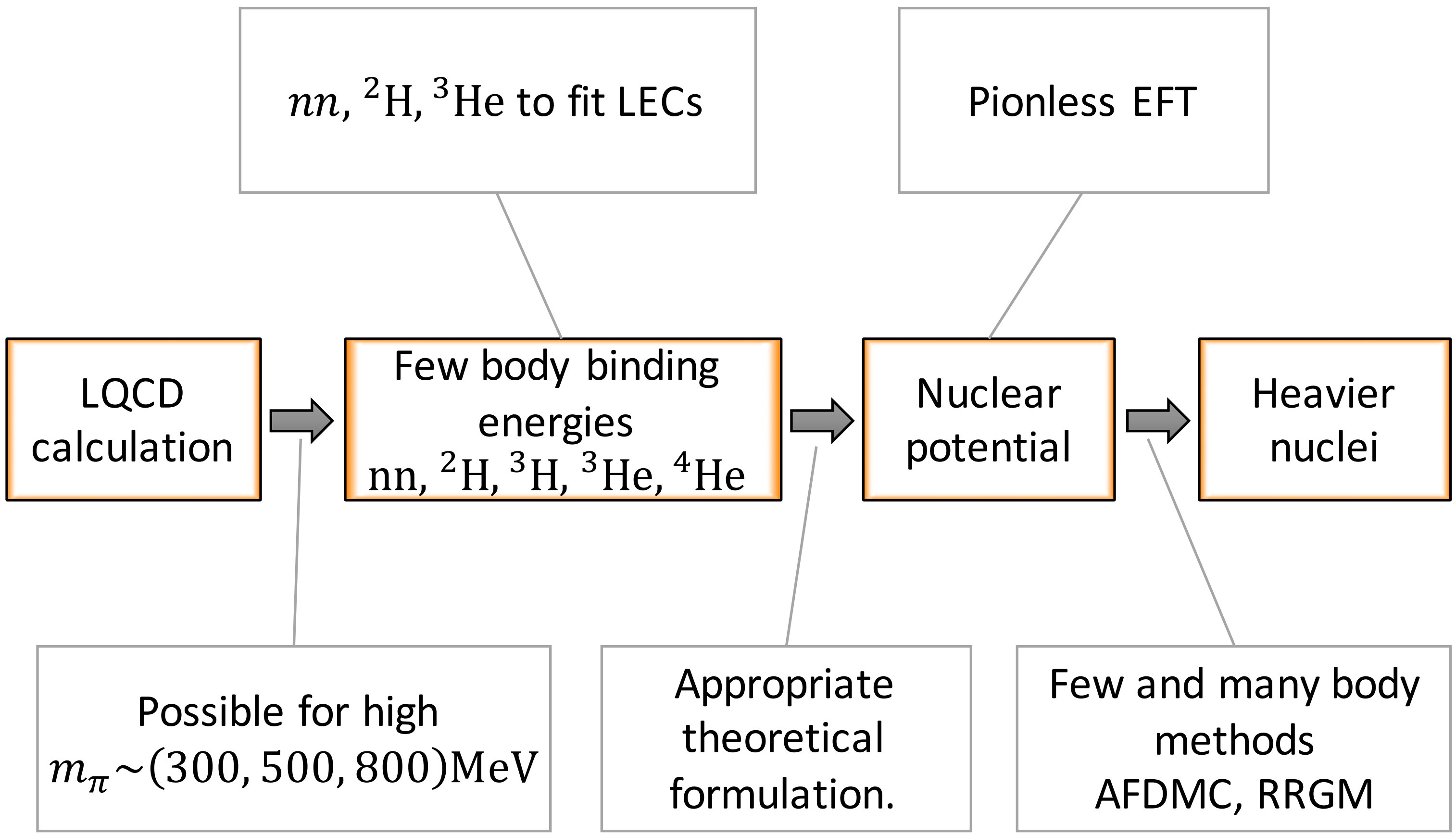

Theory formulation

- We have a good phenomenological understanding of nuclear interaction for physical m_π.
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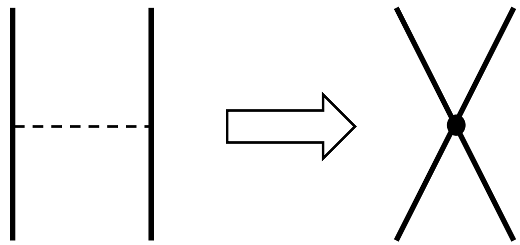
Few data available	⇨	Need a potential with few parameters as possible.
Pions are heavy.	⇨	No needs to include Pions explicitly.

Theory formulation

Pionless EFT:

- Controlled potential through power counting.
- Pionless EFT preserves relevant QCD symmetries.
- LO is simple and contains only 3 parameters.



Plus:

- Pionless theory contains only contact interactions.
- Relatively well understand power counting.

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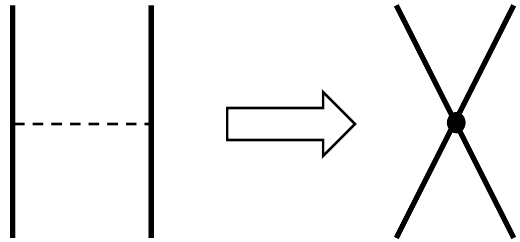

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Monte Carlo Method

Monte Carlo Method

Within Monte Carlo methods, integrals are computed using the central limit theorem:

$$S_N := \int f(\vec{r}) P(\vec{r}) d\vec{r} = \frac{1}{N} \sum_{i}^{N} f(\vec{r}_i)$$

$$S_{N \to \infty} = \frac{1}{\sqrt{2\pi\sigma_N^2}} e^{\frac{\left[S_N - \left(\int f(\vec{r}) P(\vec{r}) d\vec{r}\right)\right]^2}{2\sigma_N}}$$

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Variational Monte Carlo:

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Probability distribution to sample. ($|\psi|^2$)

Function to be computed ($\frac{H\psi}{\psi}$)

Monte Carlo Method

Diffusion Monte Carlo:

$$E_{\phi_{gs}} = \frac{\langle \phi_{gs} | H | \psi_T \rangle}{\langle \phi_{gs} | \psi_T \rangle} = \frac{\int \phi_{gs}^* \, H\psi_T}{\int \phi_{gs}^* \psi_T} = \frac{\int (\phi_{gs}^* \psi_I) \frac{H\psi_T}{\psi_I}}{\int \phi_{gs}^* \psi_T}$$

Ground state is calculated evolving in the imaginary time:

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Monte Carlo Method

Guide Wave function

Trial Wave function

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Monte Carlo Method

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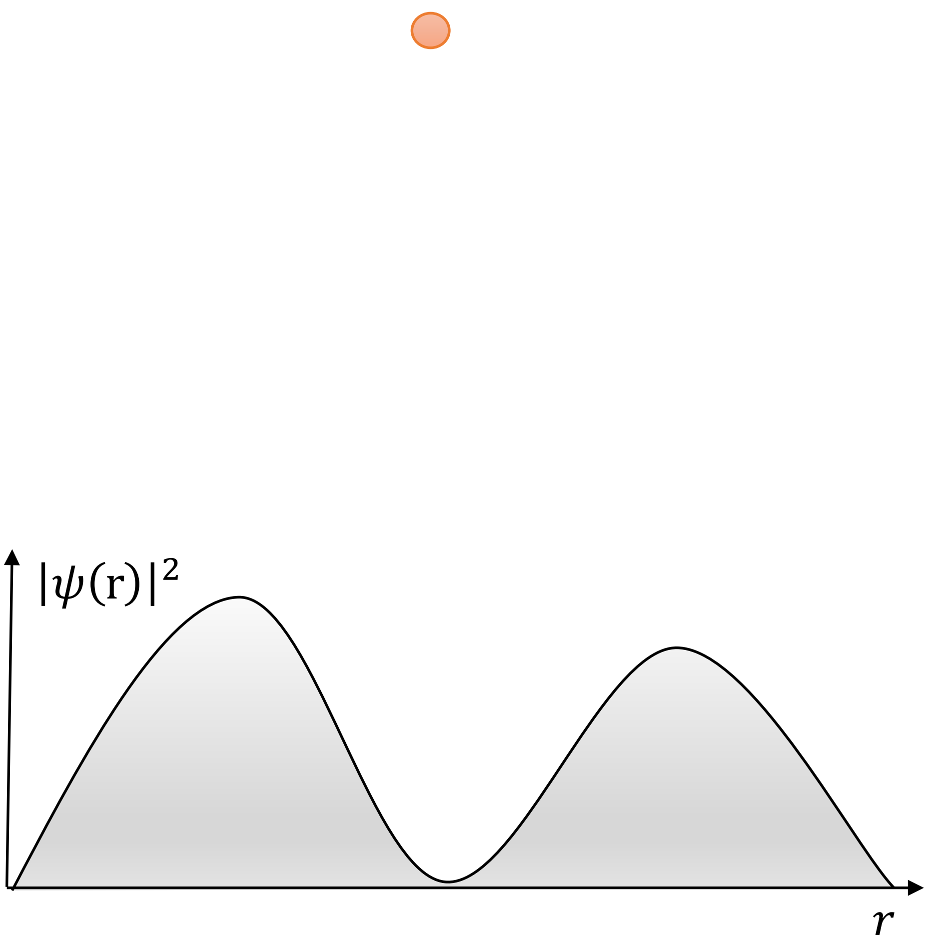

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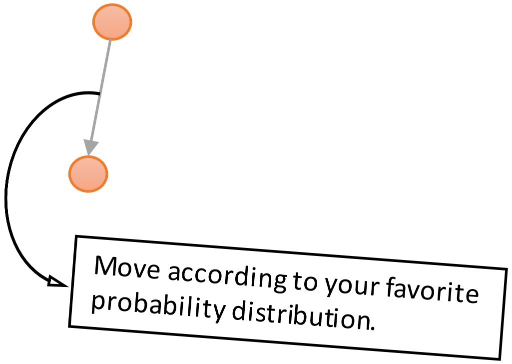

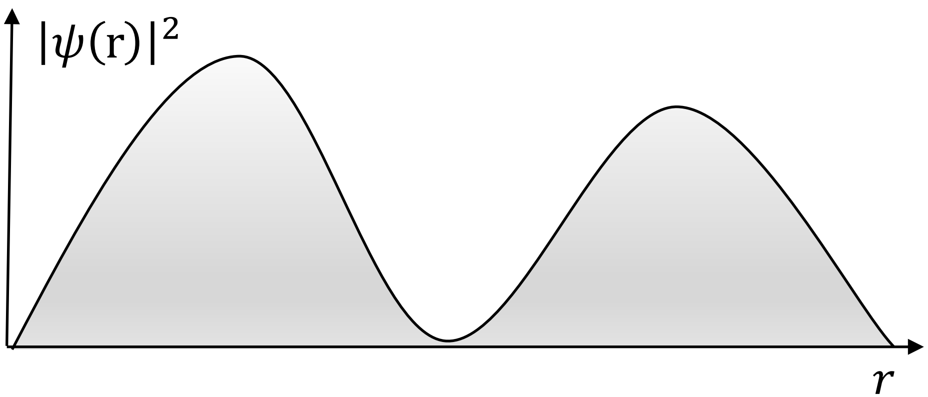

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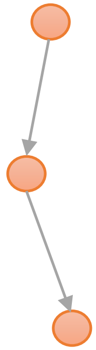

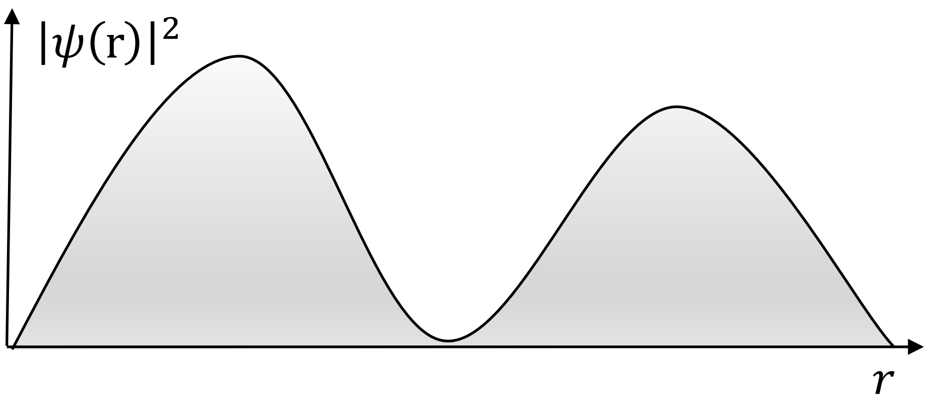

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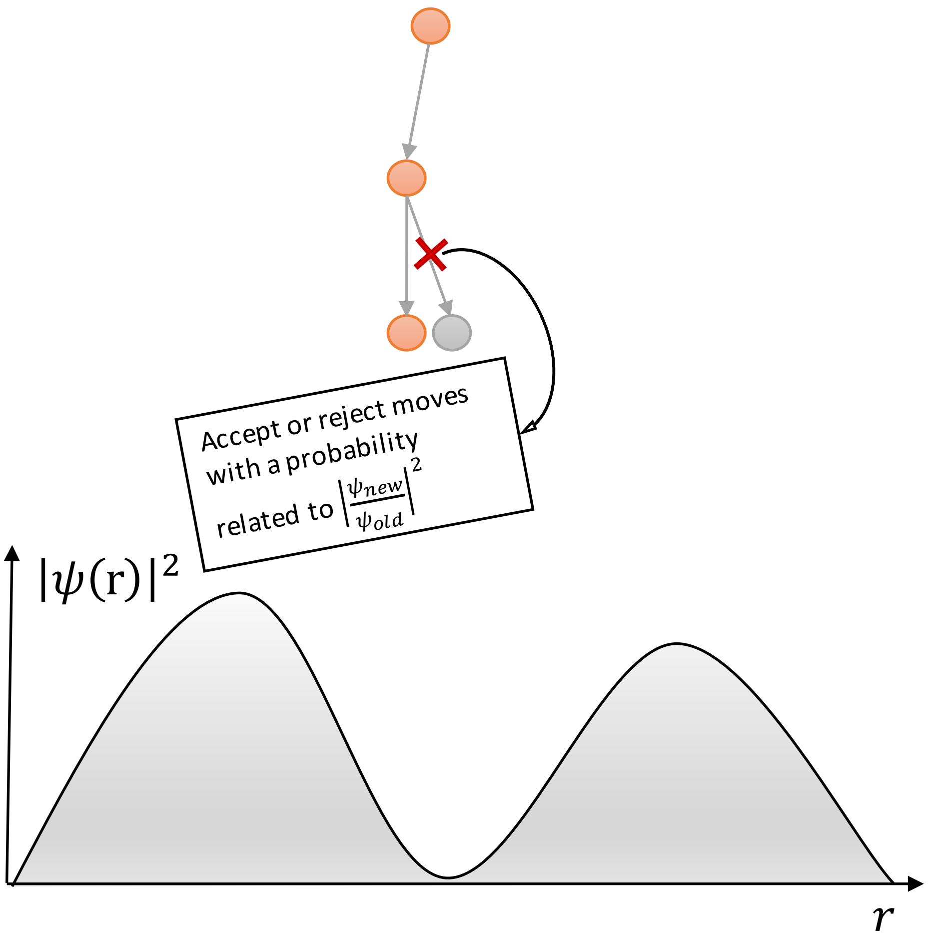

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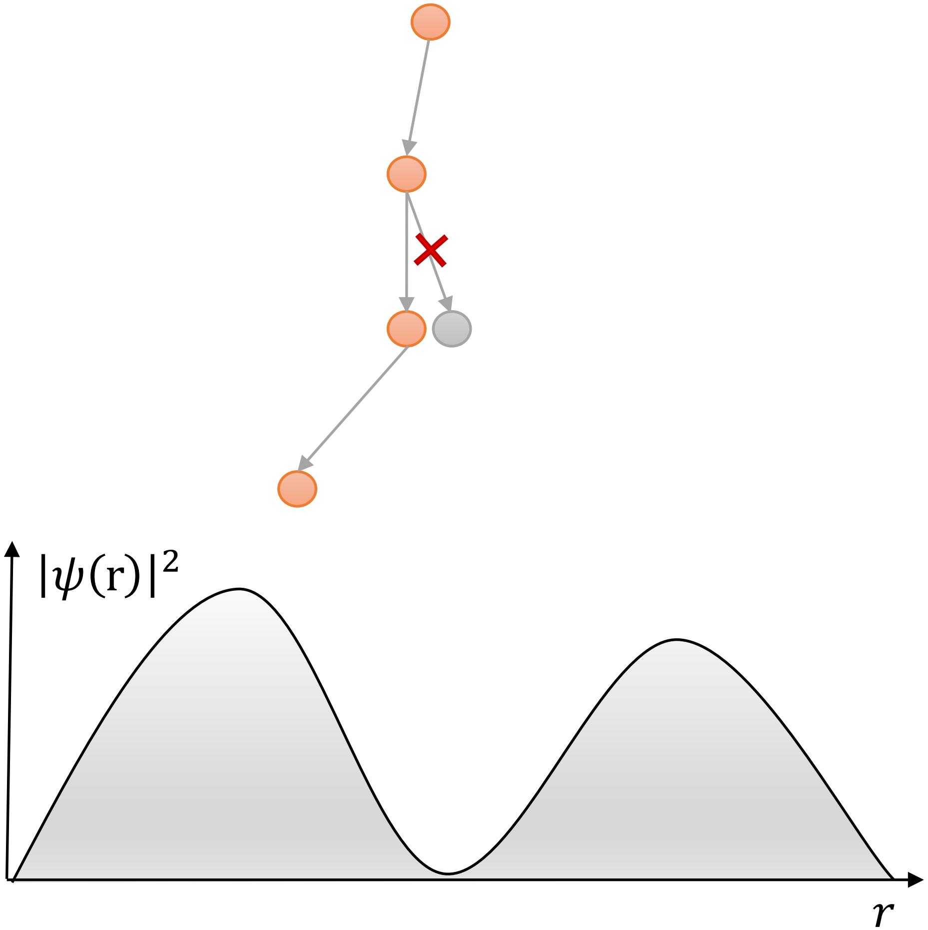

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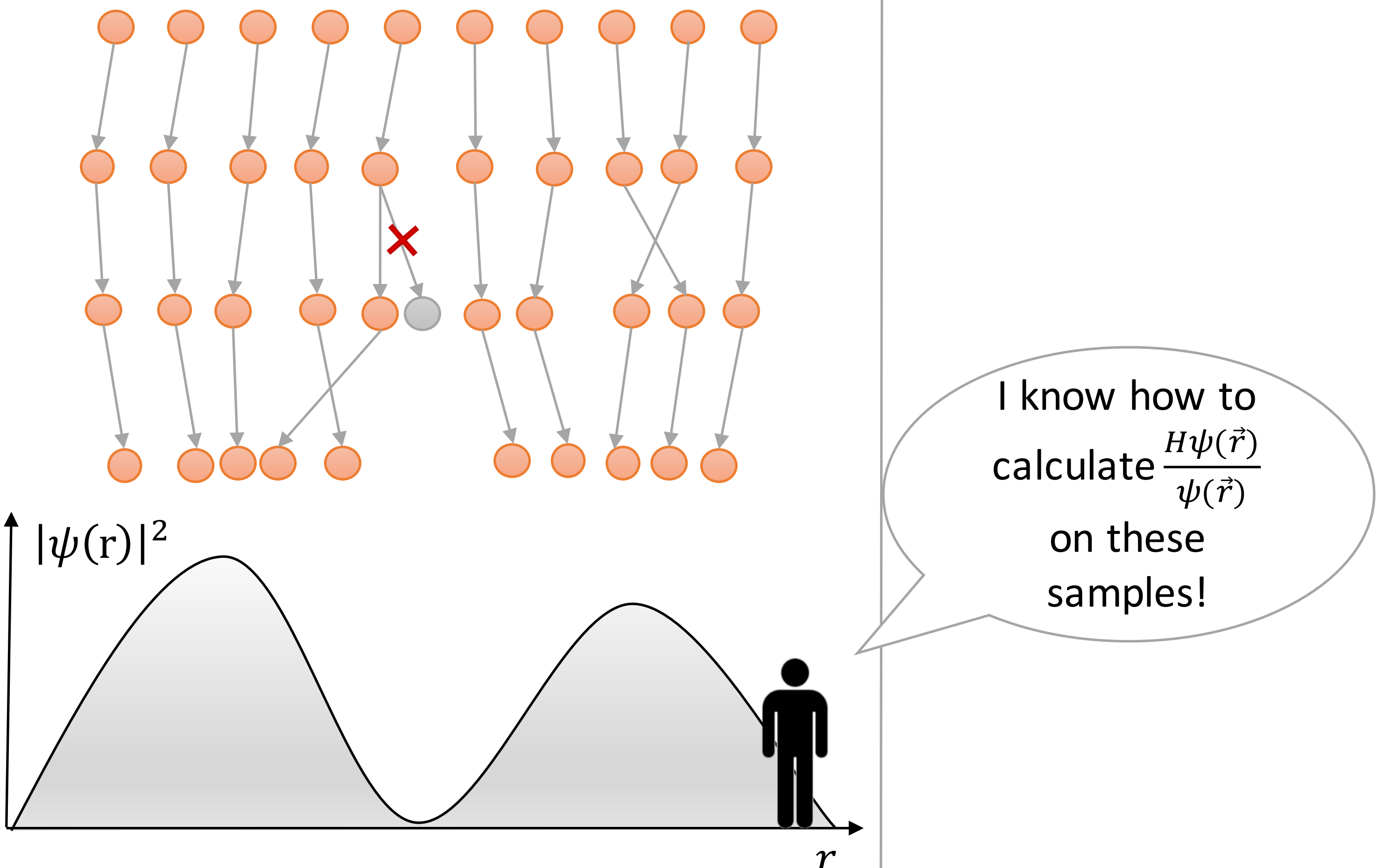

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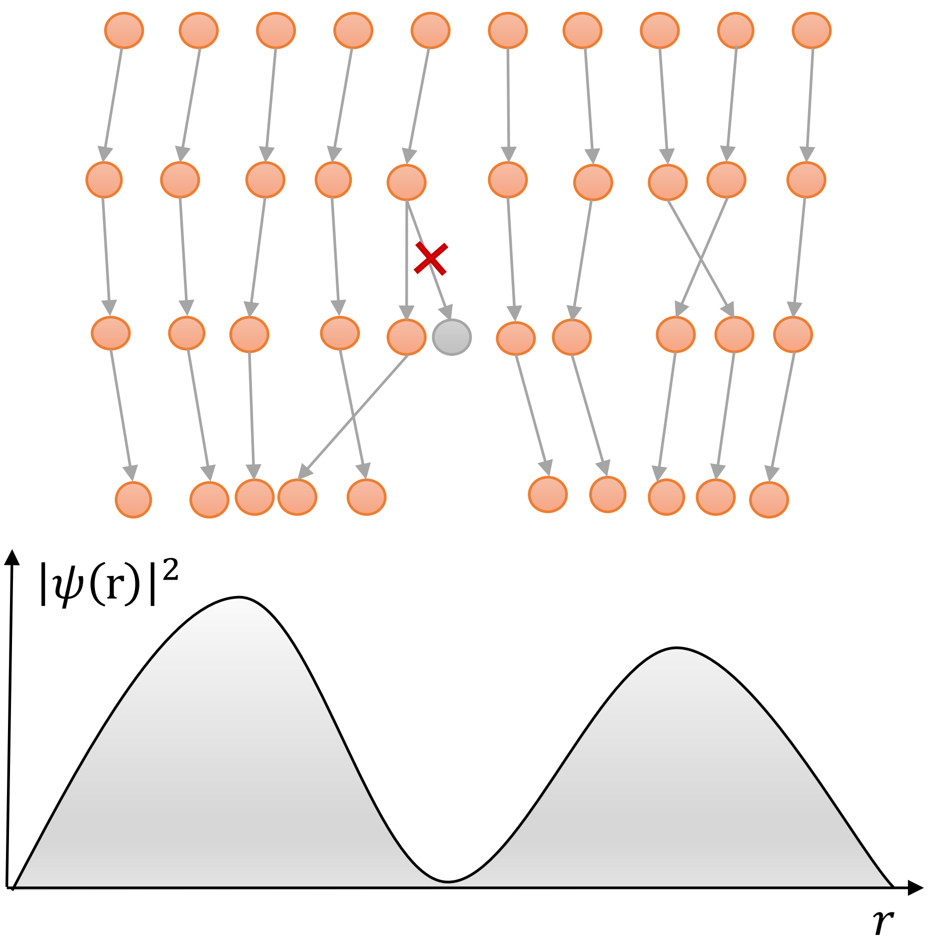

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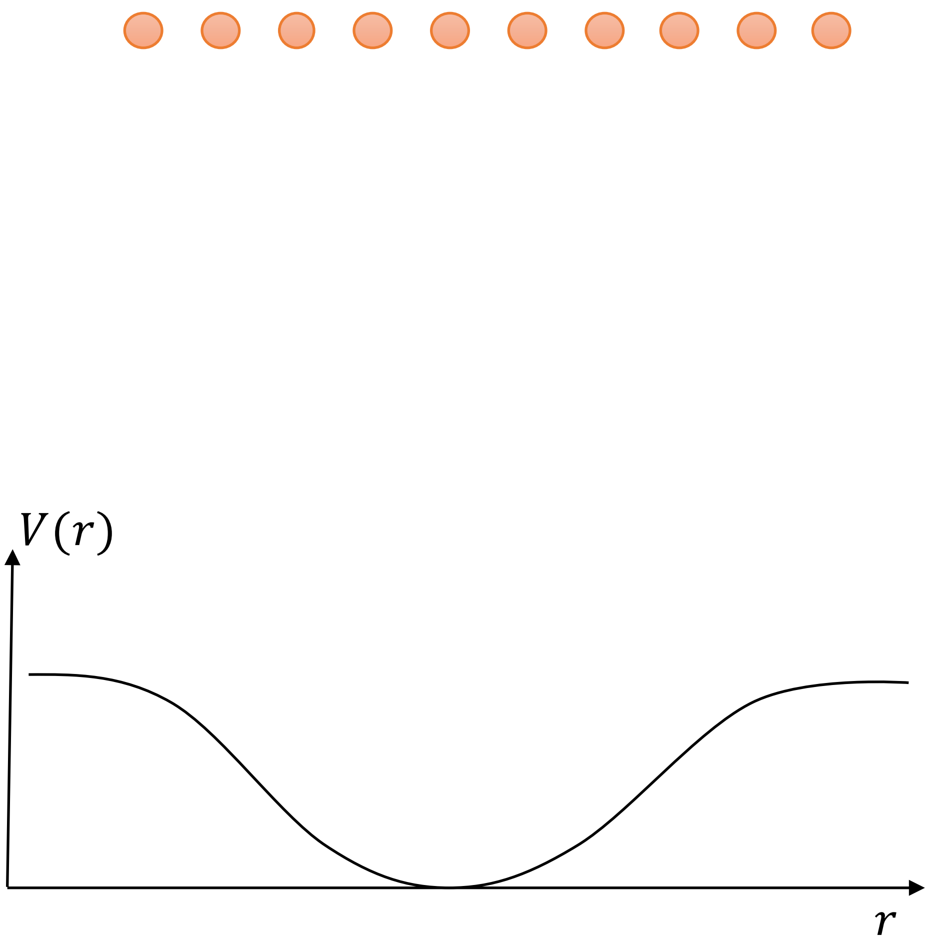

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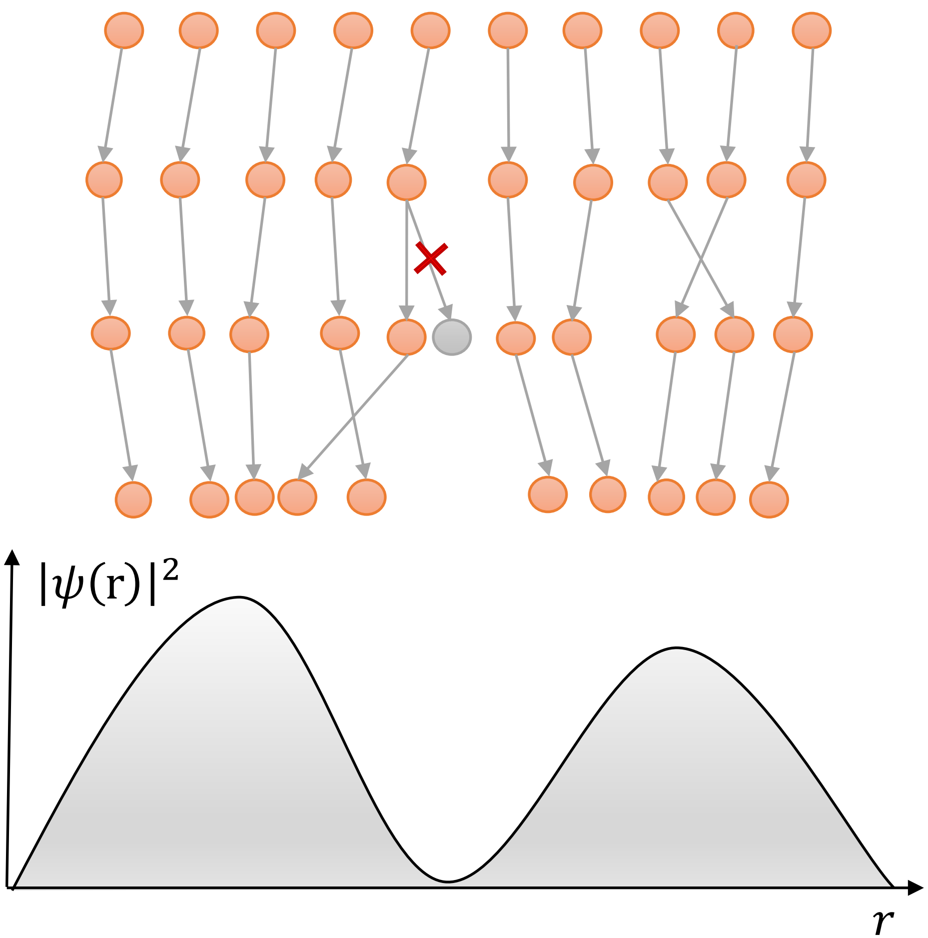

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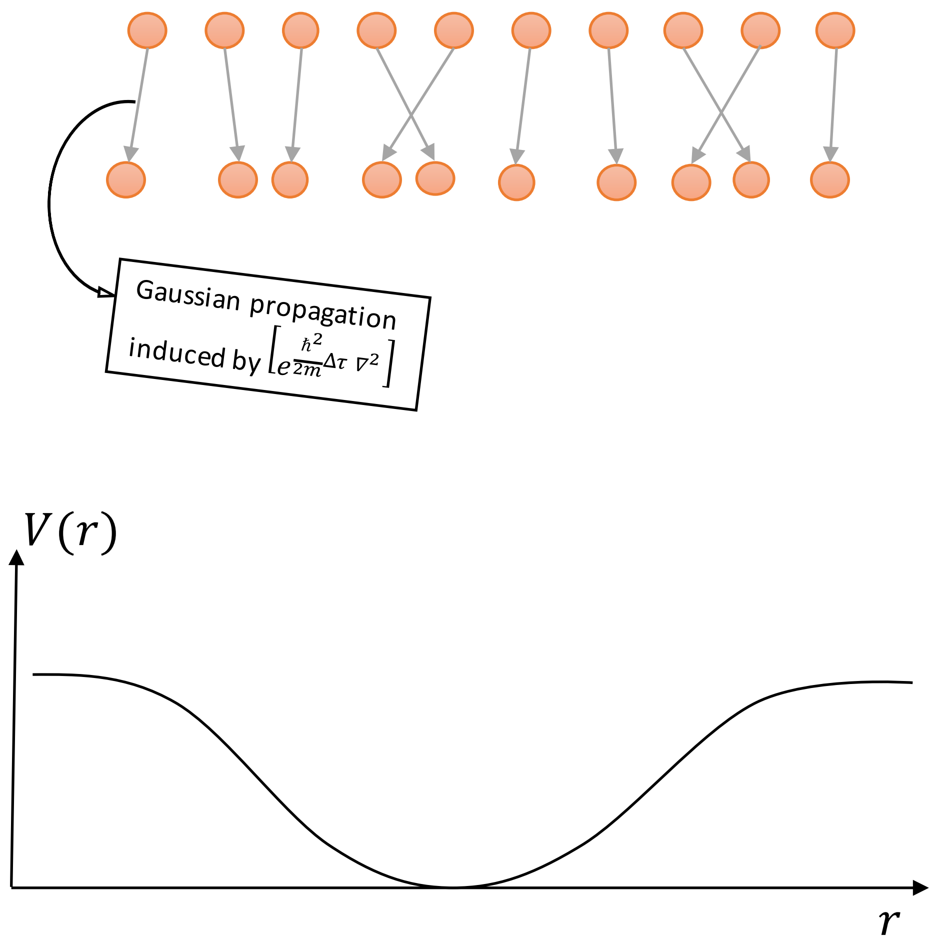

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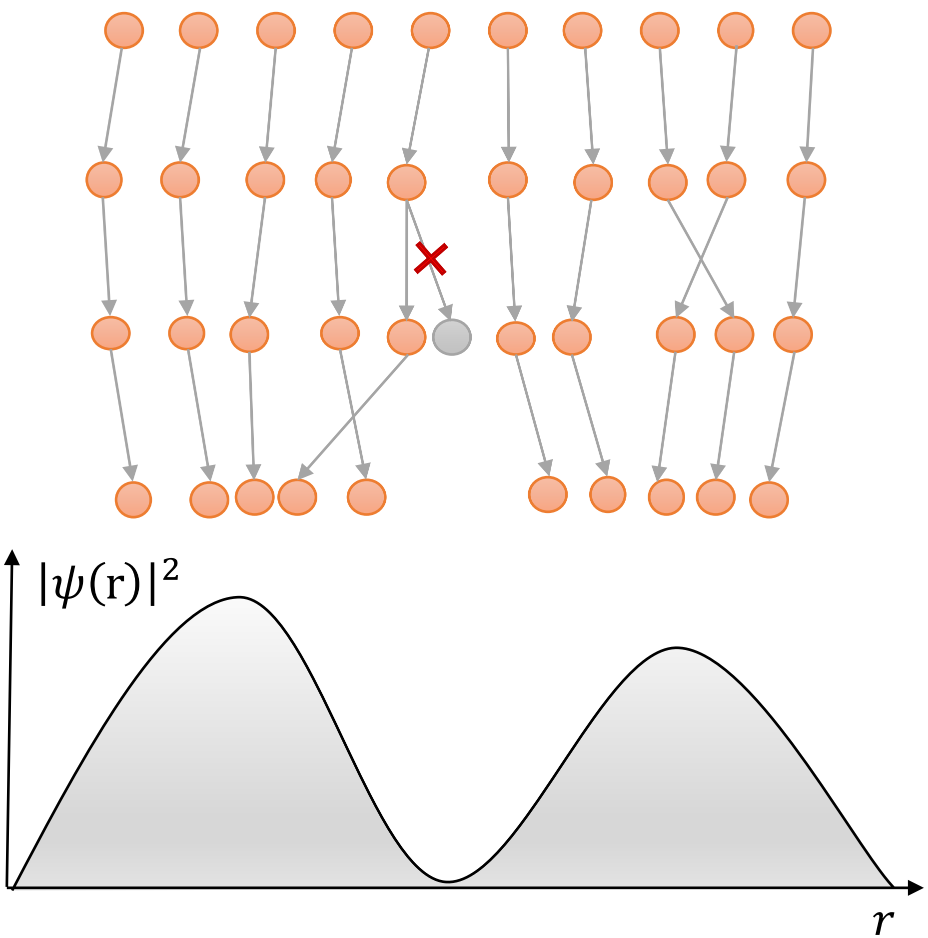

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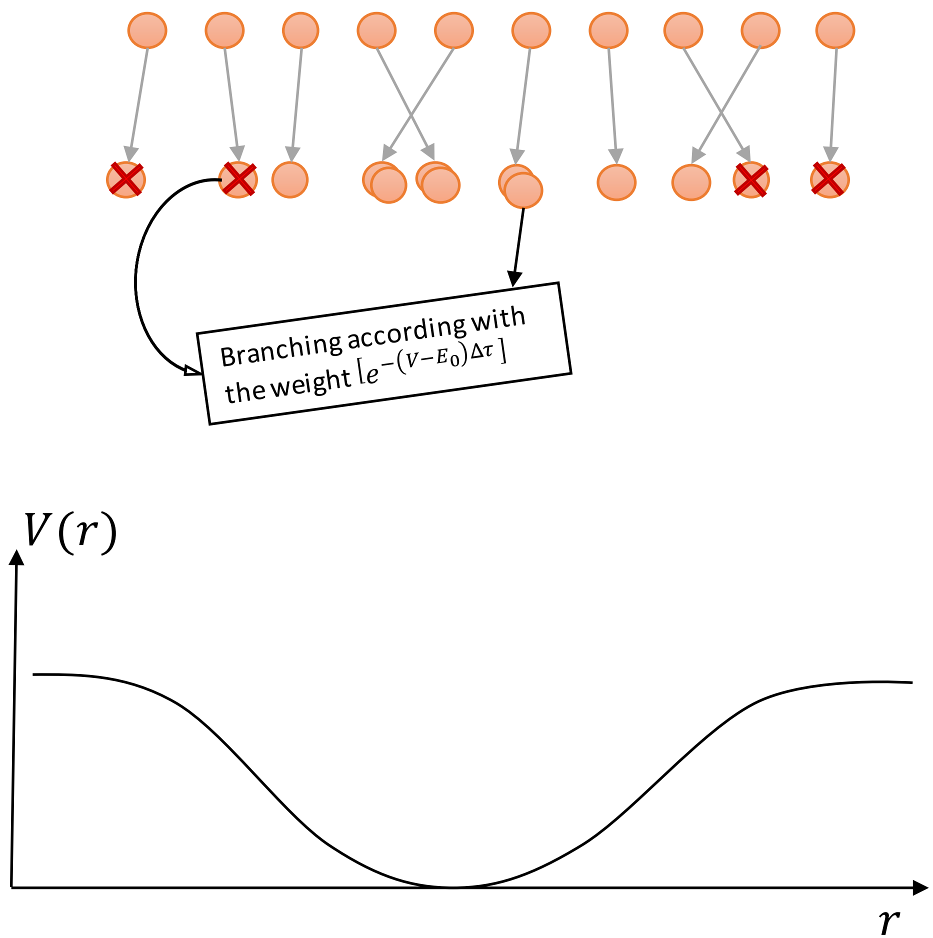

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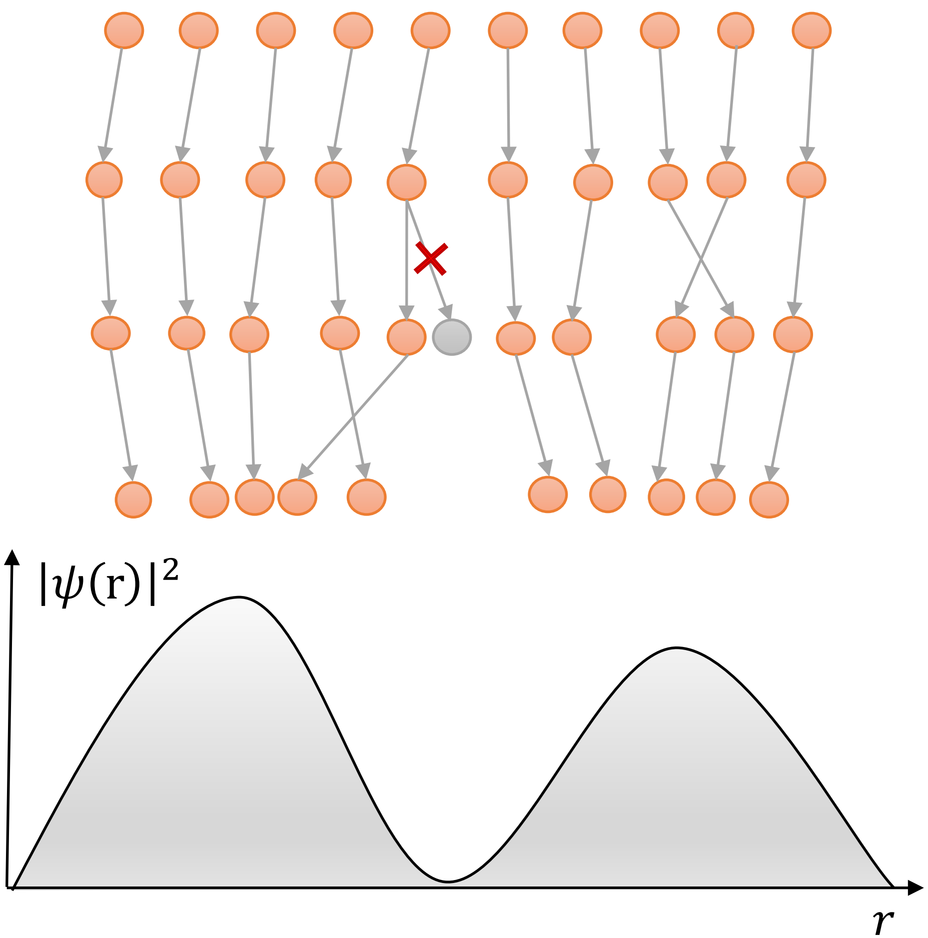

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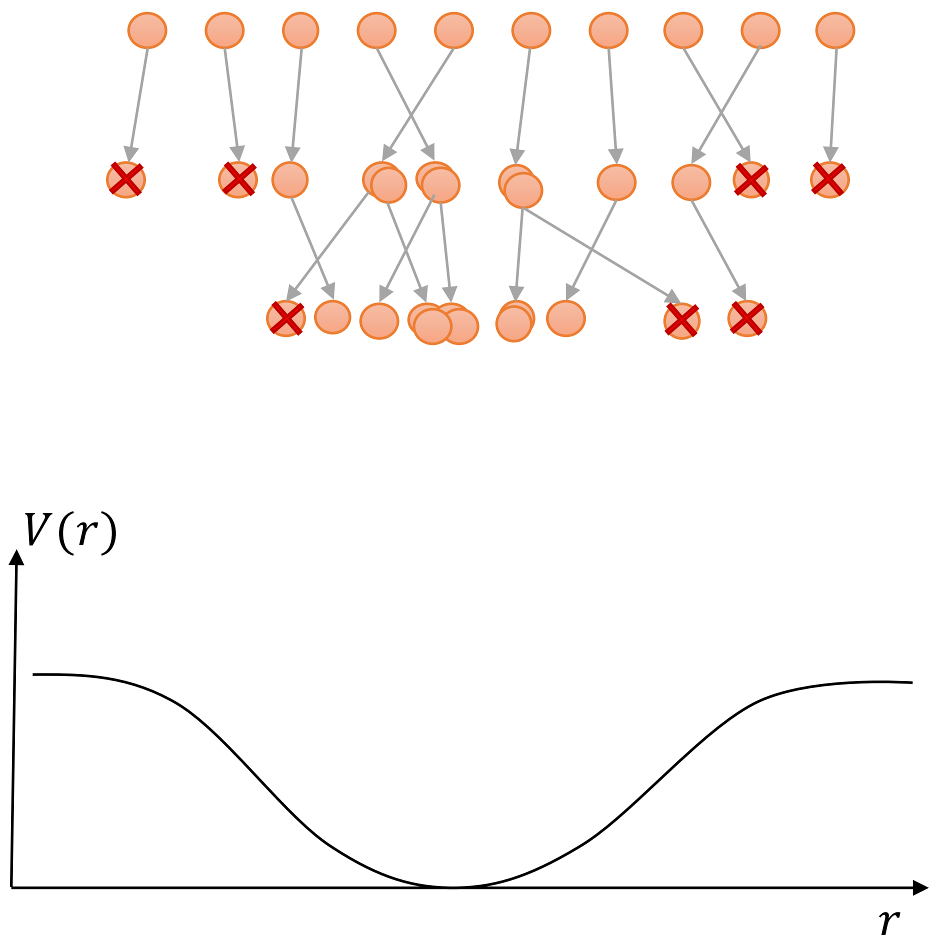

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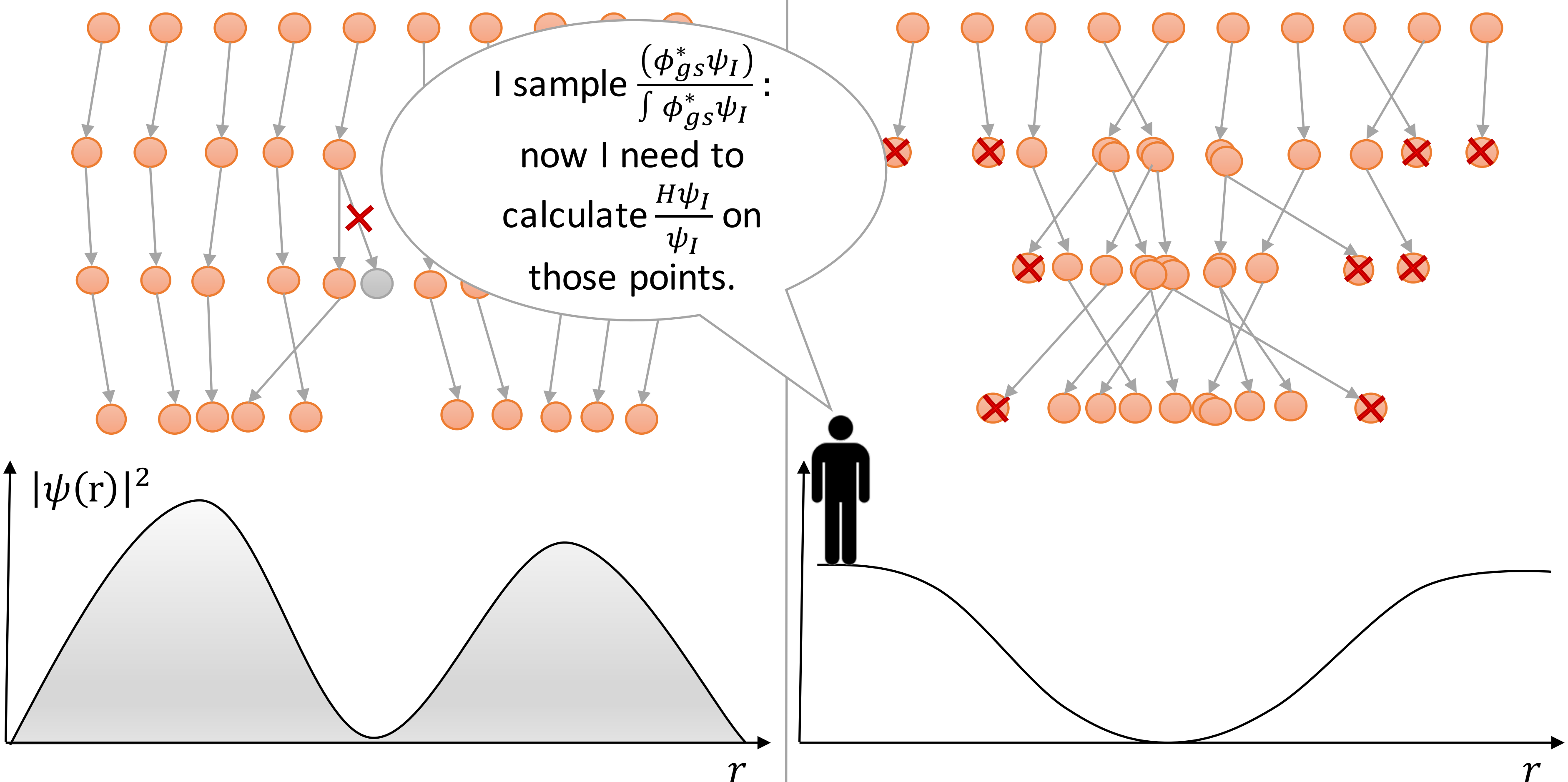

Monte Carlo Method

Sign problem:

$(\phi_{gs}^{*}\psi_{I})$ should **be real and positive to be interpreted as a probability** …

Fix node:

Only moves with **the same phase** as the **Guide wave function** ψ_I are allowed.

⇓

This will **restrict the base** on which wave function is projected, introducing a systematic error in the method.
(The system is projected on the lowest energetic state with the same **nodal surface as** ψ_I.)

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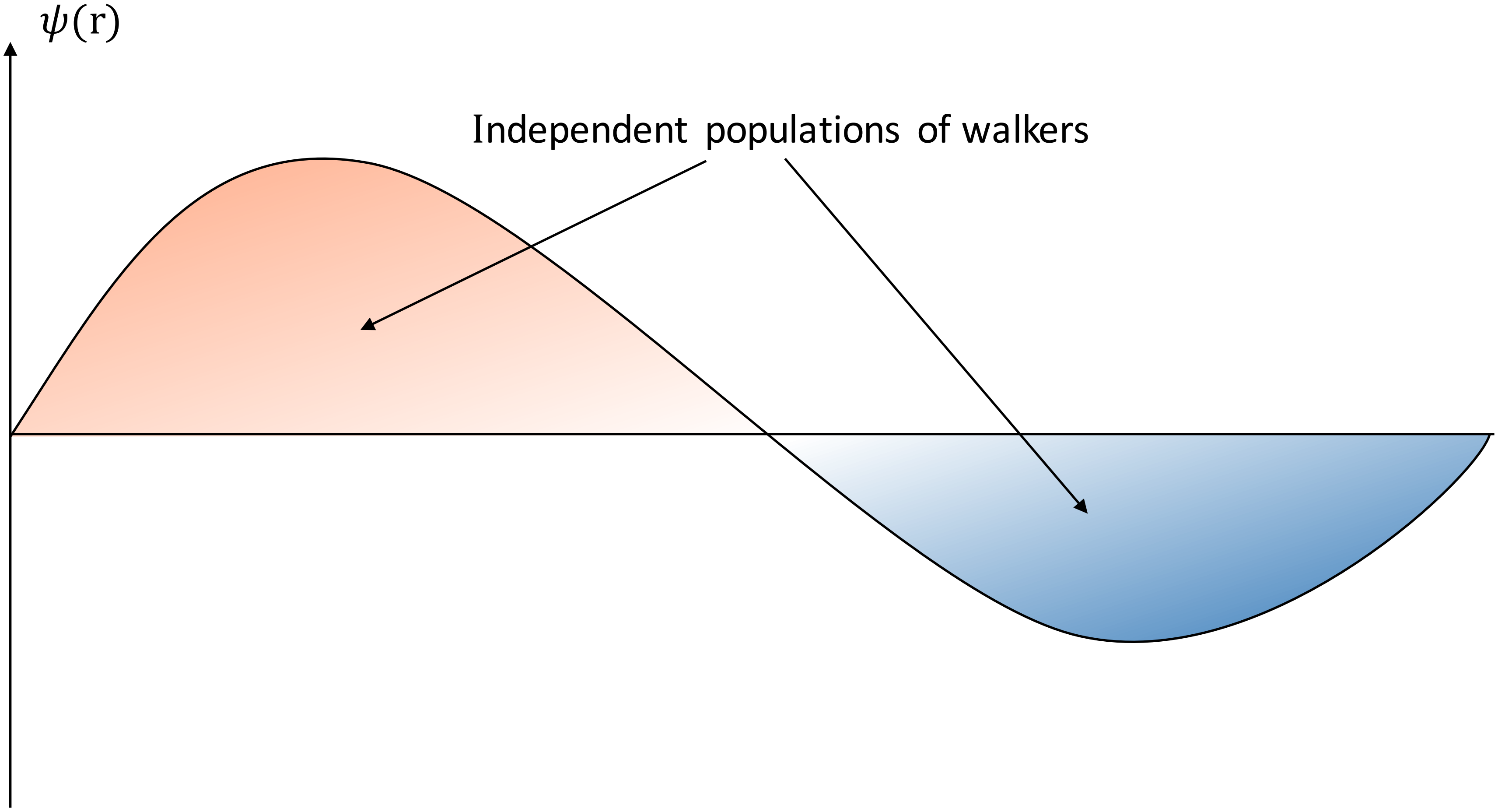


Monte Carlo Method

Guide wave function:

Linear combination of Slater determinants of single particle wave functions is used as Guide wave function.
(Scale adjustments of single particle WF can change the many body nodal surface.)

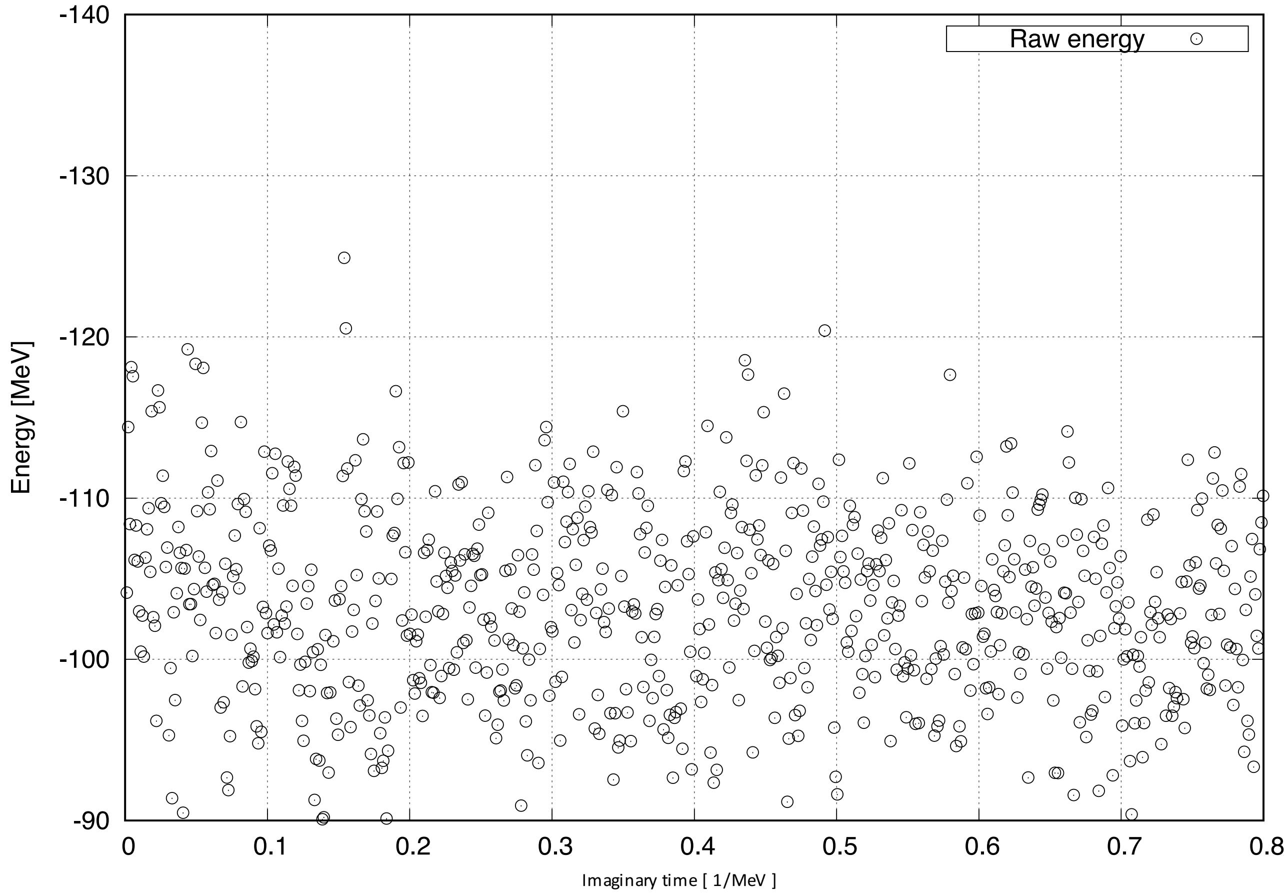
+

Correlations between particles are introduced (they are called Jastrow functions).

- **2-body correlations** can be calculated solving the two-body Schrödinger equation channel by channel runtime.
- **3-body correlations** are present only if 3-body forces are present. They are harder to be calculated during the code execution and need to be parameterized.

Monte Carlo Method

$^{4}He \mid M_{\pi} = 800 \text{ MeV} \mid \Lambda = 10\ fm^{-1}$



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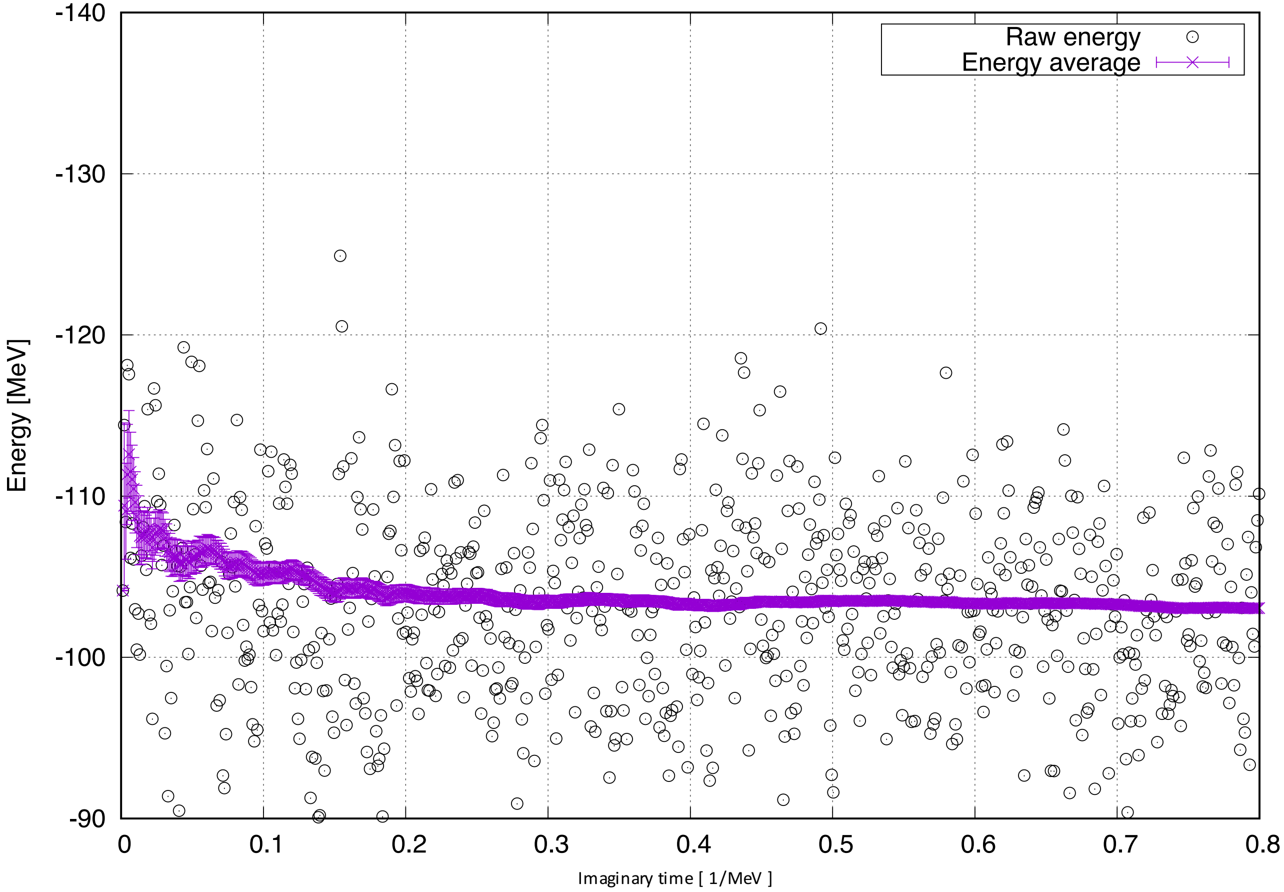

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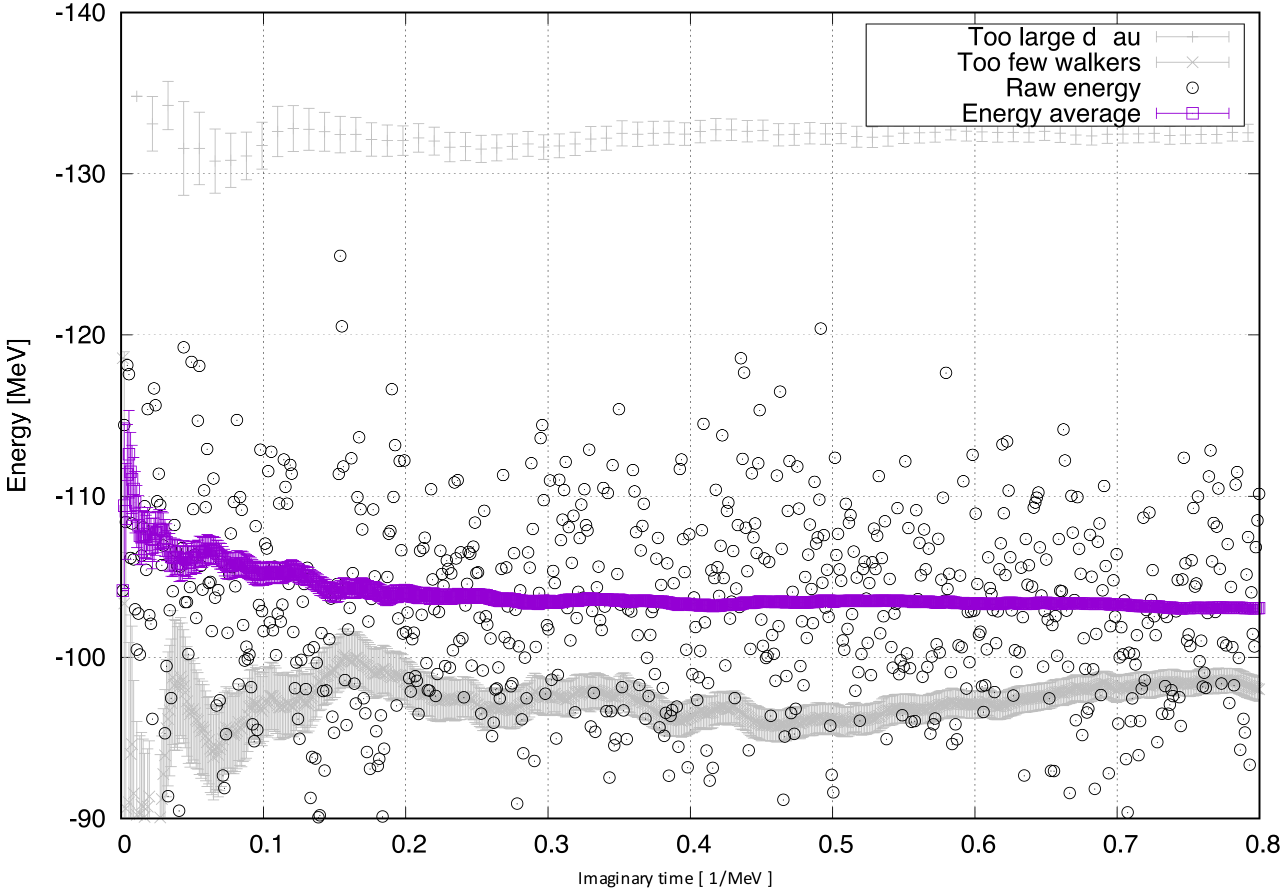


Monte Carlo Method

Spin/Isospin:

Single particle spin base is not close with respect not-quadratic spin operators.

For 3 particles:

$$(\overrightarrow{\sigma_2} \cdot \overrightarrow{\sigma_3}) \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ 2a_{\uparrow\downarrow\uparrow} - a_{\uparrow\uparrow\downarrow} \\ 2a_{\uparrow\uparrow\downarrow} - a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ 2a_{\downarrow\downarrow\uparrow} - a_{\downarrow\uparrow\downarrow} \\ 2a_{\downarrow\uparrow\downarrow} - a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} \neq \begin{pmatrix} a'_{\uparrow\uparrow\uparrow} \\ a'_{\uparrow\uparrow\downarrow} \\ a'_{\uparrow\downarrow\uparrow} \\ a'_{\uparrow\downarrow\downarrow} \\ a'_{\downarrow\uparrow\uparrow} \\ a'_{\downarrow\uparrow\downarrow} \\ a'_{\downarrow\downarrow\uparrow} \\ a'_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

n-body spinor $\rightarrow$ $\mathbf{2^N}$ components.

Monte Carlo Method

Spin/Isospin:

Using an **Hubbard-Stratonovich** transformation:

$$e^{-\frac{1}{2}\lambda O^2} = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-\frac{x^2}{2} + \sqrt{-\lambda} x\, O}$$

A quadratic operator can be transformed in a linear one,
at the price of an **integral** (per operator).

$$\vec{\sigma_i} \left(\begin{pmatrix} \alpha_1\, \widehat{p_\uparrow} \\ \beta_1\, \widehat{p_\downarrow} \\ \gamma_1\, \widehat{n_\uparrow} \\ \delta_1\, \widehat{n_\downarrow} \end{pmatrix}_1 \otimes \dots \otimes \begin{pmatrix} \alpha_i\, \widehat{p_\uparrow} \\ \beta_i\, \widehat{p_\downarrow} \\ \gamma_i\, \widehat{n_\uparrow} \\ \delta_i\, \widehat{n_\downarrow} \end{pmatrix}_i \otimes \dots \otimes \begin{pmatrix} \alpha_A\, \widehat{p_\uparrow} \\ \beta_A\, \widehat{p_\downarrow} \\ \gamma_A\, \widehat{n_\uparrow} \\ \delta_A\, \widehat{n_\downarrow} \end{pmatrix}_A \right) = \left(\begin{pmatrix} \alpha_1\, \widehat{p_\uparrow} \\ \beta_1\, \widehat{p_\downarrow} \\ \gamma_1\, \widehat{n_\uparrow} \\ \delta_1\, \widehat{n_\downarrow} \end{pmatrix}_1 \otimes \dots \otimes \begin{pmatrix} \alpha'_i\, \widehat{p_\uparrow} \\ \beta'_i\, \widehat{p_\downarrow} \\ \gamma'_i\, \widehat{n_\uparrow} \\ \delta'_i\, \widehat{n_\downarrow} \end{pmatrix}_i \otimes \dots \otimes \begin{pmatrix} \alpha_A\, \widehat{p_\uparrow} \\ \beta_A\, \widehat{p_\downarrow} \\ \gamma_A\, \widehat{n_\uparrow} \\ \delta_A\, \widehat{n_\downarrow} \end{pmatrix}_A \right)$$

Monte Carlo Method

Pro:

✓ Smart way to estimate **large integrals**.

✓ **Errors decrease with the number of sample** taken.

✓ **Diffusion** procedure samples from the **ground state** of the interaction.

✓ With **fix node** procedure, you can handle **fermion ground states.**

✓ **Auxiliary Field** procedure wipes out many coordinates, allowing **many particle calculations**.

Contra:

✗ **Intrinsic stochastic errors.**

✗ Difficult to extract **excited states**.

✗ To solve the **sign problem** only states with a particular **nodal surface** are available.

✗ **Auxiliary integrals** introduce new integrals.

Monte Carlo Method

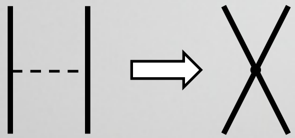
Release nodes:

- **The constraint on the phase is released.**
- Each move weighted with the **absolute value of the guide wave function**.

✓ No systematics from nodal surfaces

✗ Errors increase exponentially during the calculation.

Pionless Effective Field Theory



Regularization & Renormalization

The high energy physics is encoded in the LECs. $\overrightarrow{r_{ij}} = \overrightarrow{r_i} - \overrightarrow{r_j}$

But one has to **regularize** the potential introducing a cut-off:

$$C \cdot \delta(\overrightarrow{r_i} - \overrightarrow{r_j}) \Rightarrow C \frac{\Lambda^3}{8\pi^{3/2}} e^{\frac{-\Lambda^2 r_{ij}^2}{4}}$$

And **renormalize** it, making the LECs cut-off dependent:

$$C \frac{\Lambda^3}{8\pi^{3/2}} e^{\frac{-\Lambda^2 r_{ij}^2}{4}} \Rightarrow C(\Lambda) \frac{\Lambda^3}{8\pi^{3/2}} e^{\frac{-\Lambda^2 r_{ij}^2}{4}}$$

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About the cut-offs

Why push the cutoff high:

- **Large enough cut-off Λ** $\rightarrow$ the interaction contains all the relevant low energy physic.

Is difficult to say how large the cut-off should be:

- **Different regularizations** might show different convergence behavior.
- **The range of validity** of the theory is usually unknown and can depend from the system.

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One can (and has) to push the cutoff **higher than the supposed break scale of the theory.** ⇒ For a sufficiently large cutoff, all the relevant physics is included. ⇒ Observables will be **independent from the cutoff.**

About the cut-off

Every order will have a residual cut off dependence that will be absorbed (in part) in the next order:

› If you see a **cutoff dependence** on observables you are missing something on power counting.

Example: 3-body forces in a contact theory at LO:

Using only a 2-body attractive contact potential, the 3 (and more) body system become very bound increasing the cut-off (not cut-off independence).

› **No evidence of a 4-body** interaction at leading order.

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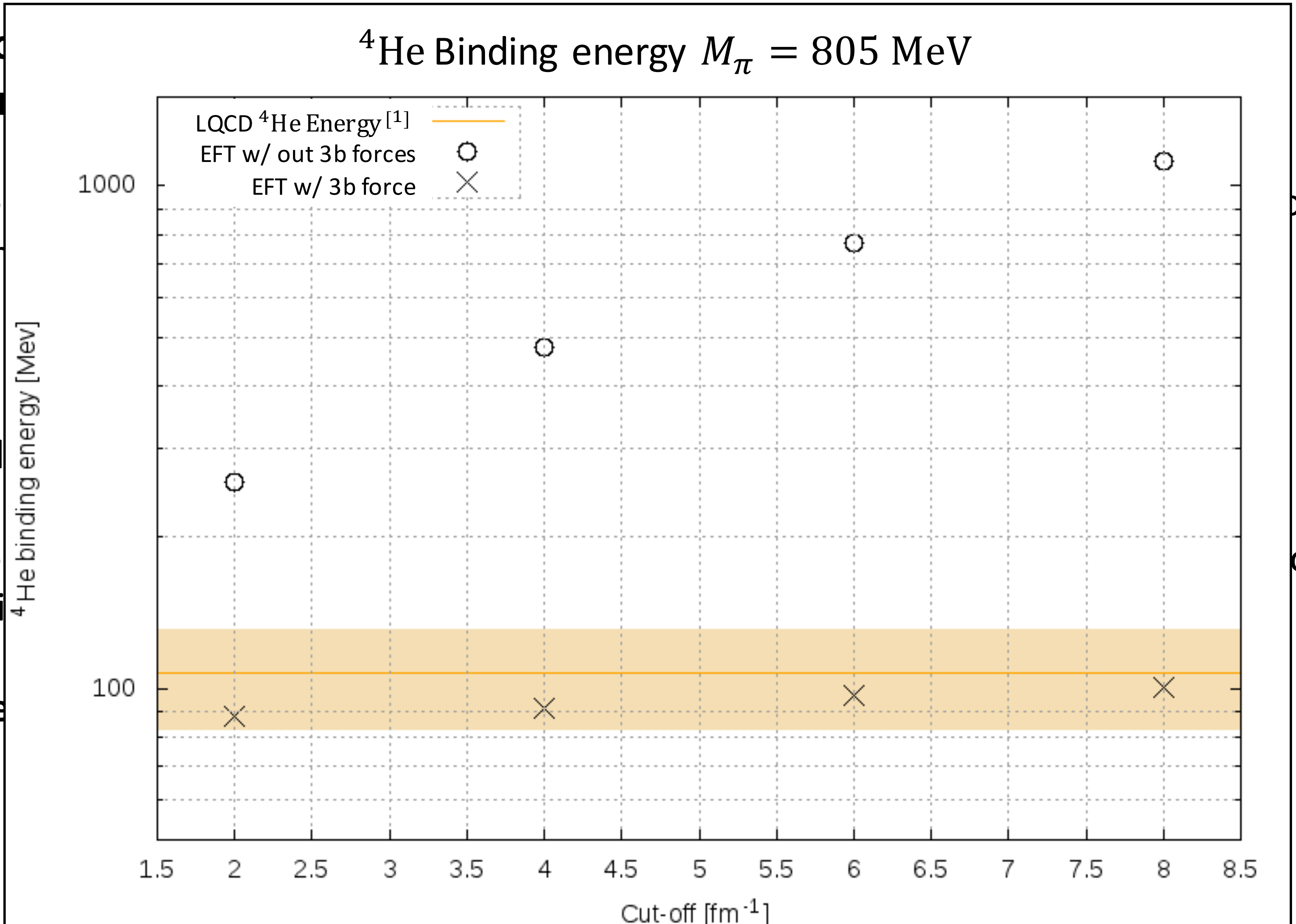

[1] - S. R. Beane, E. Chang and al. [Phys. rev. D 87, 034506 (2013)]

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You can use residual cut-off dependences to check the theory.

Contact EFT

$$q^2 = (p - p')^2$$
$$k^2 = (p + p')^2$$

$$V_{2b} = C_0 + C_1(\sigma_1 \cdot \sigma_2) + C_2(k^2 + q^2) + C_3(k^2 + q^2)(\sigma_1 \cdot \sigma_2) + \cdots$$

$$+$$

$$V_{3b} = D_0 + \cdots$$

After **regularization** in the coordinate space:

$$V^{LO} = \sum_{i<j} [C_0^\Lambda\, e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} + C_1^\Lambda\, e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} (\vec{\sigma_i} \cdot \vec{\sigma_j})\,]$$
$$+ D_0^\Lambda \sum_{(i<j)\neq k} \left[e^{-\frac{\Lambda^2}{2}\left(|r_{ij}|^2 + |r_{ik}|^2\right)} + e^{-\frac{\Lambda^2}{2}\left(|r_{ij}|^2 + |r_{jk}|^2\right)} + e^{-\frac{\Lambda^2}{2}\left(|r_{jk}|^2 + |r_{ik}|^2\right)} \right]$$

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$$V_{2b} = \overbrace{C_0 + C_1(\sigma_1 \cdot \sigma_2)}^{\text{LO}} + \overbrace{\underline{C_2(k^2 + q^2) + C_3(k^2 + q^2)(\sigma_1 \cdot \sigma_2) + \cdots}}^{\text{NLO}}$$

Perturbation theory

$$+$$

$$\underline{V_{3b} = D_0} + \cdots$$

Avoid Thomas collapse

After **regularization** in the coordinate space:

$$V^{LO} = \sum_{i<j} [C_0^\Lambda \, e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} + C_1^\Lambda \, e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} (\vec{\sigma_i} \cdot \vec{\sigma_j}) \,]$$
$$+ D_0^\Lambda \sum_{(i<j)\neq k} \left[e^{-\frac{\Lambda^2}{2}\left(|r_{ij}|^2 + |r_{ik}|^2\right)} + e^{-\frac{\Lambda^2}{2}\left(|r_{ij}|^2 + |r_{jk}|^2\right)} + e^{-\frac{\Lambda^2}{2}\left(|r_{jk}|^2 + |r_{ik}|^2\right)} \right]$$

Contact EFT

$$q^2 = (p - p')^2$$
$$k^2 = (p + p')^2$$

LO — NLO

$$V_{2b} = \underbrace{C_0 + C_1(\sigma_1 \cdot \sigma_2)}_{\text{LO}} + \underbrace{C_2(k^2 + q^2) + C_3(k^2 + q^2)(\sigma_1 \cdot \sigma_2)}_{\text{NLO}} + \cdots$$

$+$

$$V_{3b} = D_0 + \cdots$$

Perturbation theory

Avoid Thomas collapse

After **regularization** in the coordinate space:

$$V^{LO} = \sum_{i<j} [C_0^{\Lambda}\, e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} + C_1^{\Lambda}\, e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2} (\vec{\sigma_i} \cdot \vec{\sigma_j})\,]$$
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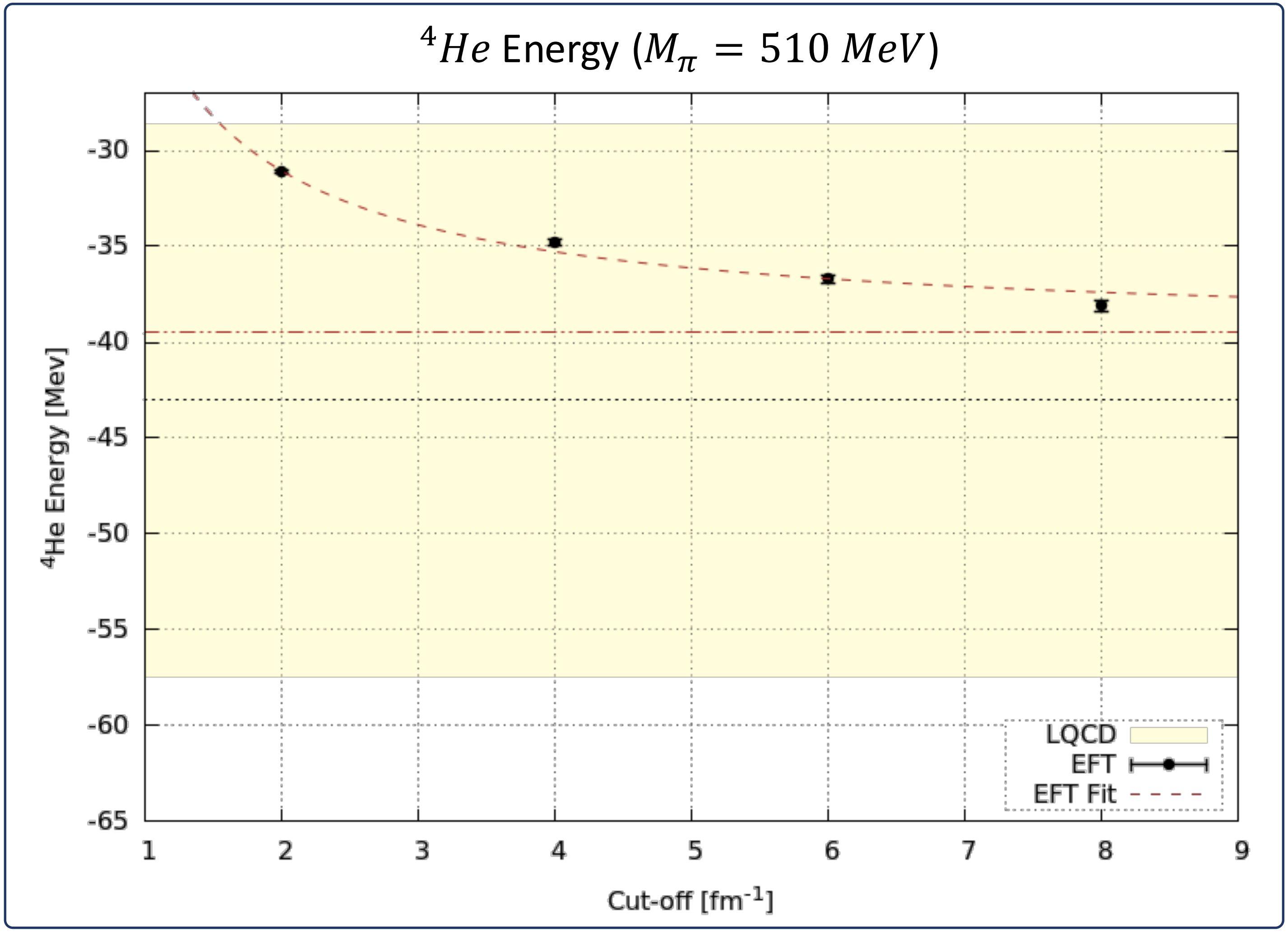
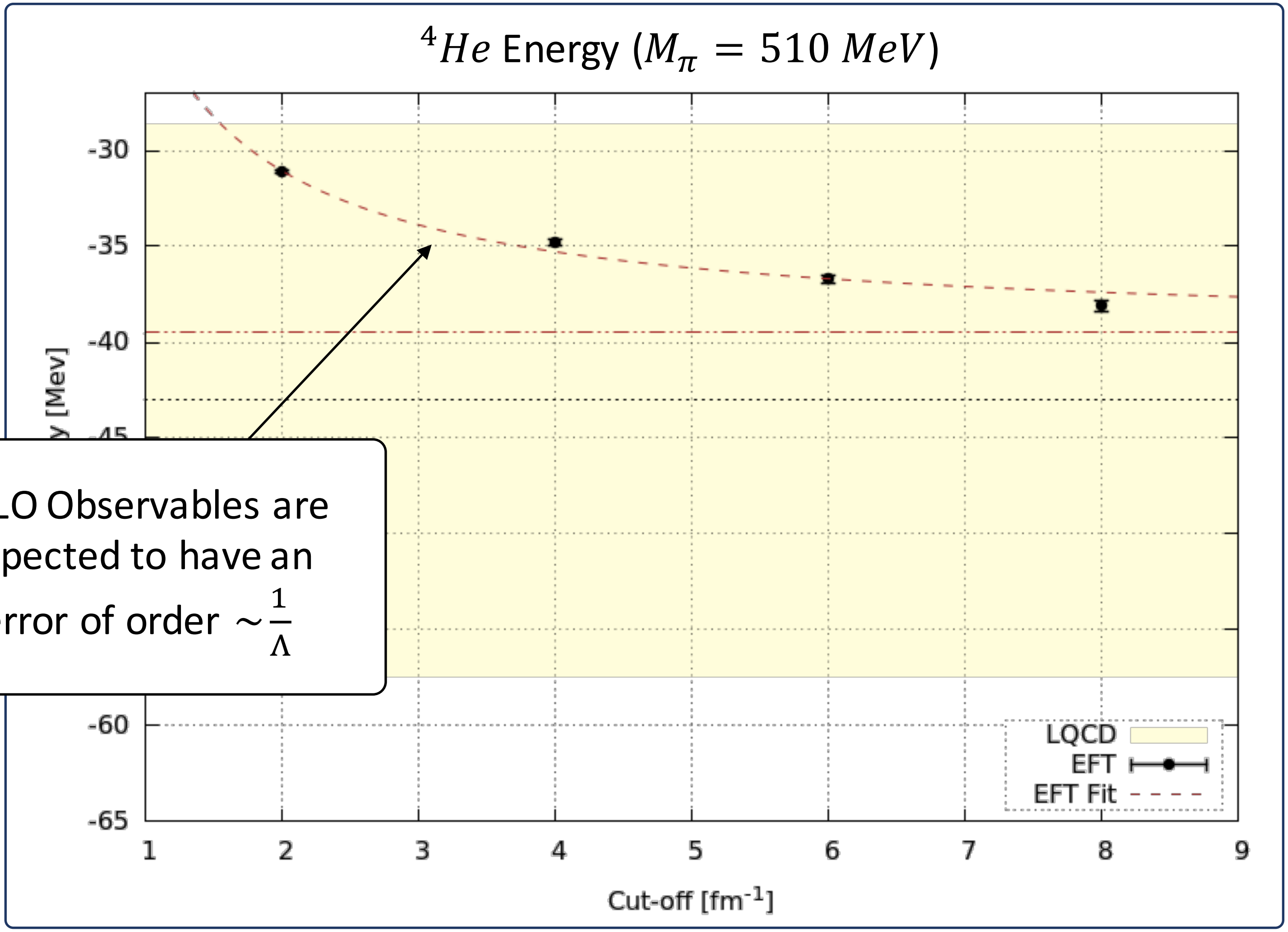
Contact EFT



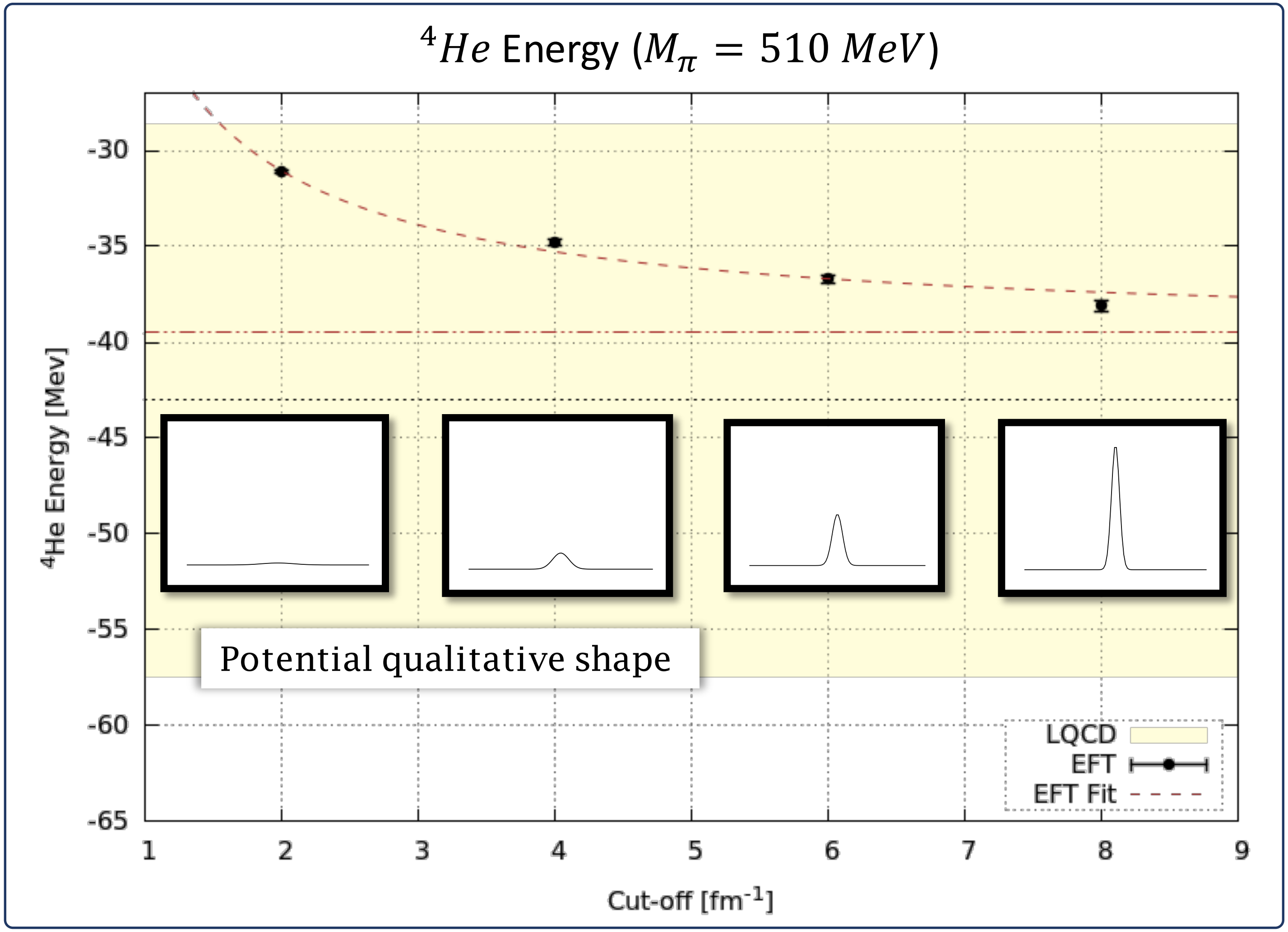
^{4}He Energy ($M_{\pi} = 510\ MeV$)
-30
-35
-40
-45
-50
-55
-60
-65
^{4}He Energy [Mev]
1
2
3
4
5
6
7
8
9
Cut-off [fm^{-1}]
LQCD
EFT
EFT Fit

Contact EFT



At LO Observables are expected to have an error of order $\sim\frac{1}{\Lambda}$

Contact EFT



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1
2
3
4
5
6
7
8
9
Cut-off [fm^{-1}]
Potential qualitative shape
LQCD
EFT
EFT Fit

LQCD few-body data

Nucleus	**Nature**	$m_\pi = 510\ MeV$ [1]	$m_\pi = 805\ MeV$ [2]
N (mass)	939.6	1320.0	1634.0
P (mass)	938.3	1320.0	1634.0
$n - p$	2.224	11.5(1.3)	19.5(4.8)
$n - n$	---------	7.4(1.4)	15.9(3.8)
^3H	8.482	20.3(4.5)	53.9(10.7)
^3He	7.718	20.3(4.5)	53.9(10.7)
^4He	28.296	43.0(14.4)	107.0(24.2)

[1] - Takeshi Yamazaki, Ken-ichi Ishikawa and al. [Phys. rev. D 86, 074514 (2012)]
[2] - S. R. Beane, E. Chang and al. [Phys. rev. D 87, 034506 (2013)]

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2b LECs

3b LEC

Benchmark

[1] - Takeshi Yamazaki, Ken-ichi Ishikawa and al. [Phys. rev. D 86, 074514 (2012)]
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α

$m_\pi = 140\ MeV$	
Λ $[\mathrm{fm}^{-1}]$	^{4}He Energy [MeV]
2	-23.3(1)
4	-23.4(2)
6	-24.8(3)
8	-26.0(3)
∞	-28.3(5)
Exp	-28.296

$m_\pi = 510\ MeV$	
Λ $[\mathrm{fm}^{-1}]$	^{4}He Energy [MeV]
2	-31.1(1)
4	-34.8(2)
6	-36.7(2)
8	-38.1(3)
∞	-38.8(1.0)
LQCD	-43(14)

$m_\pi = 805\ MeV$	
Λ $[\mathrm{fm}^{-1}]$	^{4}He Energy [MeV]
2	-87.9(2)
4	-91.3(3)
6	-96.4(4)
8	-101.3(5)
∞	-114(15)
LQCD	-107(24)

- Results has been checked using Monte Carlo and diagonalization methods.
- Extrapolation done using $f(x) = a + \frac{b}{\Lambda} + \frac{c}{\Lambda^2}$ excluding $\Lambda = 2\ \mathrm{fm}^{-1}$.
- All the shown errors are statistical errors from Monte Carlo method and extrapolation errors.
- Physical m_π LECs have been fitted using B(d), a(p - n) and B(^{3}H)

^{16}O

Preliminary

$m_\pi = 140\ MeV$			$m_\pi = 510\ MeV$			$m_\pi = 805\ MeV$		
Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]	Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]	Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]
2	-97(1)	-93.2(1)	2	-114.6(2)	-124.4(3)	2	-347(1)	-351(1)
4	-58(1)	-94.0(8)	4	-113.8(2)	-139.1(7)	4	-335(1)	-365(1)
6	-50(1)	-100(1)	6	-109.7(1)	-147(1)	6	-326(1)	-385(2)
8	-52(1)	-104(2)	8	-105.7(5)	-153(1)	8	-315(1)	-405(2)

- All the shown errors are statistical errors from Monte Carlo method.

Calculation issues.

Preliminary

- **Oxygen is not bound** with respect of 4α system.
- DMC can find only ground states.
- The Oxygen energy is far from the threshold.

- We are not getting the correct ground state (4α is more bound than our ^{16}O).
- The error is probably due to the **Fixed phase** approximation that force the nucleus to be in wrong ground state.

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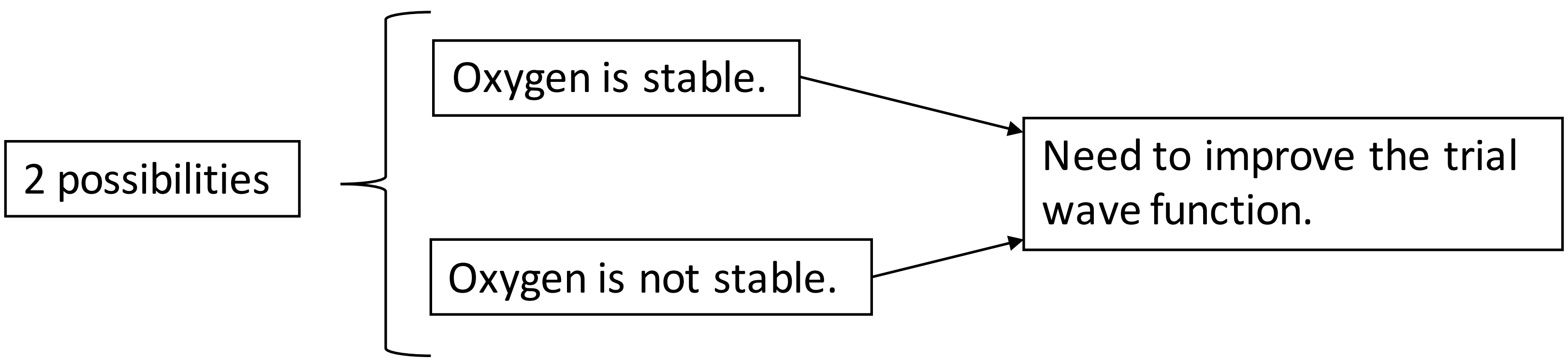


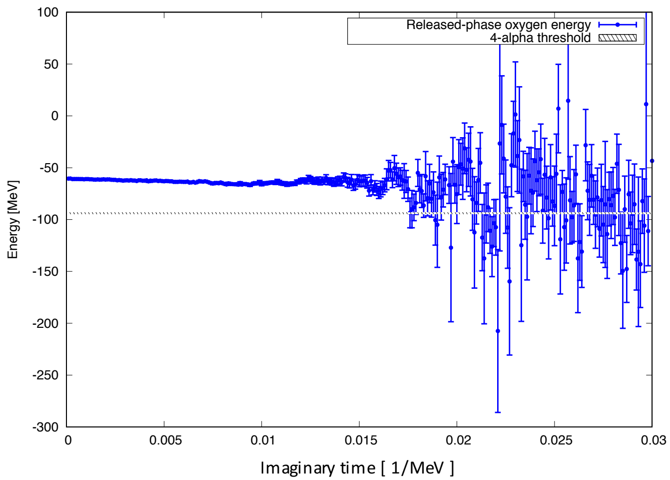
Release nodes

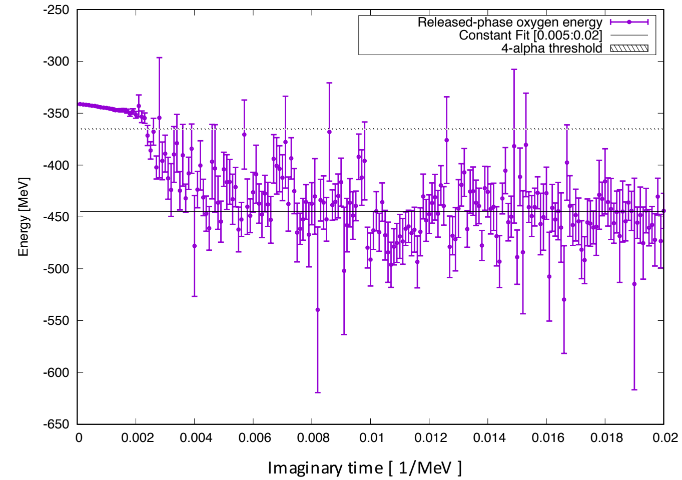
Preliminary

M_π 140 MeV 800 MeV

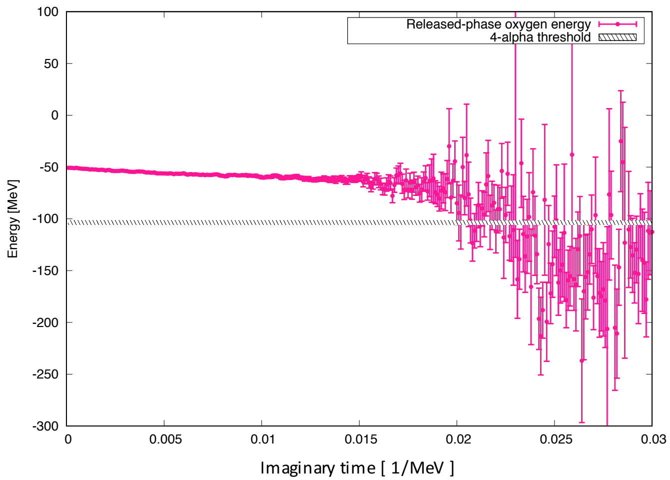
Cut-off

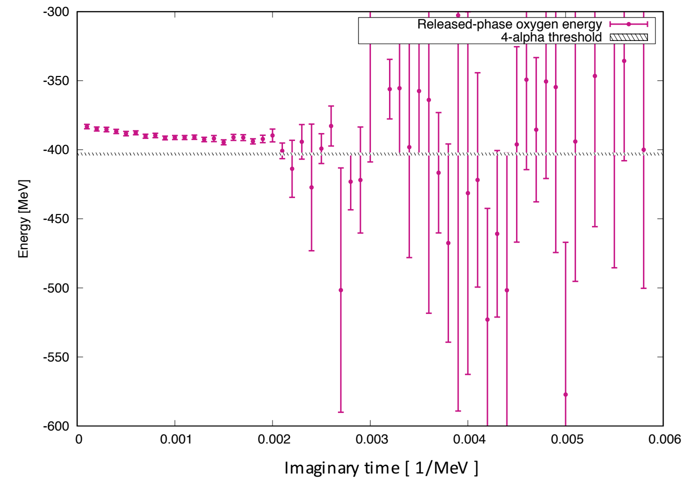
$4\ \mathrm{fm}^{-1}$





$8\ \mathrm{fm}^{-1}$





Conclusions:

- ^{4}He seems to **converge** in the cut-off, and **agrees with LQCD result**.
- Oxygen seems **to be unstable with respect 4α** for $m_\pi = 140, 510$ and 805 MeV.
- **Release node can recover** 4α state for $m_\pi = 140$ MeV .
- **Evidence for a bound state** for $m_\pi = 805$ MeV and $\Lambda = 4\ \text{fm}^{-1}$

What's next:

- Accumulate **more statistics** for $m_\pi = 805$ MeV and $\Lambda = 8\ \text{fm}^{-1}$.
- Look ^{16}O at **different Cut-offs** for $m_\pi = 805$ MeV.
- **Next to leading order.**

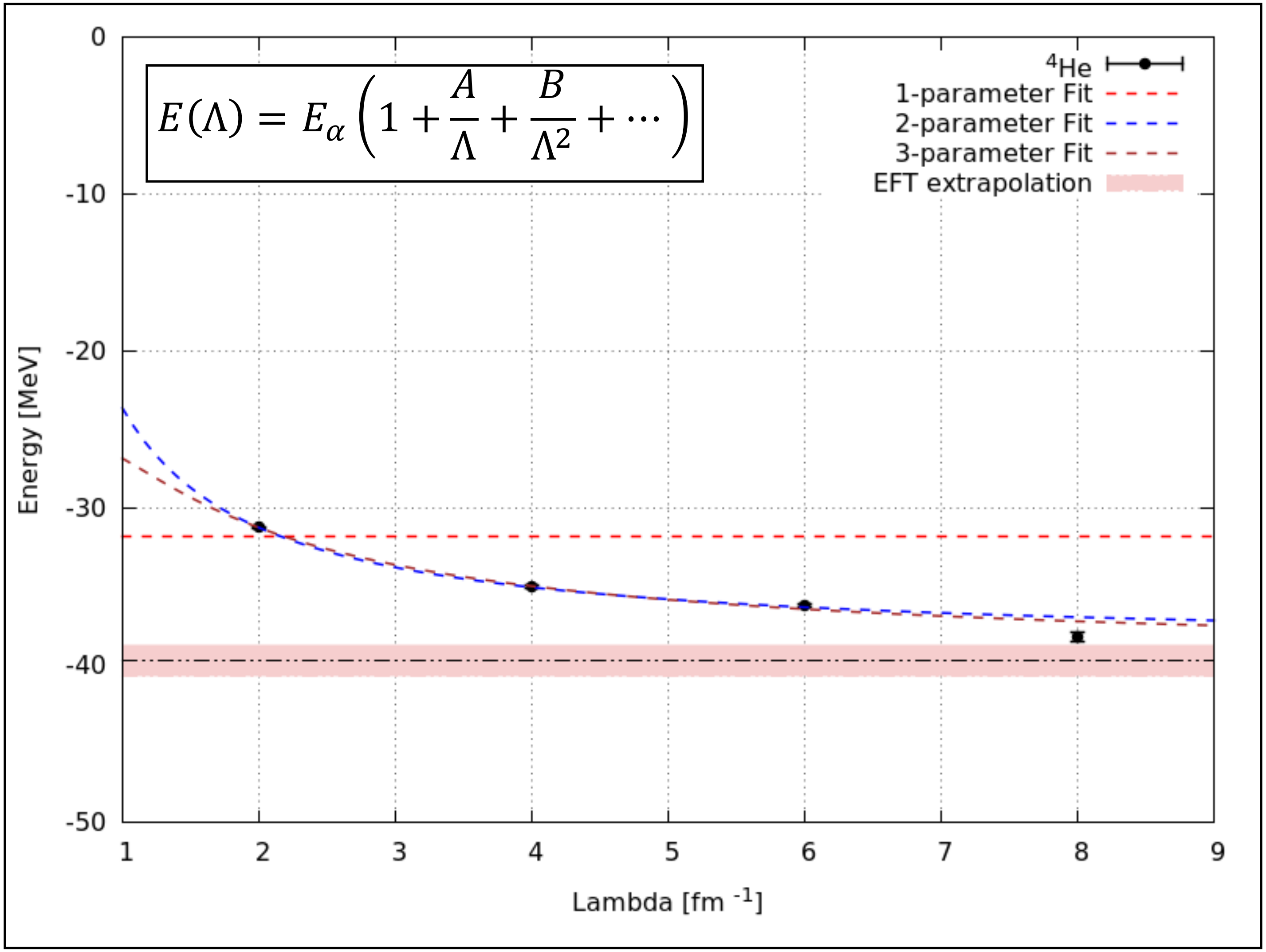
Other interesting things:

- Look at **intermediate nuclei**.
- Probe **$\alpha - \alpha$ interaction**.

Thanks for your attention

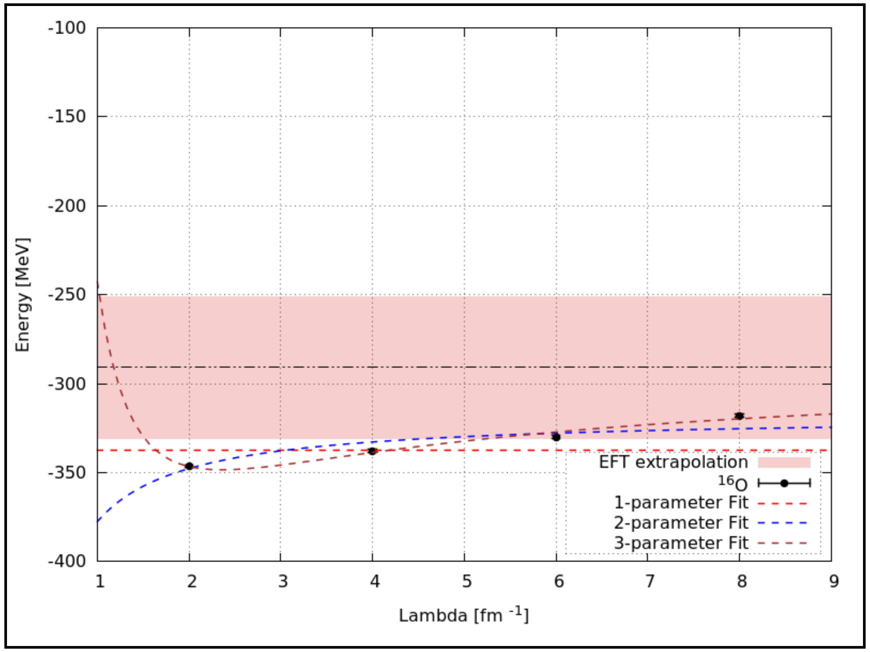
Convergences of data $m_\pi = 500\ MeV$

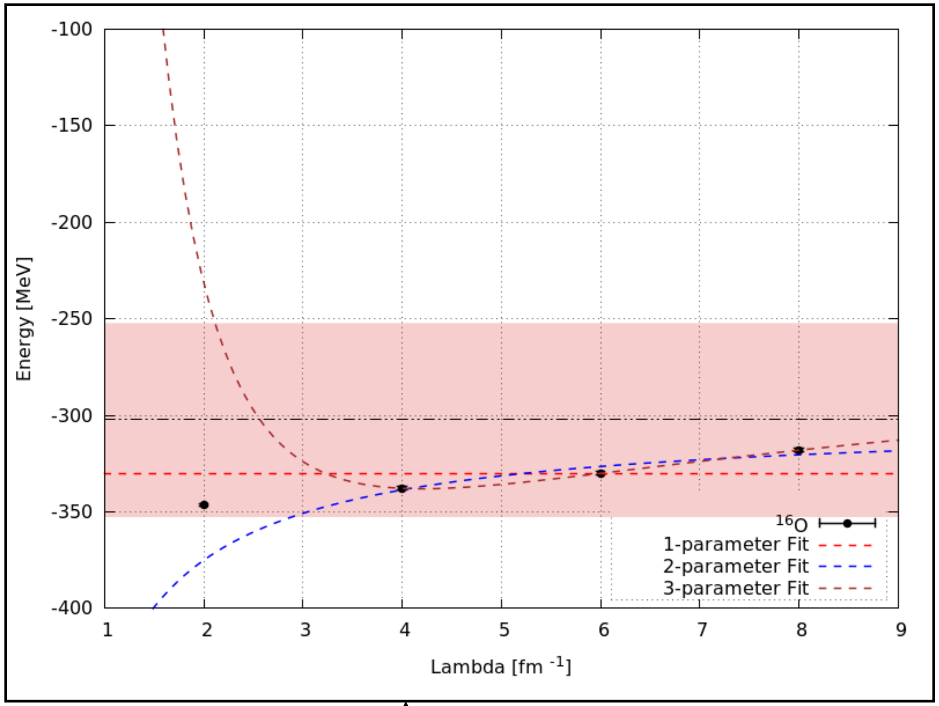
^4He energy



Convergences of data $m_\pi = 800\ MeV$

^{16}O energy





Excluding $\Lambda = 2\ fm^{-1}$ from fit.

Convergences of data at physical m_π

$$V_{Lo} = \sum_{ij}[C_0 + C_1(\sigma_1 \cdot \sigma_2)]\delta_{r_i,r_j} + \sum_{ijk} D_0\, \delta_{r_i,r_j,r_k}$$

$n-p$
scattering lenght
and binding energy

^3H binding energy

Λ $[\mathrm{fm}^{-1}]$	$^4He\ Energy$ $[MeV]$
2	-23.3(1)
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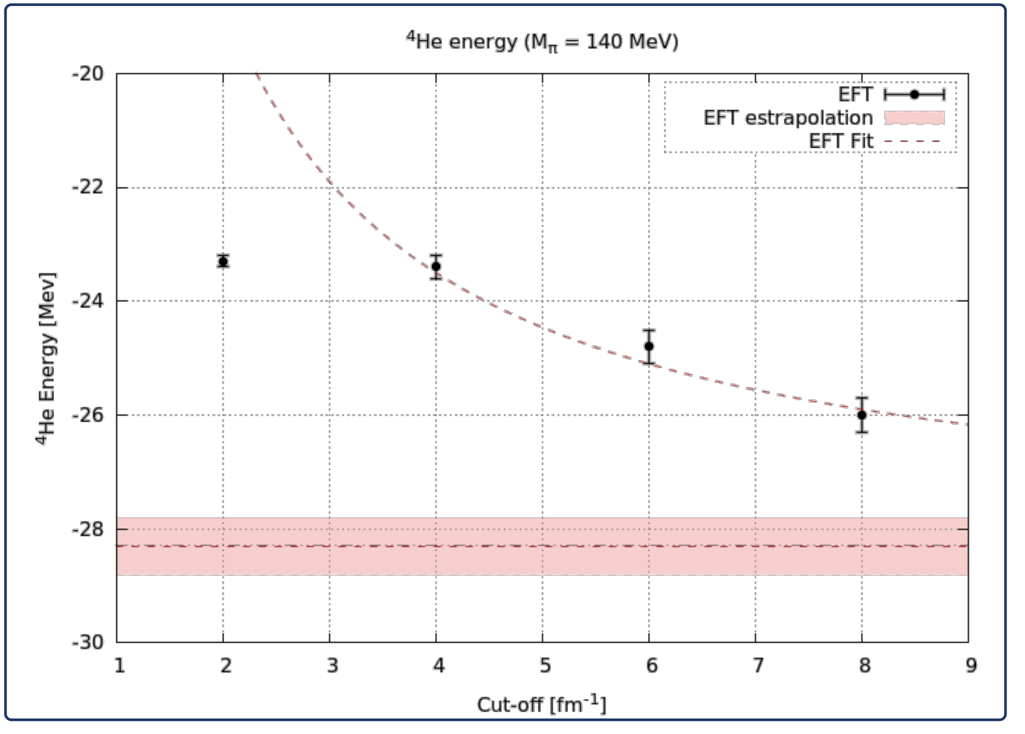
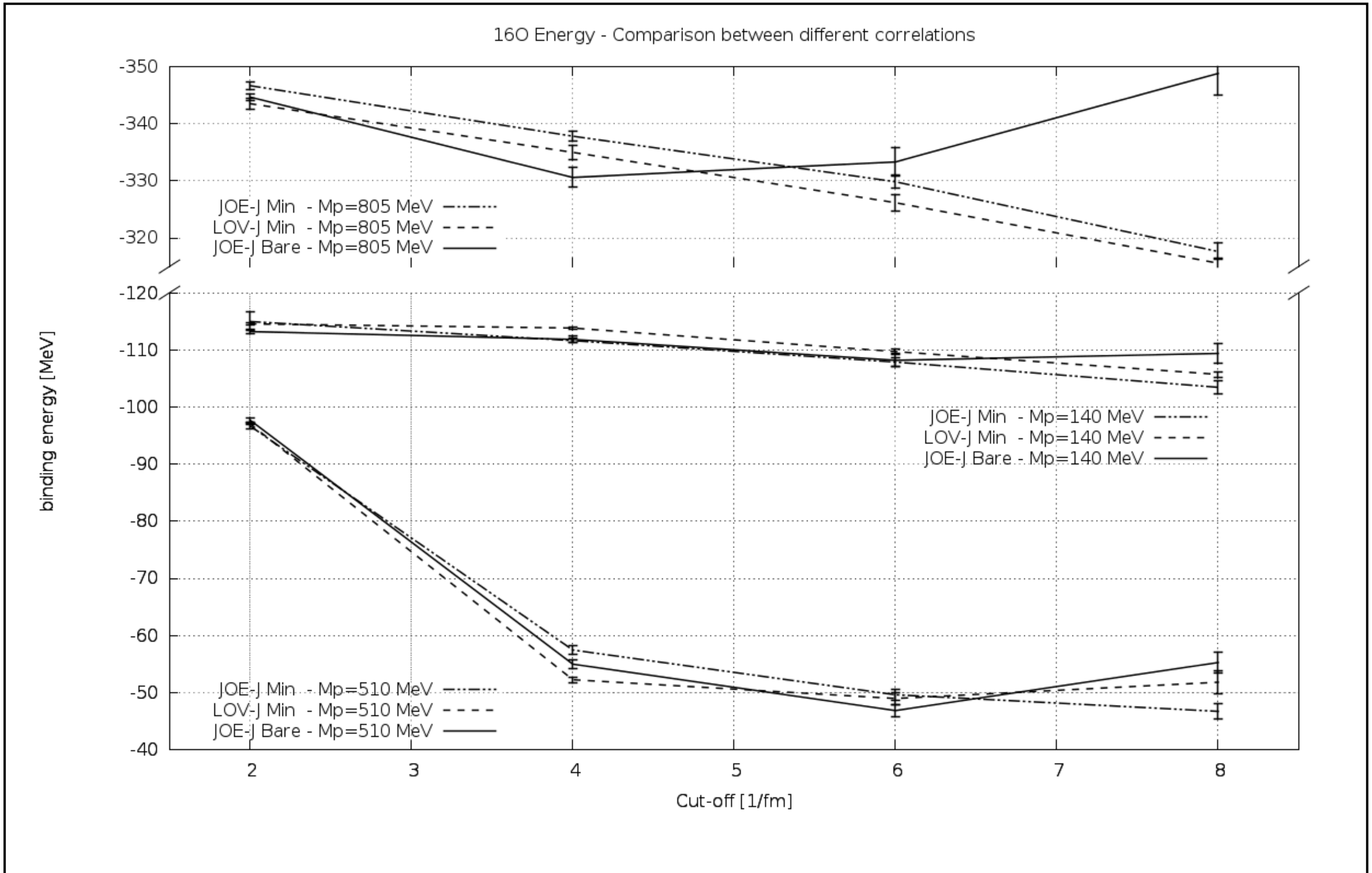


Different correlations in AFDMC



^{40}Ca

$m_\pi = 510\ MeV$		
Λ $[\mathrm{fm}^{-1}]$	$^{40}\mathrm{Ca}$ $Energy$ $[MeV]$	10α $treshold$ $[MeV]$
2	-279.1(9)	-311(1)
4	-260(2)	-348(2)
6	-243(4)	-367(2)
8	-186(5)	-381(3)
∞	-	-388(1)
LQCD	-	-