

Effective theory for lattice nuclei

(using Monte Carlo methods)

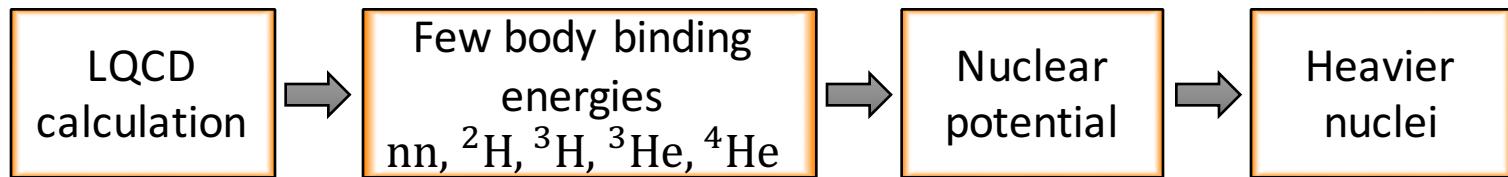
Lorenzo Contessi
(TIFPA, Università degli studi di Trento)

Overview:

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

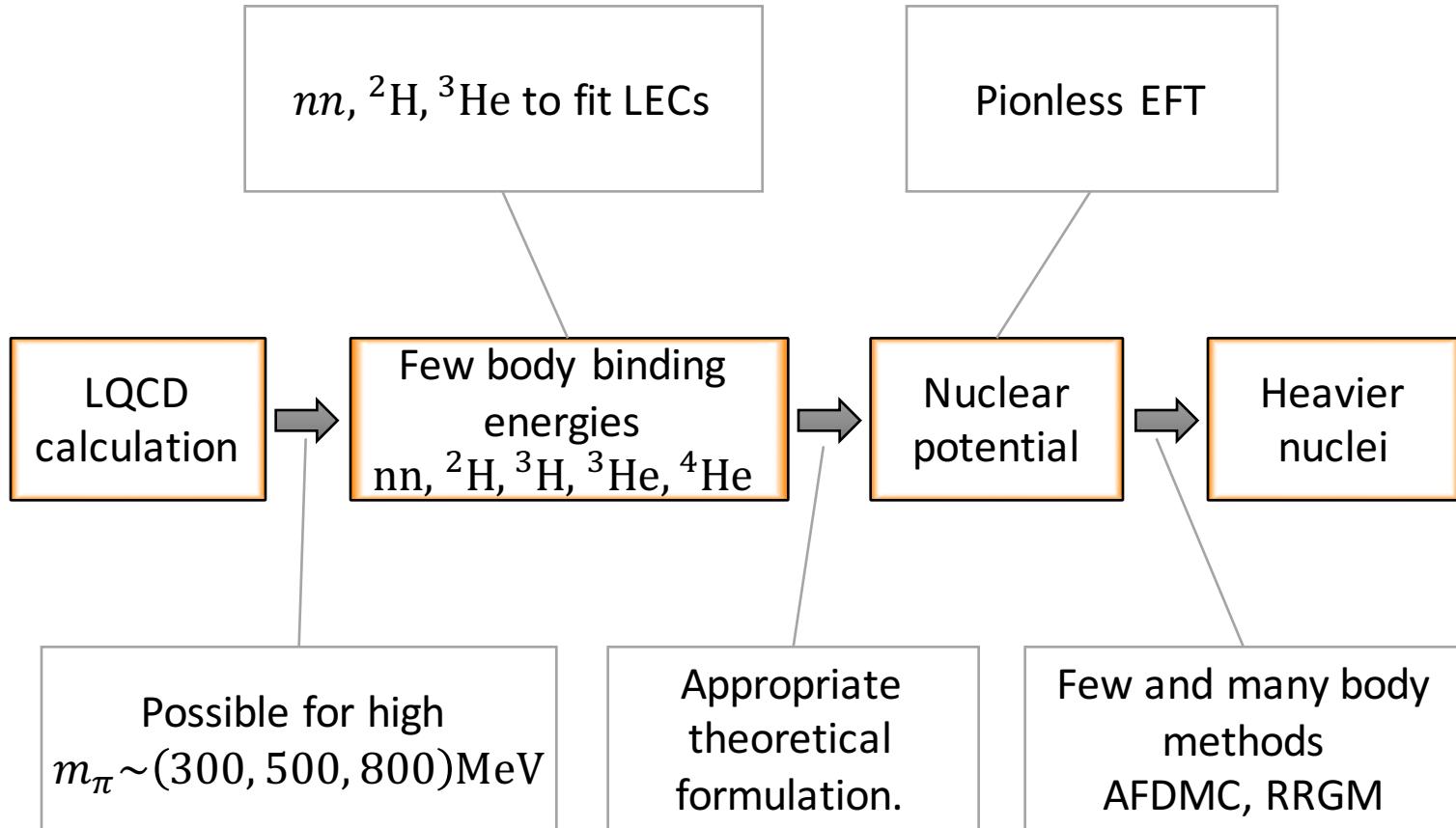


Connect nuclear physics with QCD





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Theory formulation



- We have a good phenomenological understanding of nuclear interaction for physical m_π .
- It is difficult to have a phenomenological description changing m_π .

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Few data available



Need a potential with few parameters as possible.

Pions are heavy.



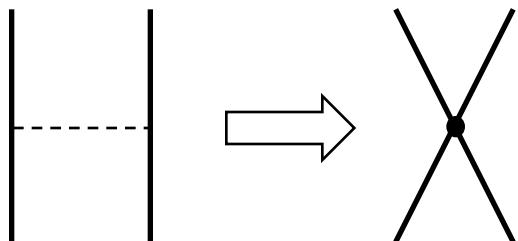
No needs to include Pions explicitly.

Theory formulation



Pionless EFT:

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



Plus:

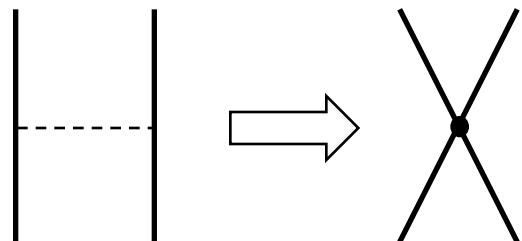
- Pionless theory contains only contact interactions.
- Relatively well understand power counting.

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Monte Carlo Method



20/04/16

INT: Nuclear Physics from Lattice QCD -
Effective theory for lattice nuclei

Monte Carlo Method



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

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

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

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$$E_\psi = \langle \psi | H | \psi \rangle = \int \psi^* H \psi = \int |\psi|^2 \frac{H\psi}{\psi}$$

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Probability distribution
to sample.

Function to be
computed

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:

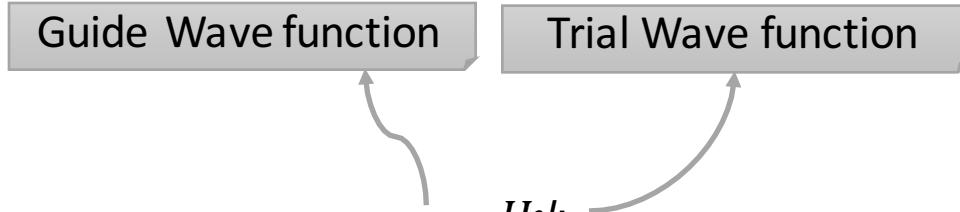
$$\begin{aligned} |\phi_{gs}\rangle &= e^{-(H-E_0)\tau} |\psi\rangle = \sum_{n=0}^{\infty} c_n e^{-(H-E_0)\tau} |\psi_n\rangle = c_0 |\phi_{gs}\rangle + \sum_{n=1}^{\infty} c_n e^{-(En-E_0)\tau} |\psi_n\rangle \\ e^{-(H-E_0)\tau} |\psi\rangle &\cong (e^{-(H-E_0)\Delta\tau})^N |\psi\rangle \cong (e^{\frac{\hbar}{2m}\Delta\tau \nabla^2} e^{-(V-E_0)\Delta\tau})^N |\psi\rangle \end{aligned}$$

Monte Carlo Method



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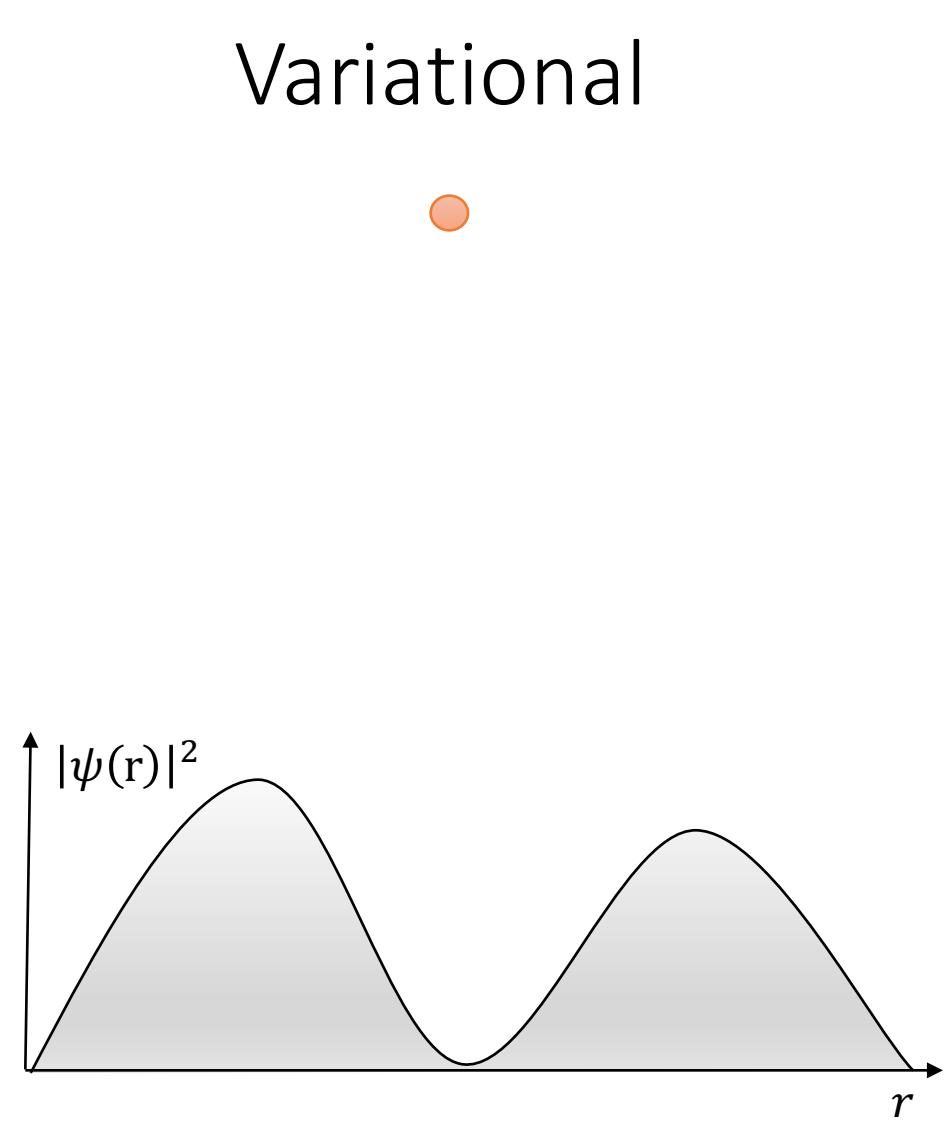
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Monte Carlo Method



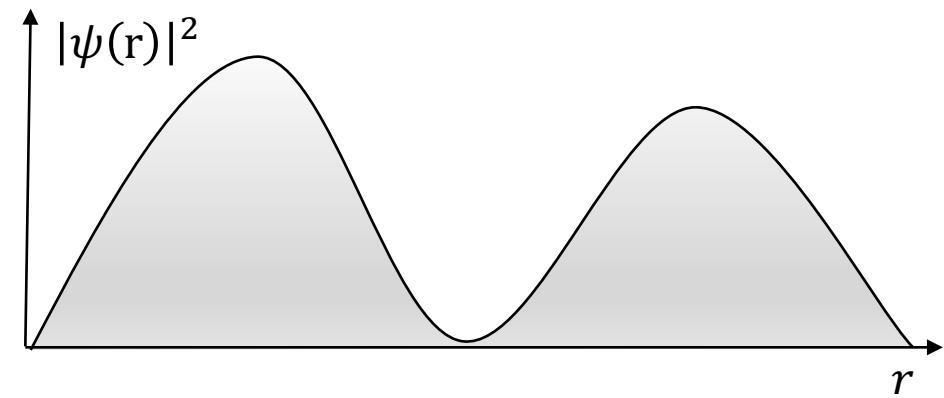
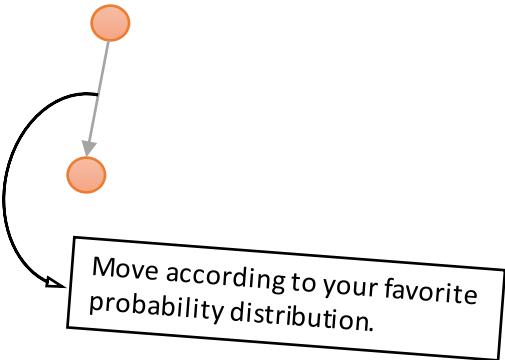
Variational



Monte Carlo Method



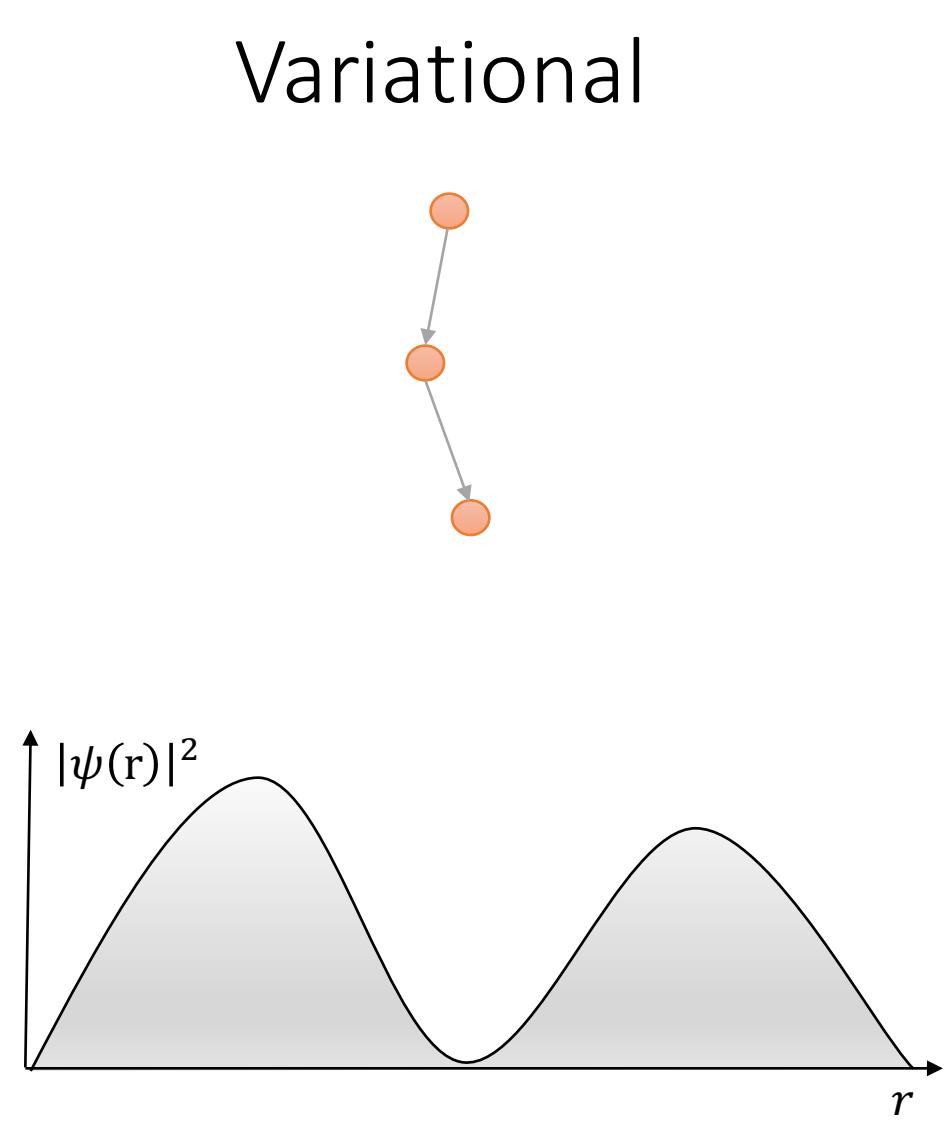
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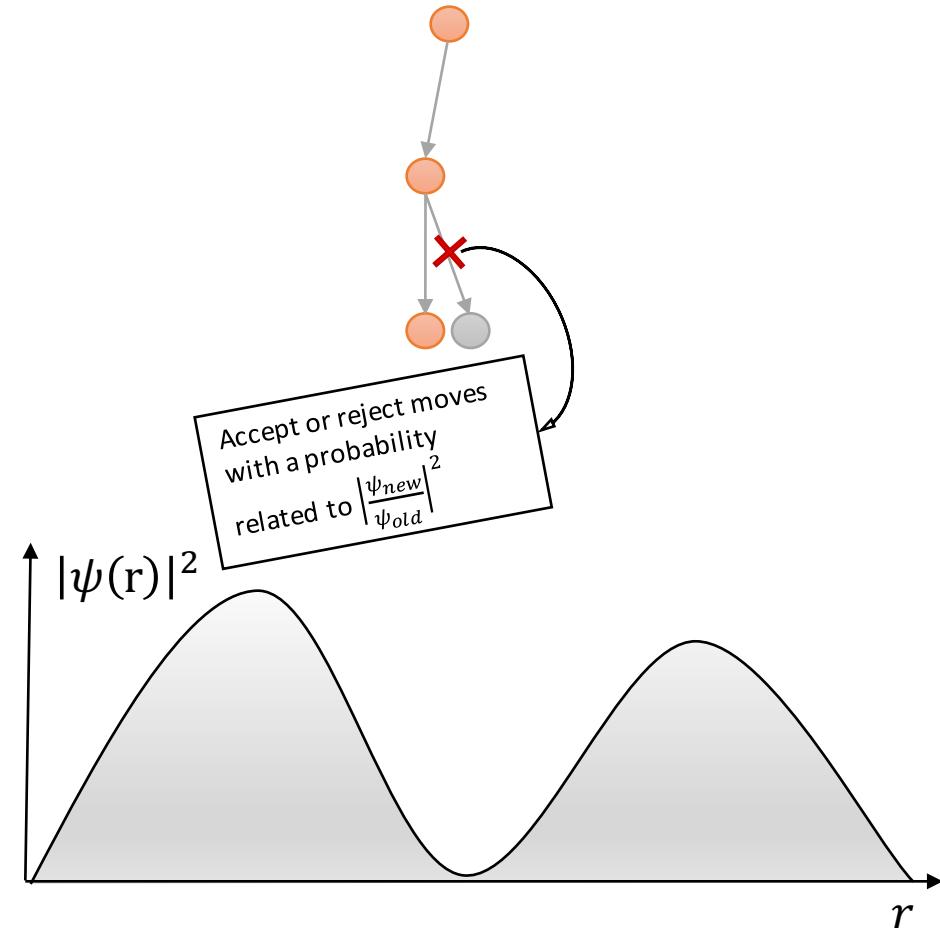
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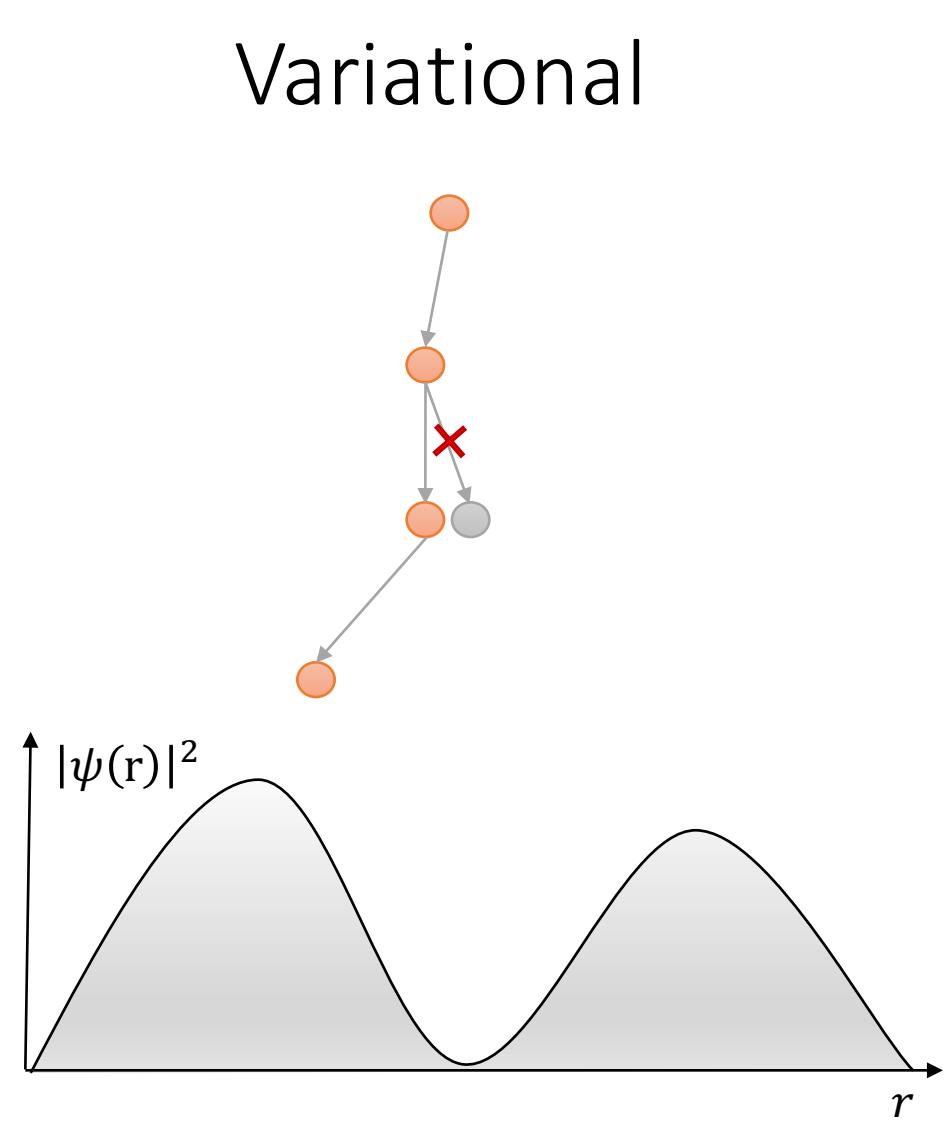
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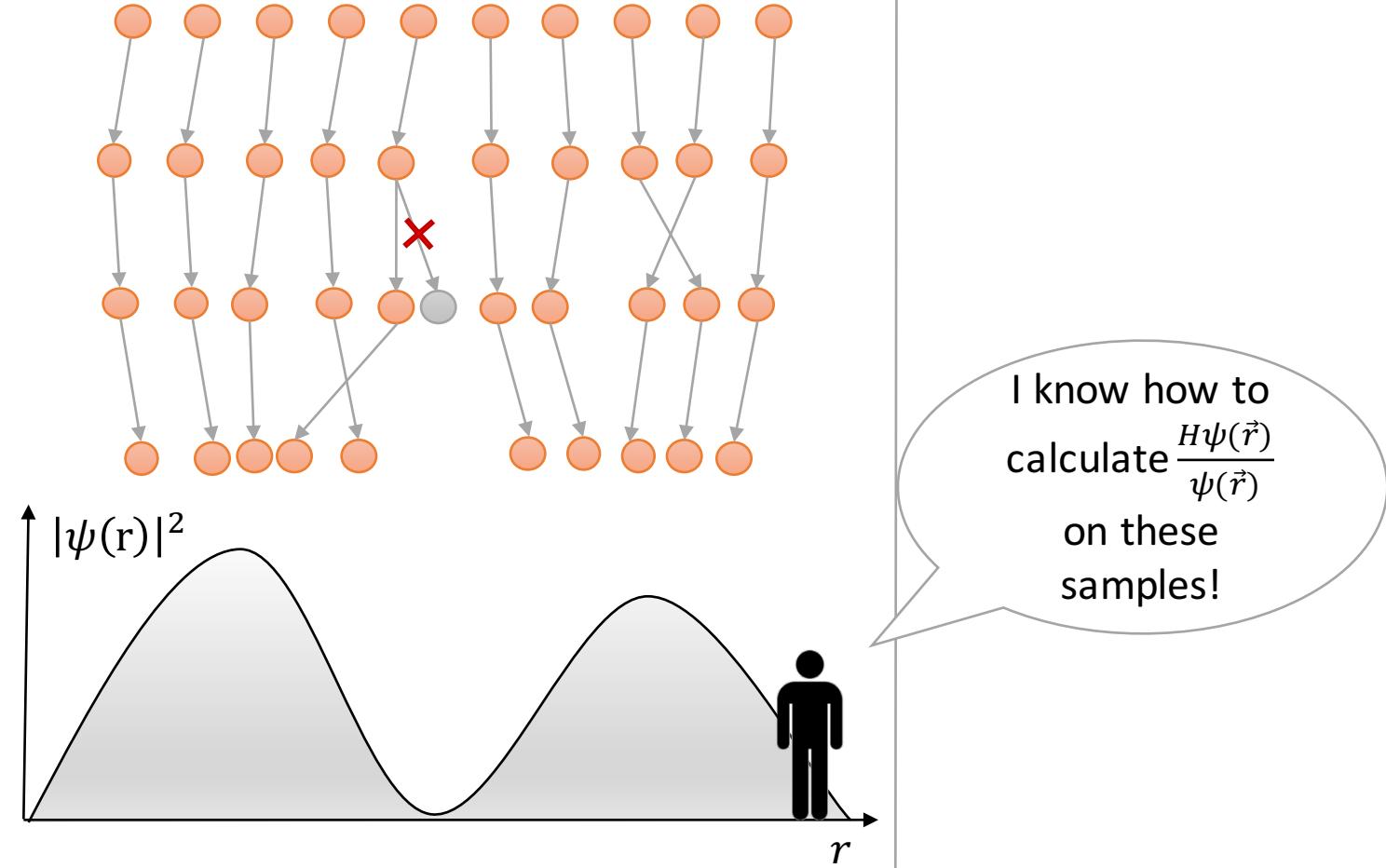
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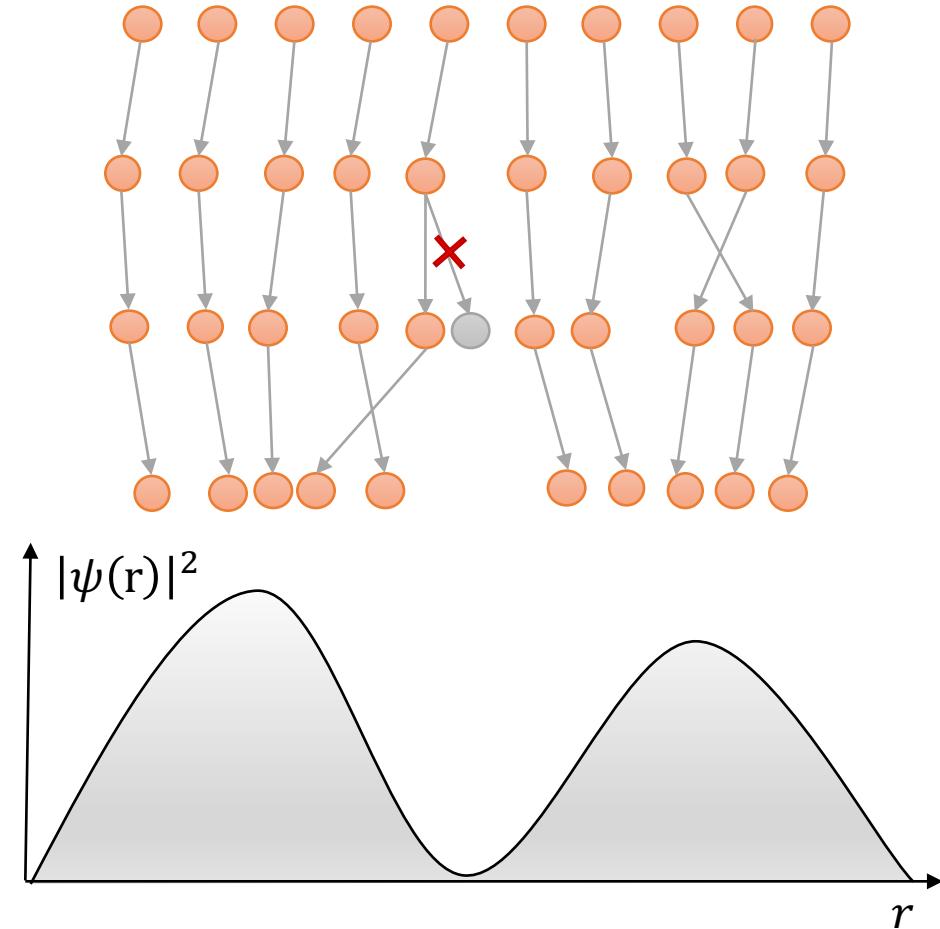
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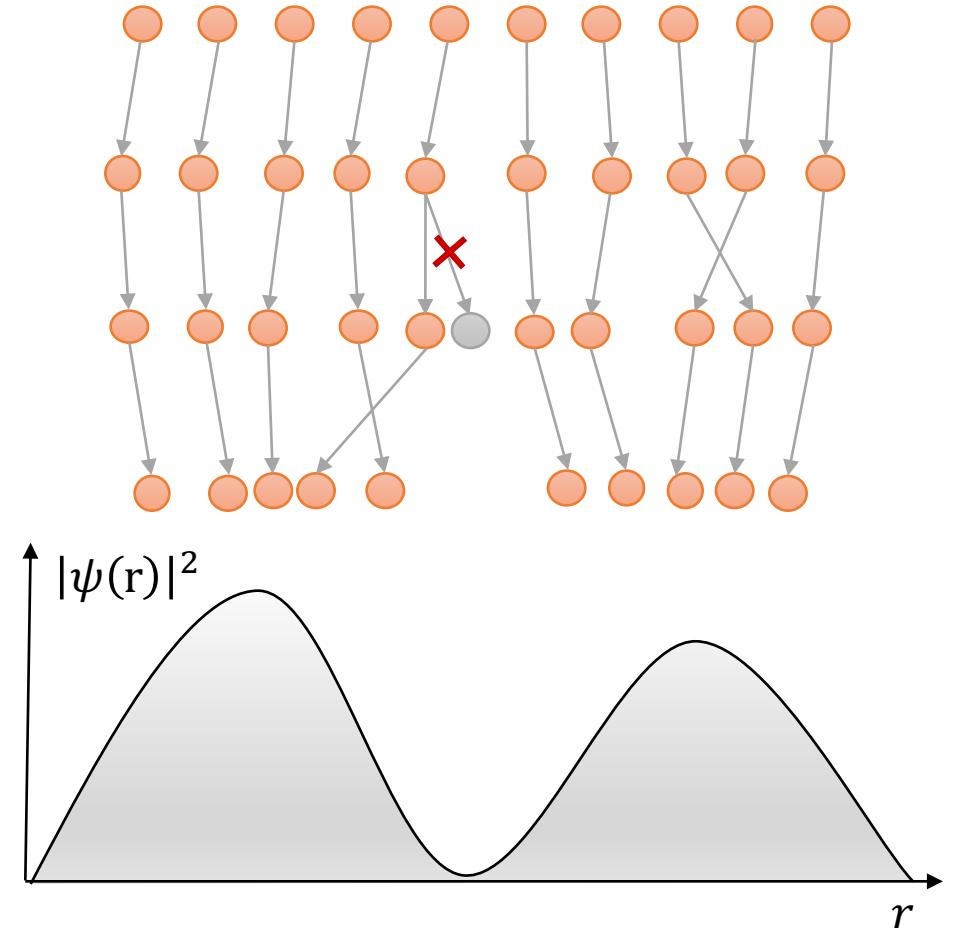
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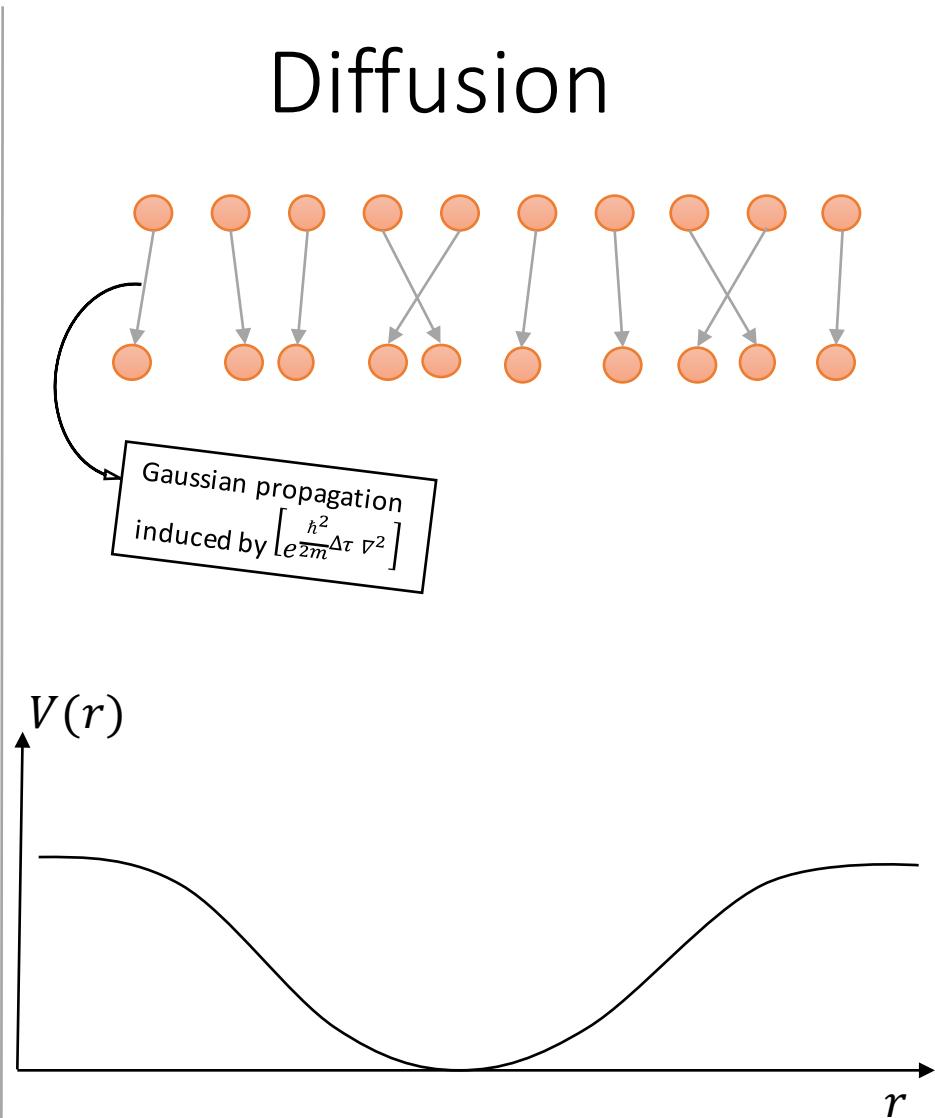
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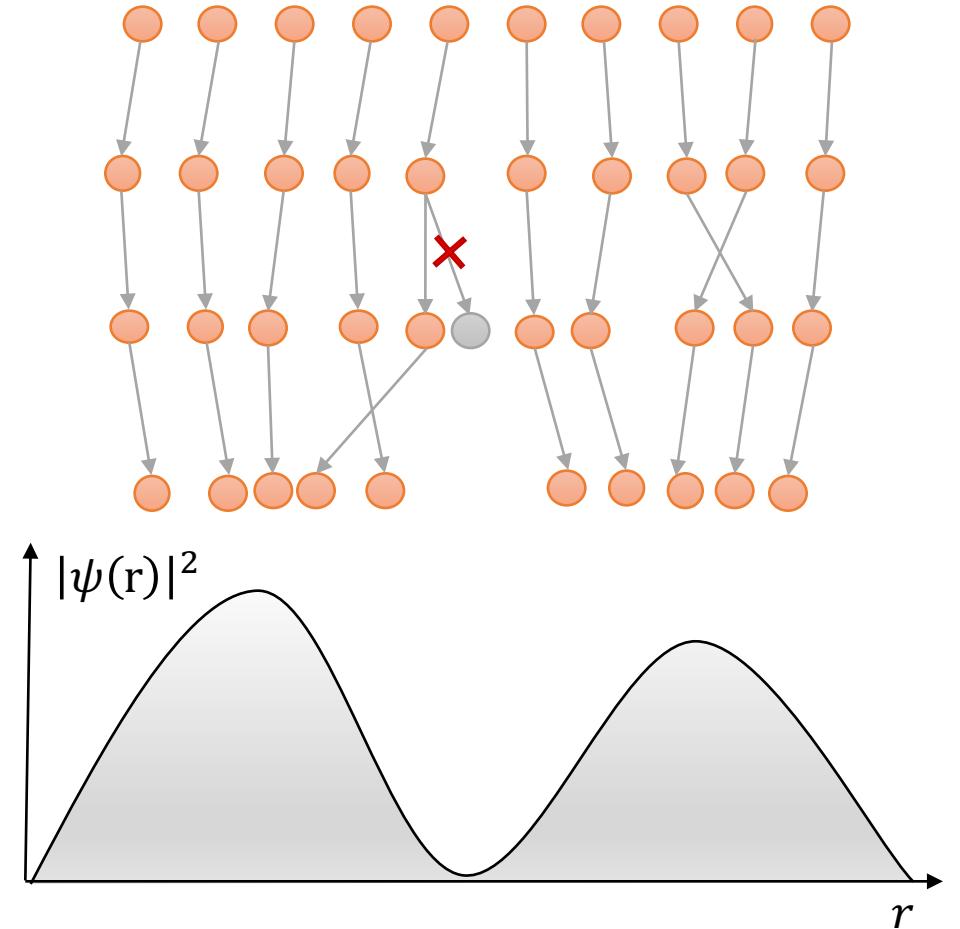
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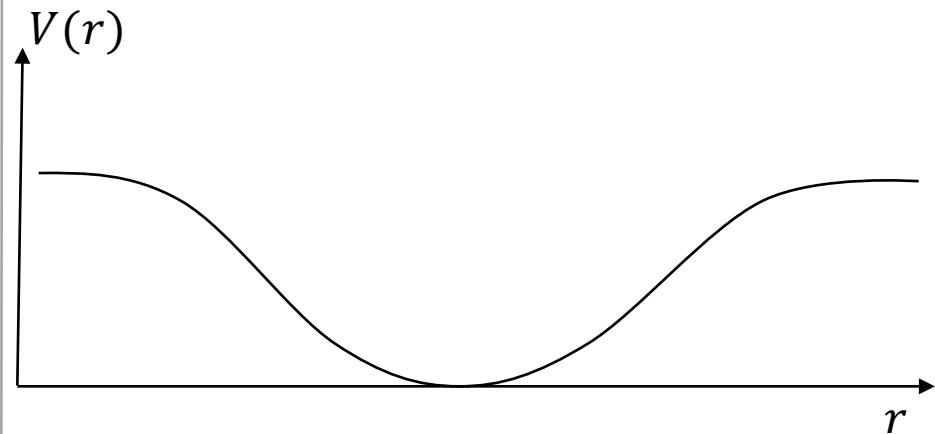
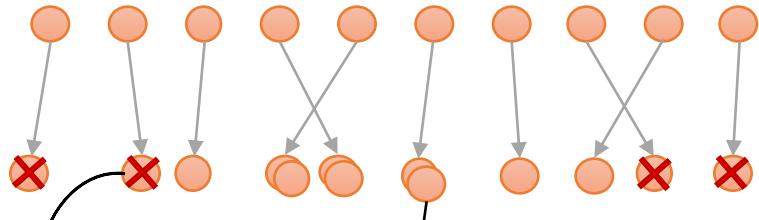
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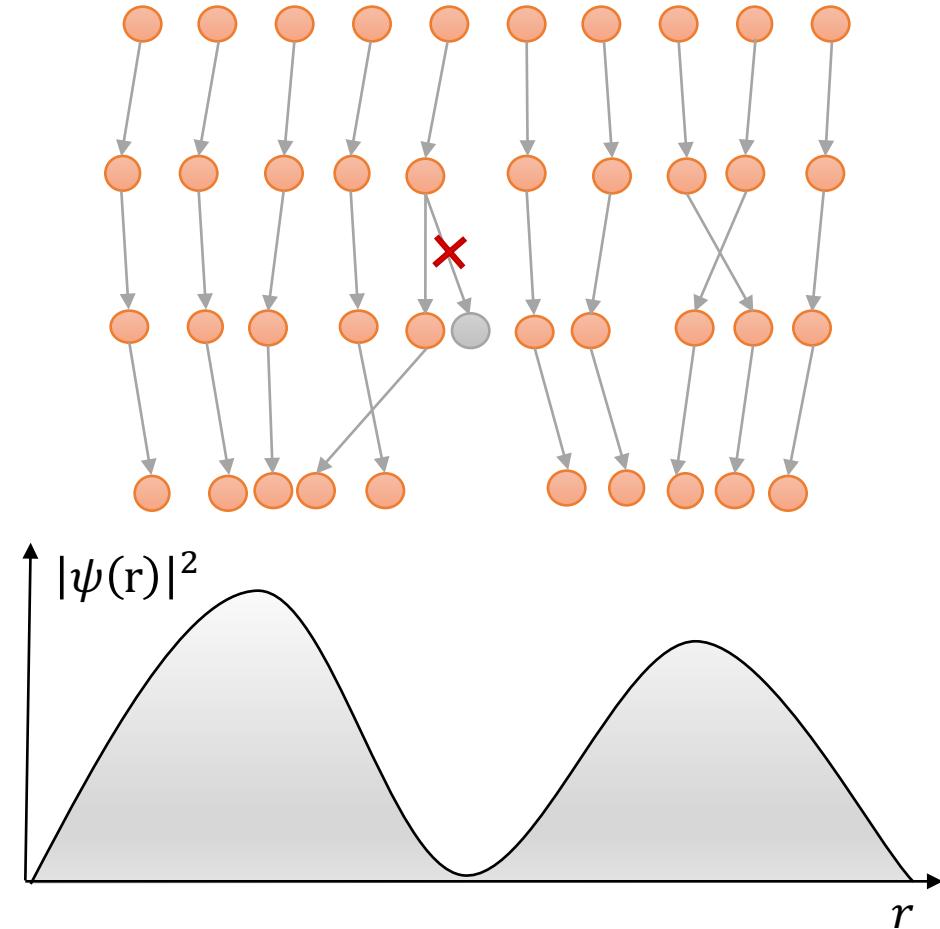
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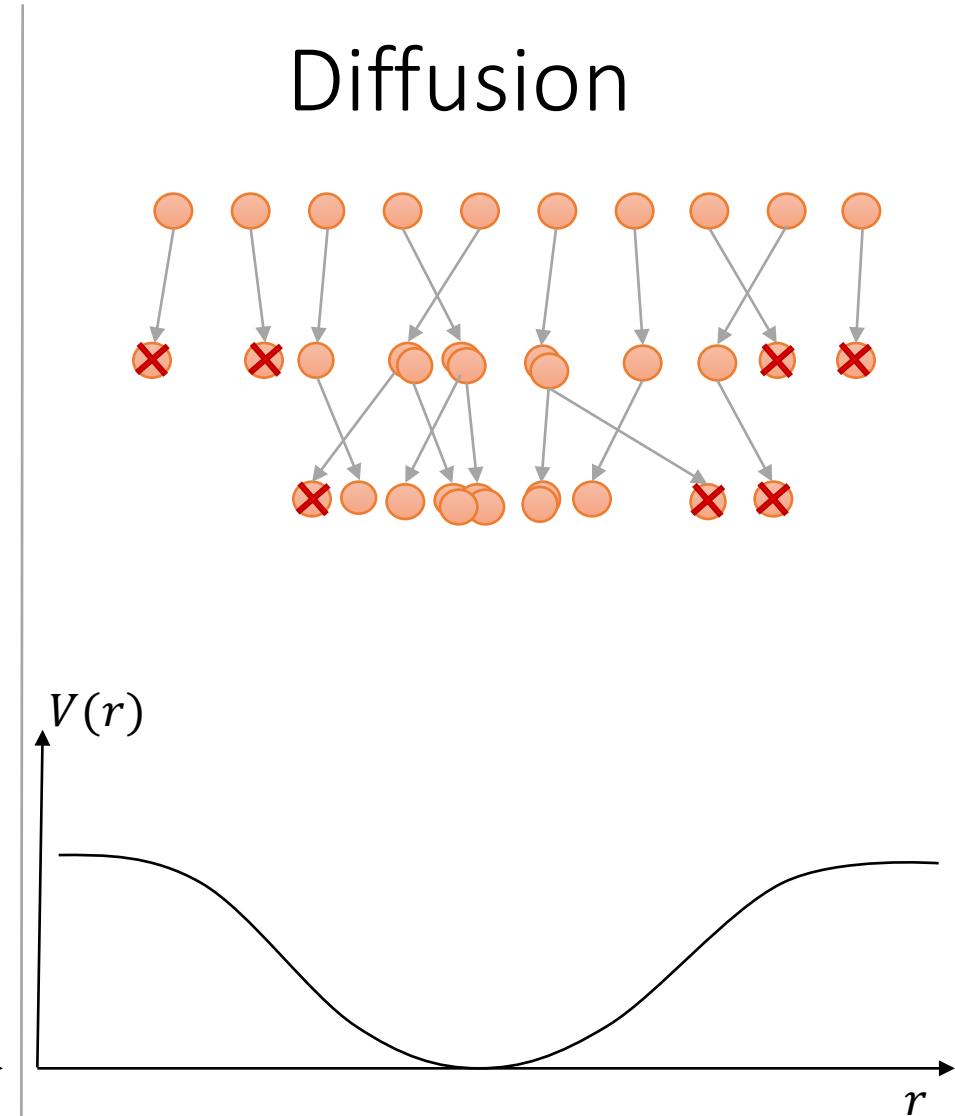
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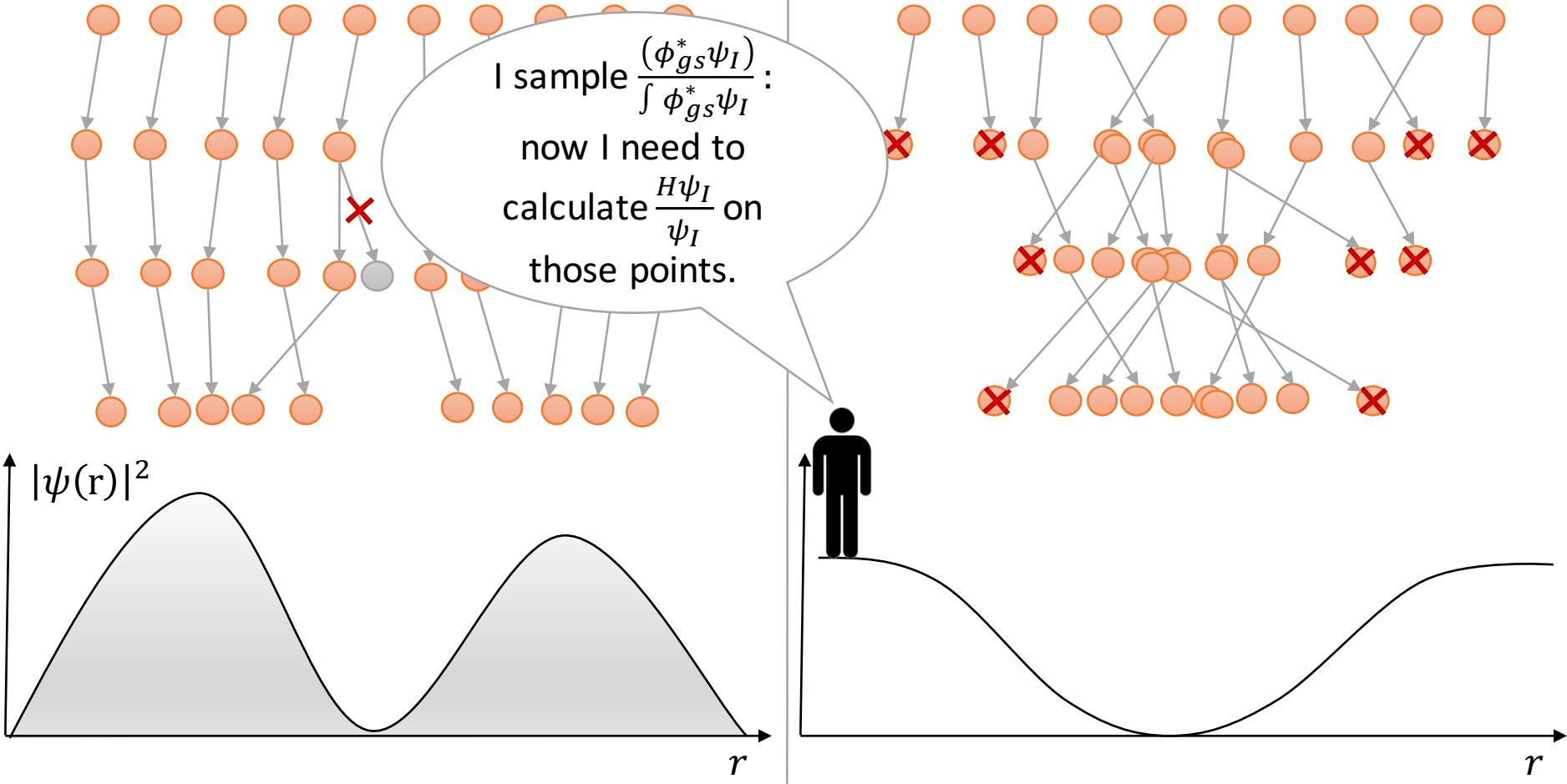
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Monte Carlo Method



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 .)

Monte Carlo Method

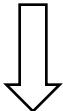


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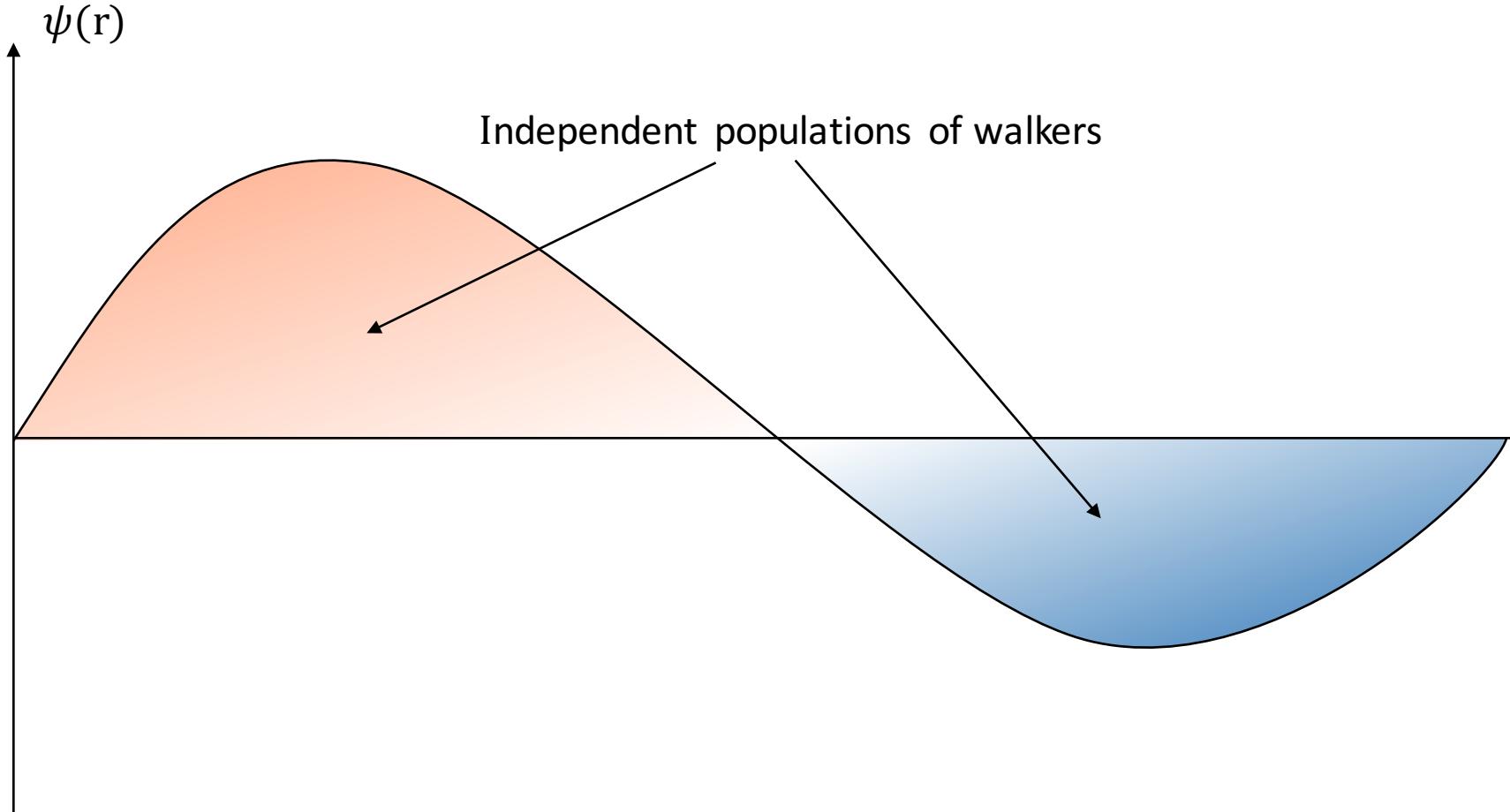
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Monte Carlo Method



Fix node:



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.)

+

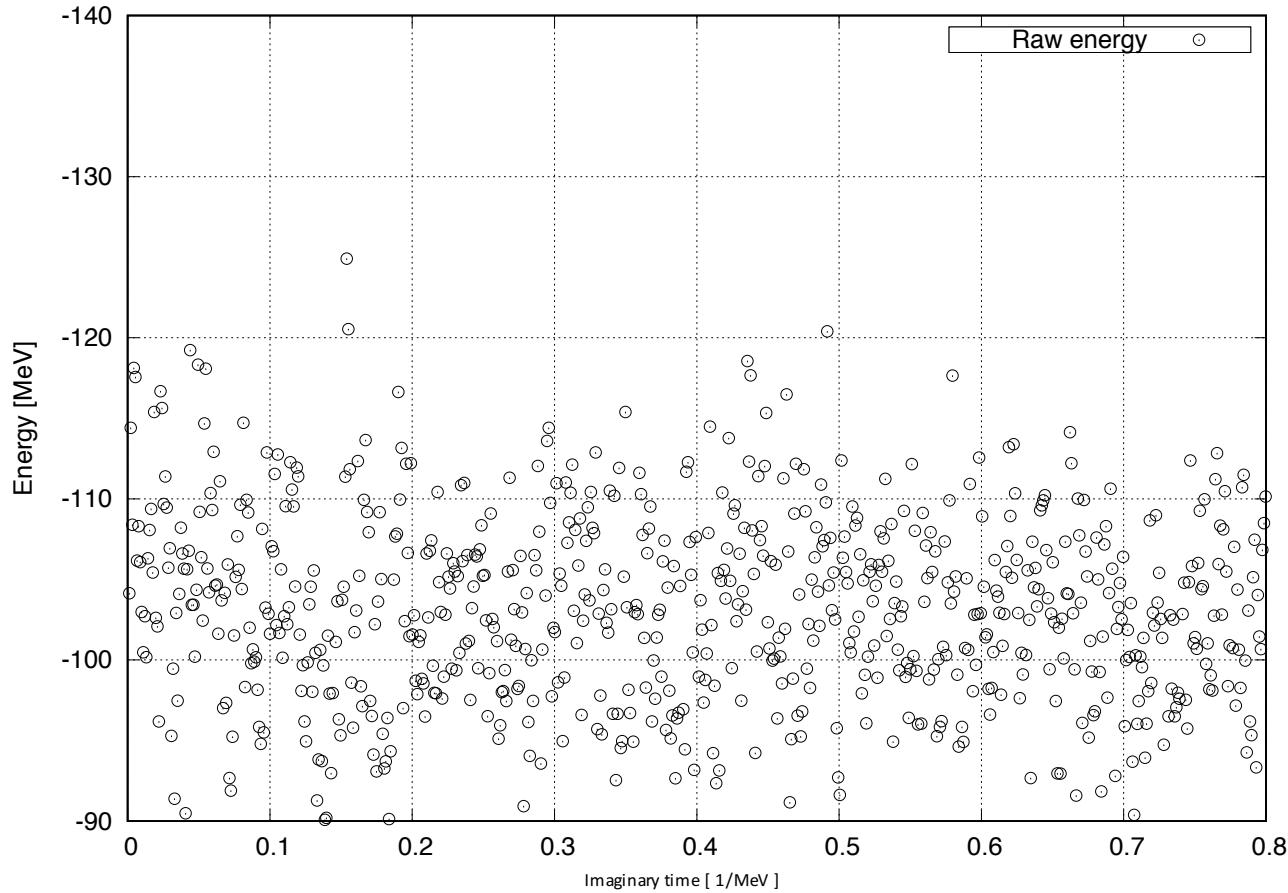
Correlations between particles are introduced (they are called Jastrow functions).

- **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



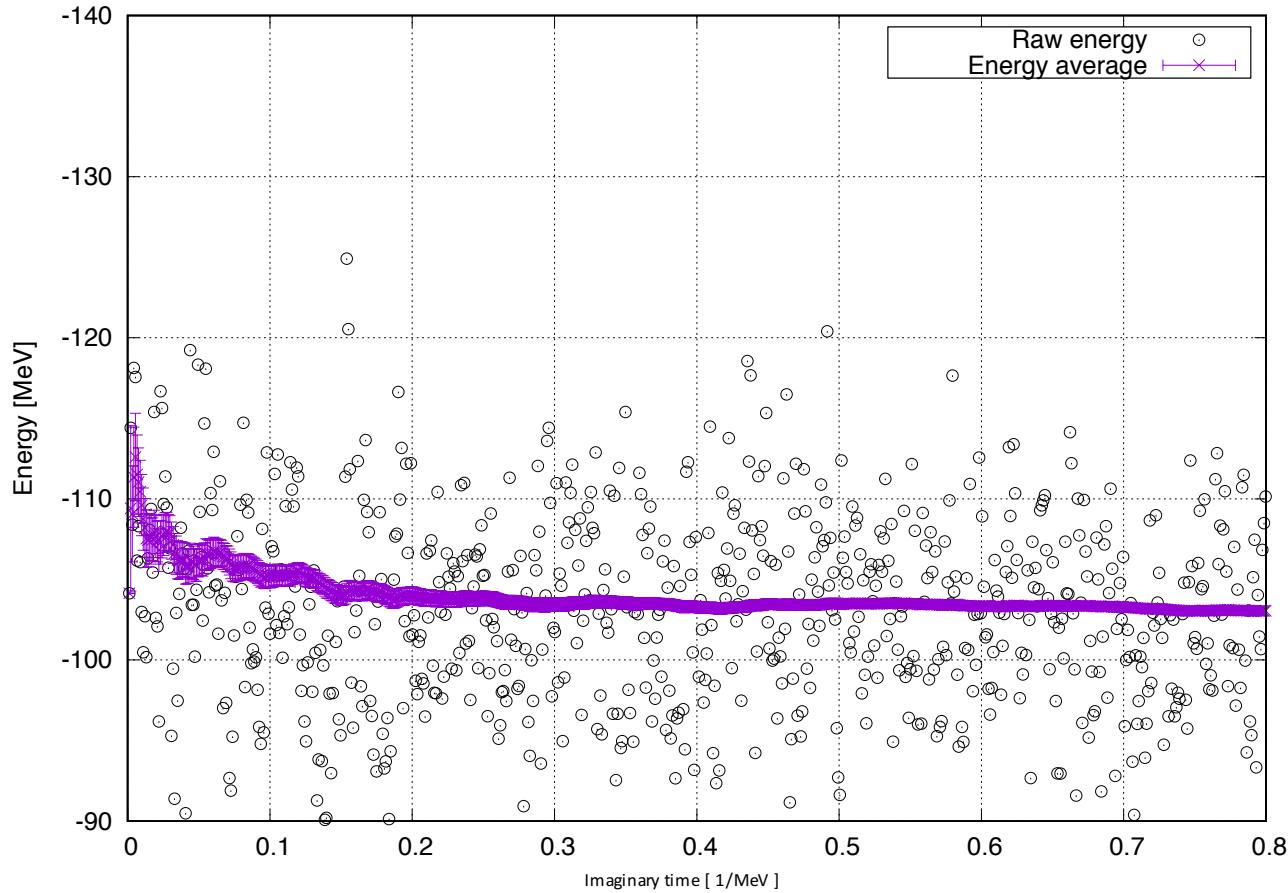
${}^4He \mid M_\pi = 800 \text{ MeV} \mid \Lambda = 10 \text{ fm}^{-1}$



Monte Carlo Method



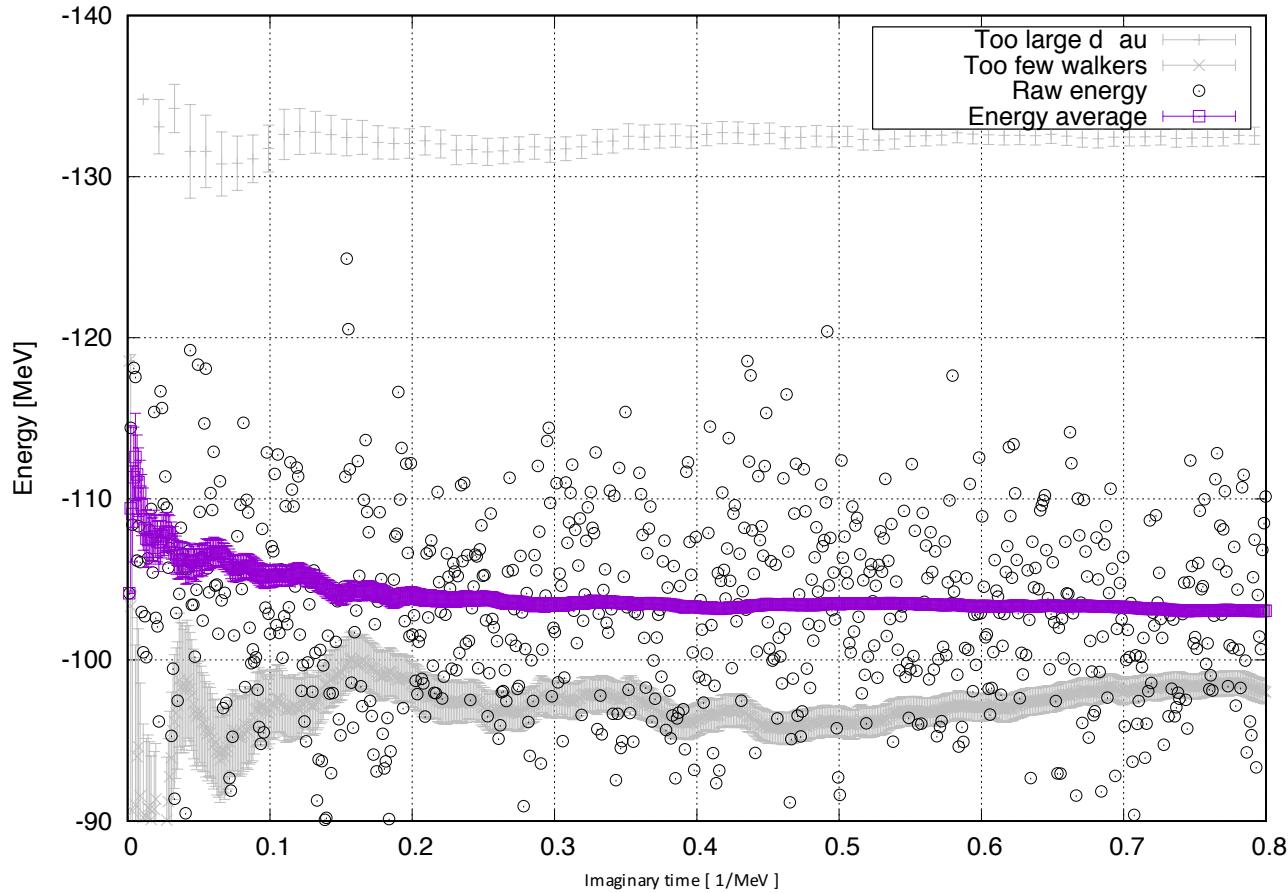
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Monte Carlo Method



Spin/Isospin:

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

For 3 particles:

$$(\vec{\sigma}_2 \cdot \vec{\sigma}_3) \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ 2a_{\uparrow\downarrow\uparrow} - a_{\uparrow\uparrow\downarrow} \\ 2a_{\uparrow\uparrow\downarrow} - a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ 2a_{\downarrow\downarrow\uparrow} - a_{\downarrow\uparrow\downarrow} \\ 2a_{\downarrow\downarrow\downarrow} - a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} \neq \begin{pmatrix} a'_{\uparrow\uparrow\uparrow} \\ a'_{\uparrow\uparrow\downarrow} \\ a'_{\uparrow\downarrow\uparrow} \\ a'_{\uparrow\downarrow\downarrow} \\ a'_{\downarrow\uparrow\uparrow} \\ a'_{\downarrow\uparrow\downarrow} \\ a'_{\downarrow\downarrow\uparrow} \\ a'_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

n-body spinor \rightarrow 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).

$$\vec{\sigma}_i \left(\begin{pmatrix} \alpha_1 \hat{p}_\uparrow \\ \beta_1 \hat{p}_\downarrow \\ \gamma_1 \hat{n}_\uparrow \\ \delta_1 \hat{n}_\downarrow \end{pmatrix}_1 \otimes \dots \otimes \begin{pmatrix} \alpha_i \hat{p}_\uparrow \\ \beta_i \hat{p}_\downarrow \\ \gamma_i \hat{n}_\uparrow \\ \delta_i \hat{n}_\downarrow \end{pmatrix}_i \otimes \dots \otimes \begin{pmatrix} \alpha_A \hat{p}_\uparrow \\ \beta_A \hat{p}_\downarrow \\ \gamma_A \hat{n}_\uparrow \\ \delta_A \hat{n}_\downarrow \end{pmatrix}_A \right) = \left(\begin{pmatrix} \alpha_1 \hat{p}_\uparrow \\ \beta_1' \hat{p}_\downarrow \\ \gamma_1' \hat{n}_\uparrow \\ \delta_1' \hat{n}_\downarrow \end{pmatrix}_1 \otimes \dots \otimes \begin{pmatrix} \alpha_i' \hat{p}_\uparrow \\ \beta_i' \hat{p}_\downarrow \\ \gamma_i' \hat{n}_\uparrow \\ \delta_i' \hat{n}_\downarrow \end{pmatrix}_i \otimes \dots \otimes \begin{pmatrix} \alpha_A \hat{p}_\uparrow \\ \beta_A \hat{p}_\downarrow \\ \gamma_A \hat{n}_\uparrow \\ \delta_A \hat{n}_\downarrow \end{pmatrix}_A \right)$$

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.

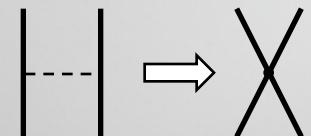
Monte Carlo Method



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.

$$\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

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

$$C \cdot \delta(\vec{r}_i - \vec{r}_j) \Rightarrow C \frac{\Lambda^3}{8\pi^{3/2}} e^{\frac{-\Lambda^2 r_{ij}^2}{4}}$$

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** → 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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- **The range of validity** of the theory is usually unknown and can depend from the system.

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.



About the cut-off

Every day
in the office

> If you
course

Example

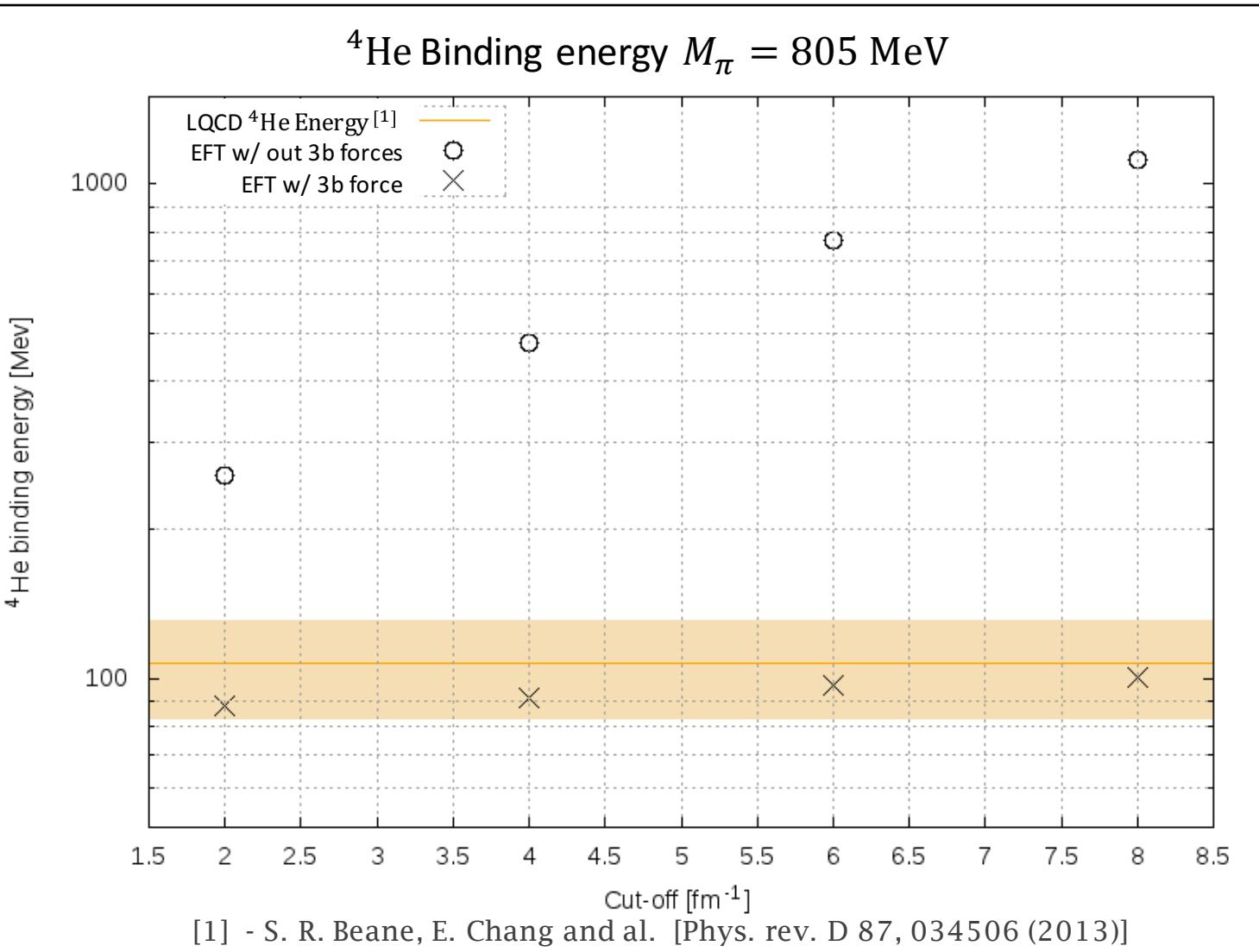
Using only
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You can use residual cut-off dependences to check the theory.

Contact EFT

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



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

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

After regularization in the coordinate space:

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

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LO		NLO
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+		
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	Avoid Thomas collapse	

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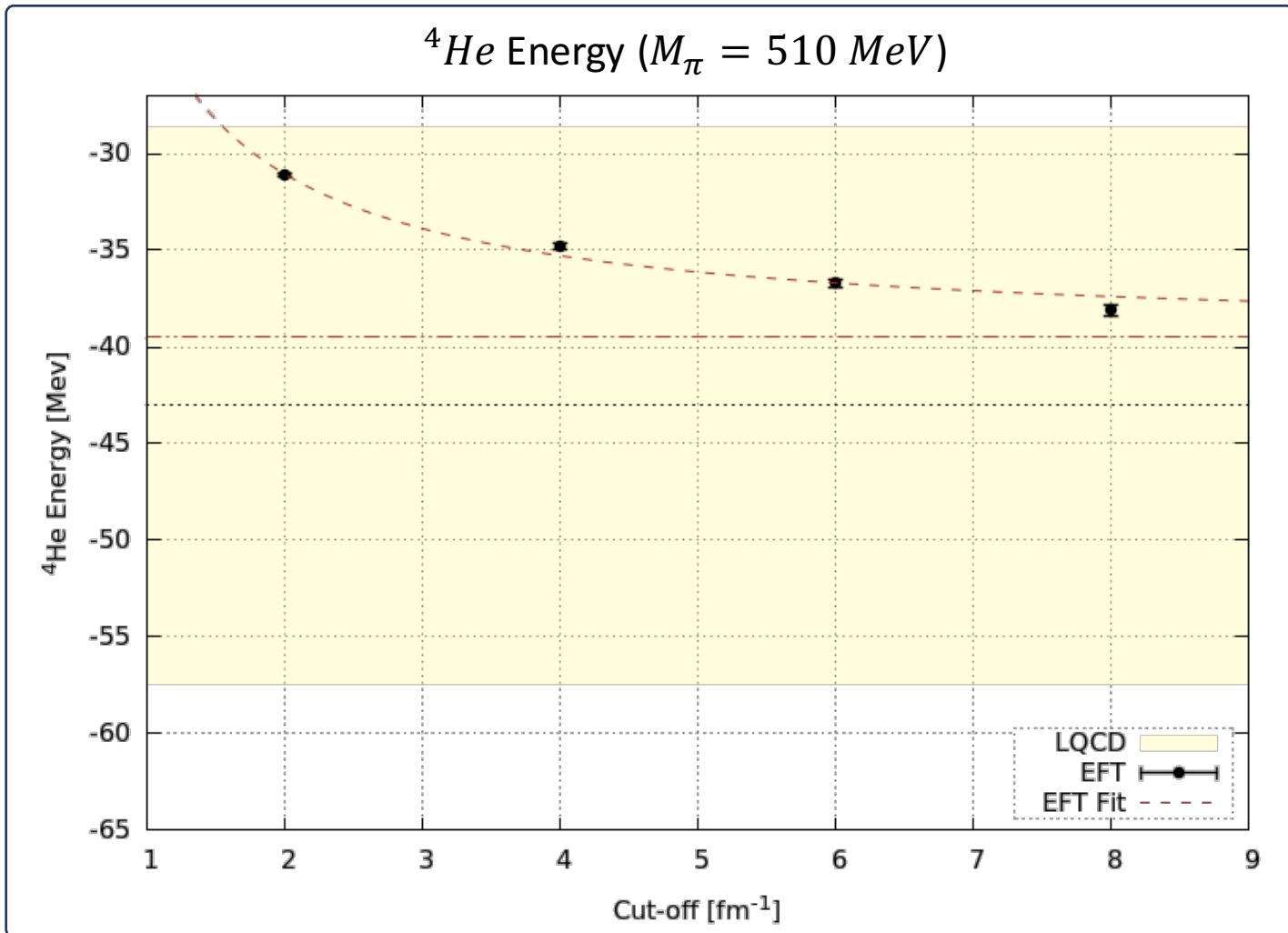
LO		NLO
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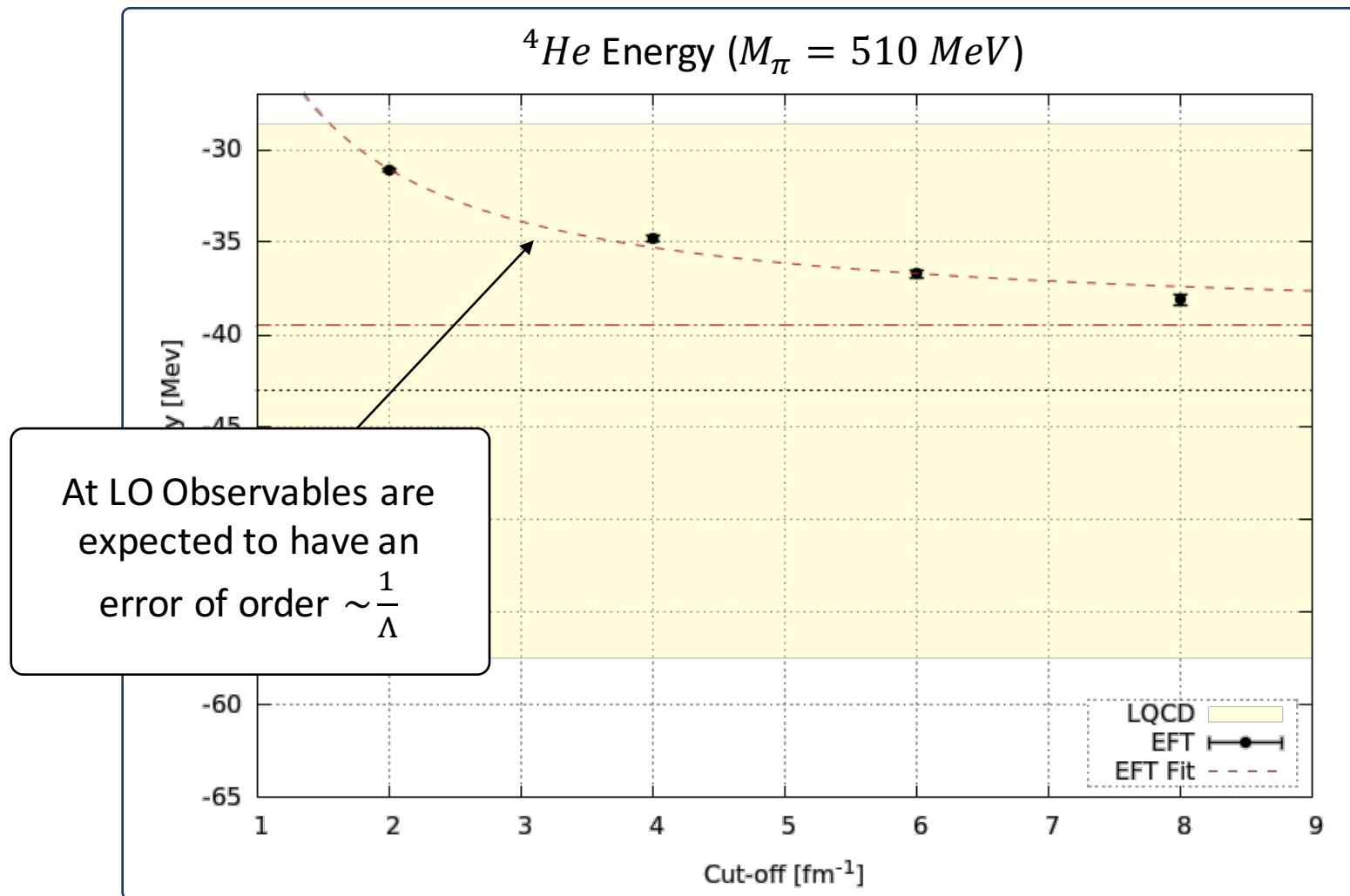
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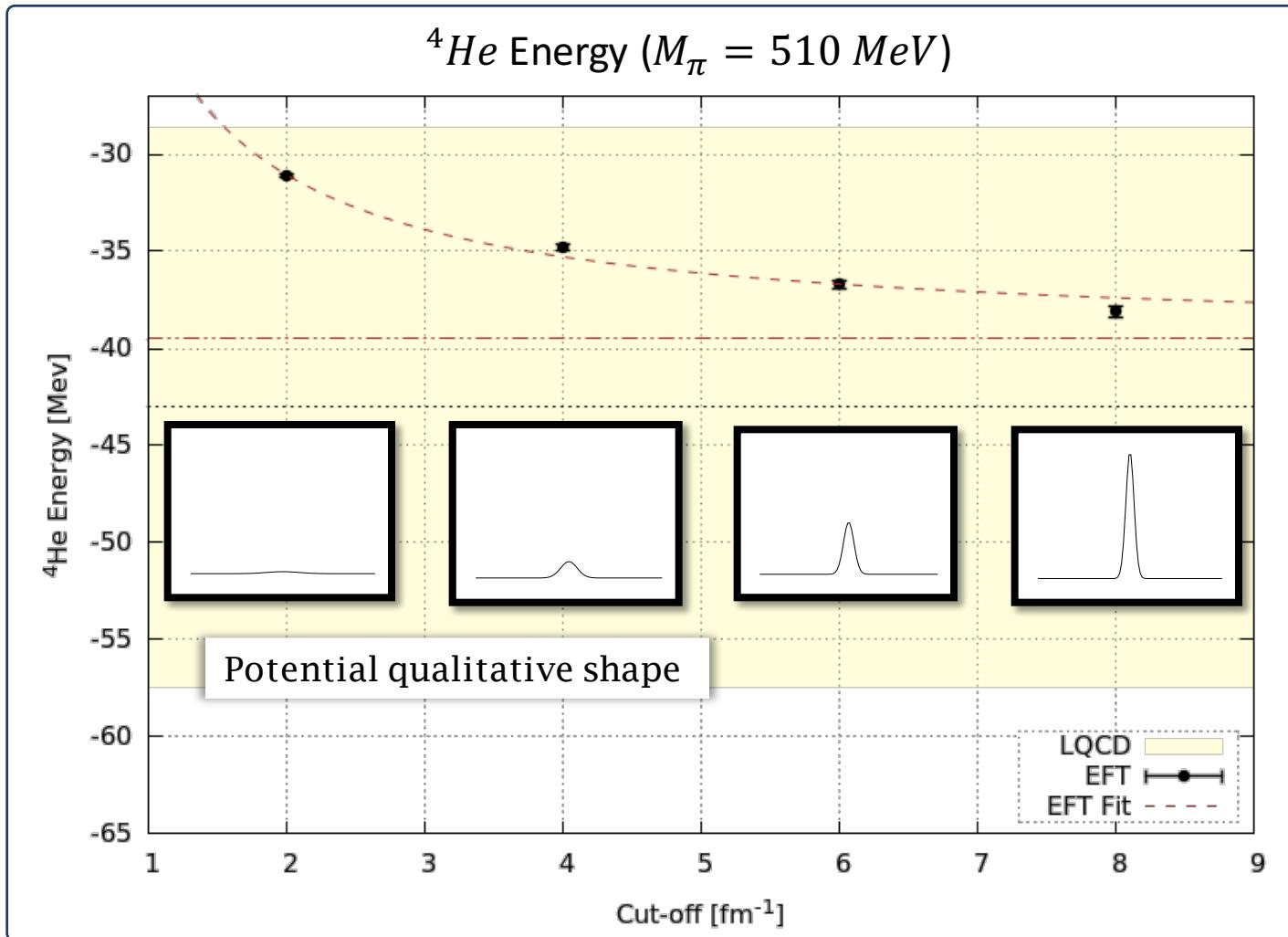
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Contact EFT





LQCD few-body data

Nucleus	Nature	$m_\pi = 510 \text{ MeV}$ [1]	$m_\pi = 805 \text{ MeV}$ [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)

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[2] - S. R. Beane, E. Chang and al.

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2b LECs
3b LEC
Benchmark

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 α

$m_\pi = 140 \text{ MeV}$		$m_\pi = 510 \text{ MeV}$		$m_\pi = 805 \text{ MeV}$	
Λ [fm $^{-1}$]	^4He Energy [MeV]	Λ [fm $^{-1}$]	^4He Energy [MeV]	Λ [fm $^{-1}$]	^4He Energy [MeV]
2	-23.3(1)	2	-31.1(1)	2	-87.9(2)
4	-23.4(2)	4	-34.8(2)	4	-91.3(3)
6	-24.8(3)	6	-36.7(2)	6	-96.4(4)
8	-26.0(3)	8	-38.1(3)	8	-101.3(5)
∞	-28.3(5)	∞	-38.8(1.0)	∞	-114(15)
Exp	-28.296	LQCD	-43(14)	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 $\Lambda = 2 \text{ fm}^{-1}$.
- 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 $B(^3\text{H})$

^{16}O

$m_\pi = 140 \text{ MeV}$			$m_\pi = 510 \text{ MeV}$			$m_\pi = 805 \text{ MeV}$		
Λ [fm $^{-1}$]	^{16}O Energy [MeV]	4α threshold [MeV]	Λ [fm $^{-1}$]	^{16}O Energy [MeV]	4α threshold [MeV]	Λ [fm $^{-1}$]	^{16}O Energy [MeV]	4α threshold [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.

- **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.

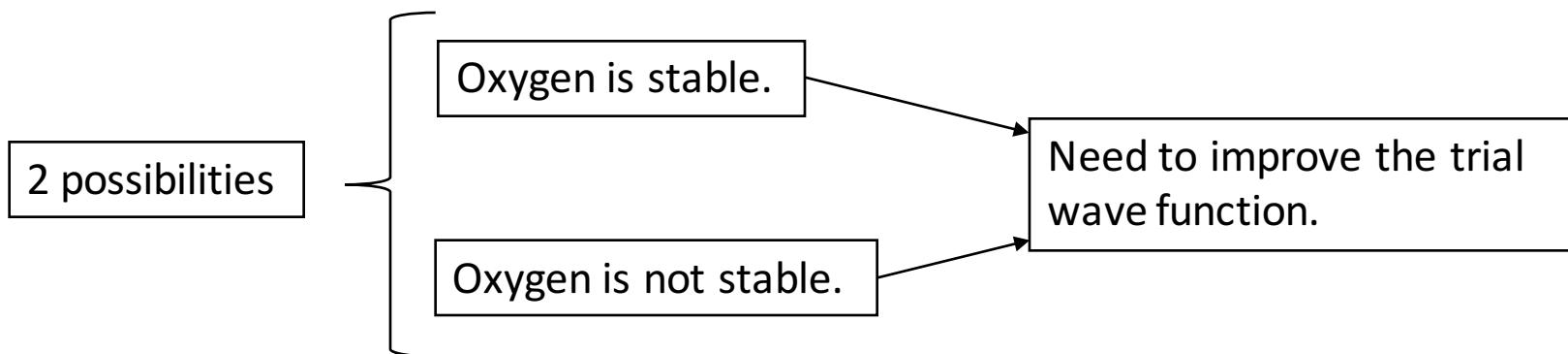
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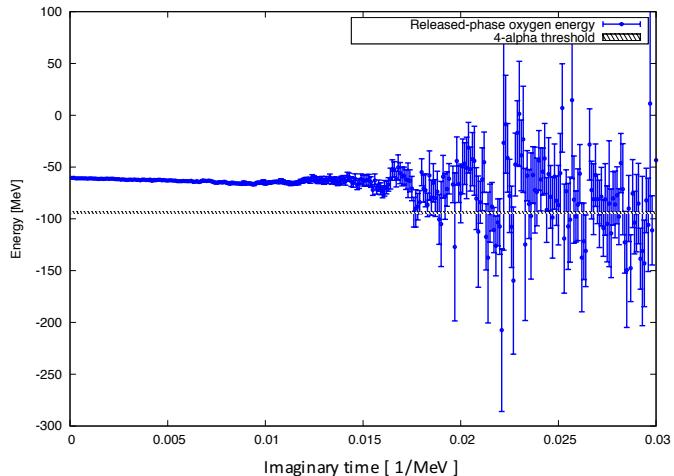
Release nodes

M_π

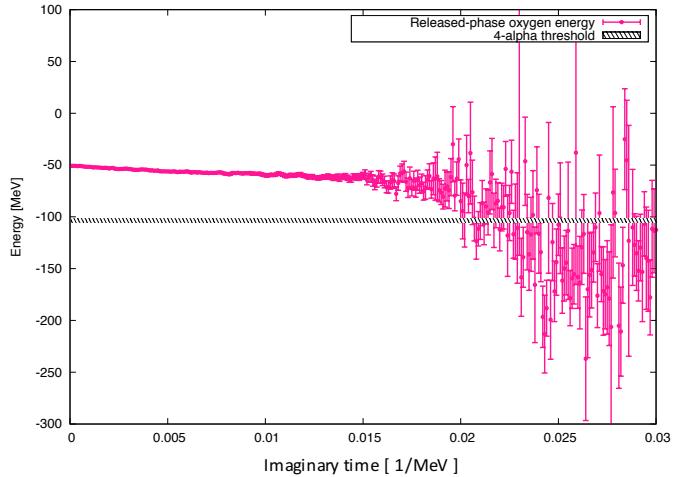
140 MeV

Cut-off

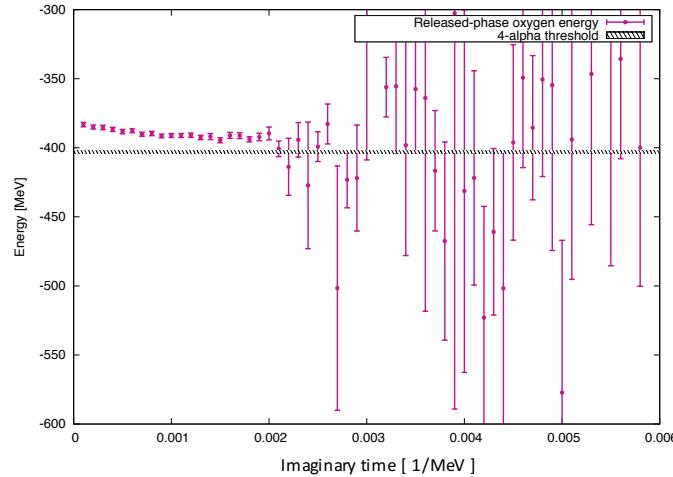
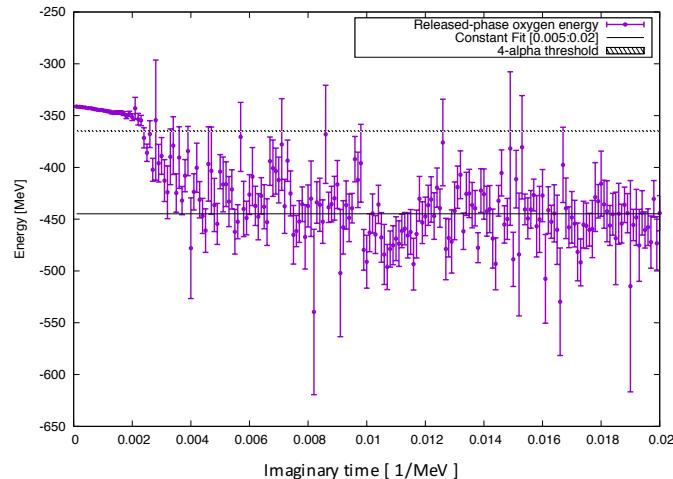
4 fm^{-1}



8 fm^{-1}



800 MeV



Conclusions:

- ^4He 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 $m_\pi = 140 \text{ MeV}$.
- **Evidence for a bound state** for $m_\pi = 805 \text{ MeV}$ and $\Lambda = 4 \text{ fm}^{-1}$

What's next:

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

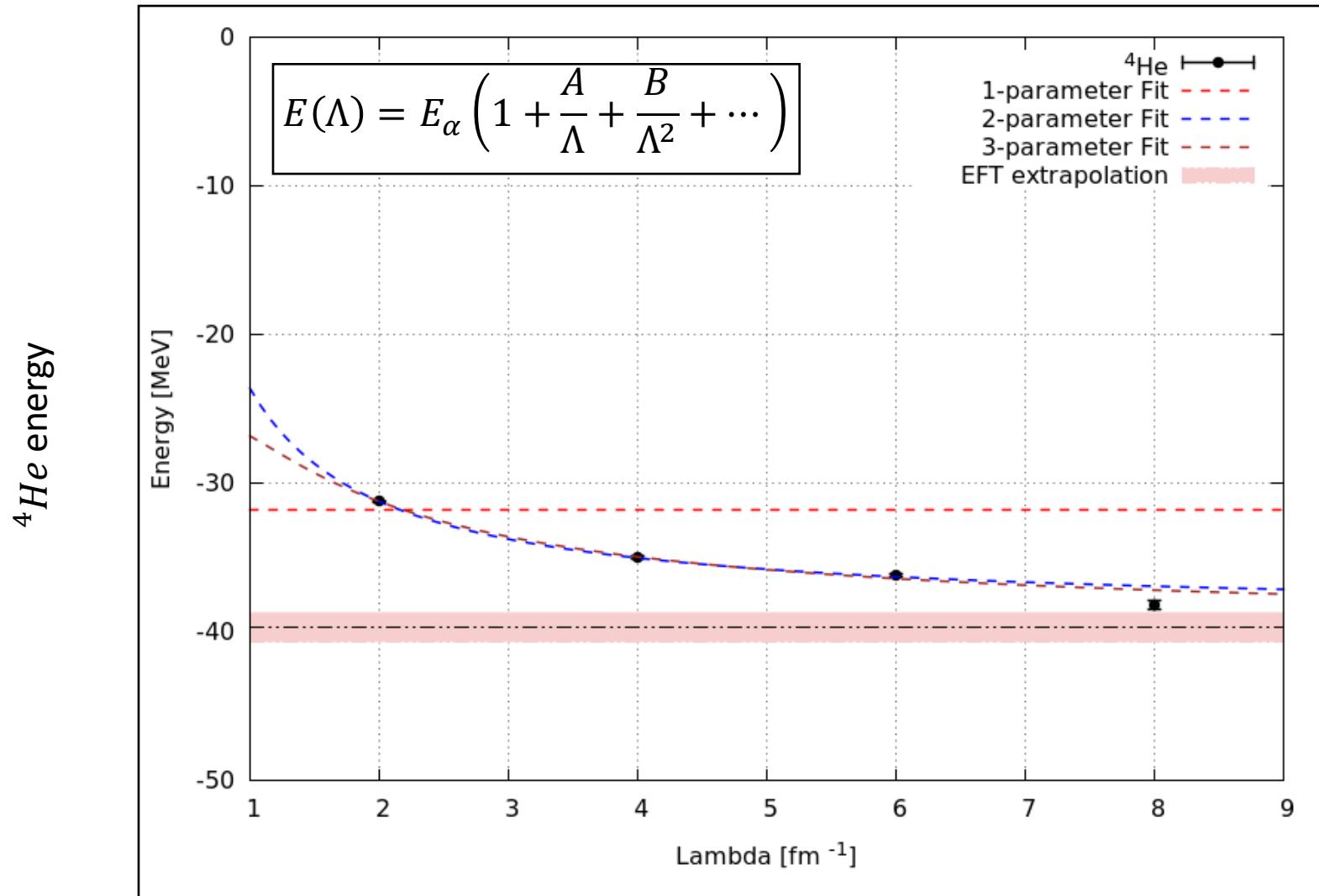
Other interesting things:

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

Thanks for your attention

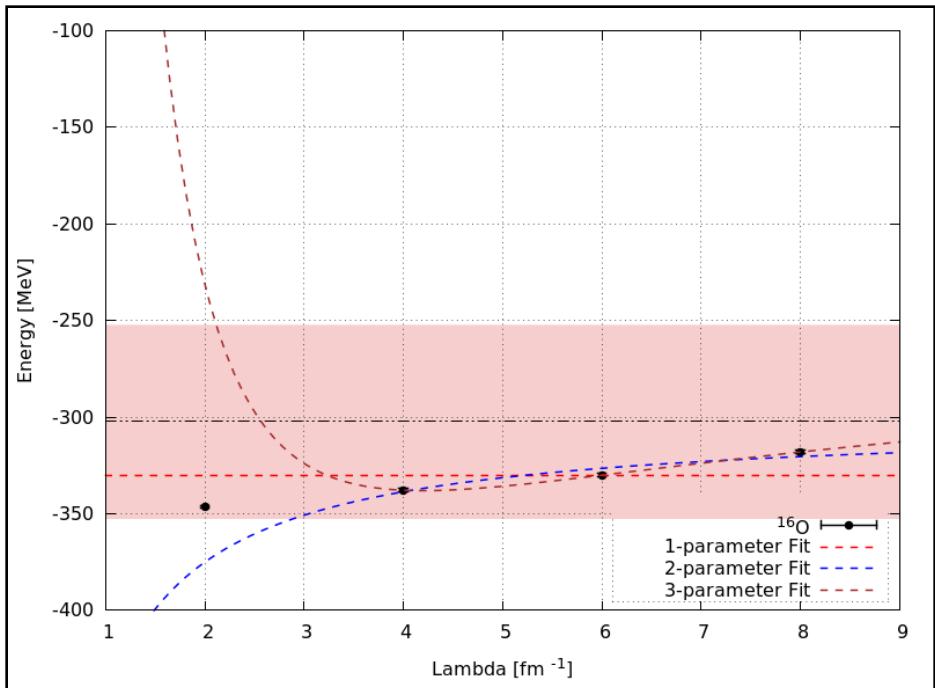
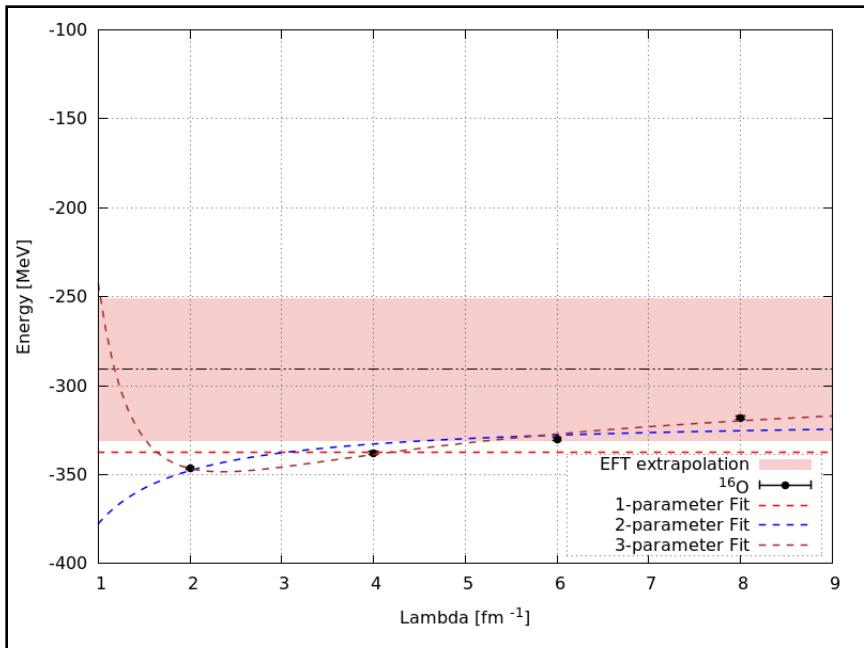


Convergences of data $m_\pi = 500 \text{ MeV}$



Convergences of data $m_\pi = 800 \text{ MeV}$

^{16}O energy



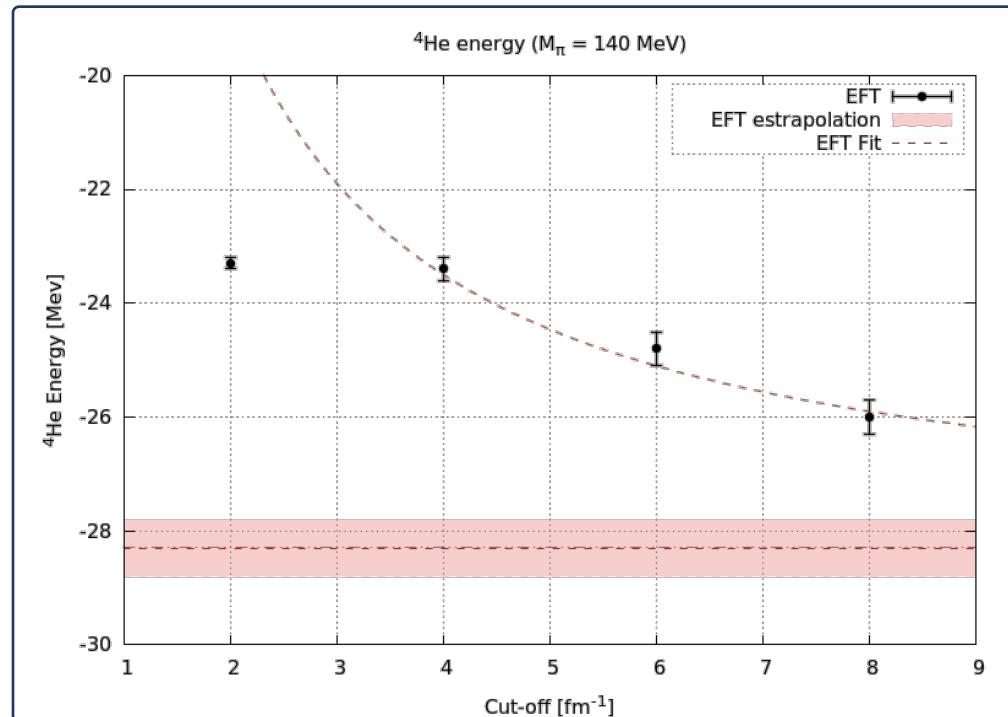
Excluding $\Lambda = 2 \text{ fm}^{-1}$ from fit.

Convergences of data at physical m_π

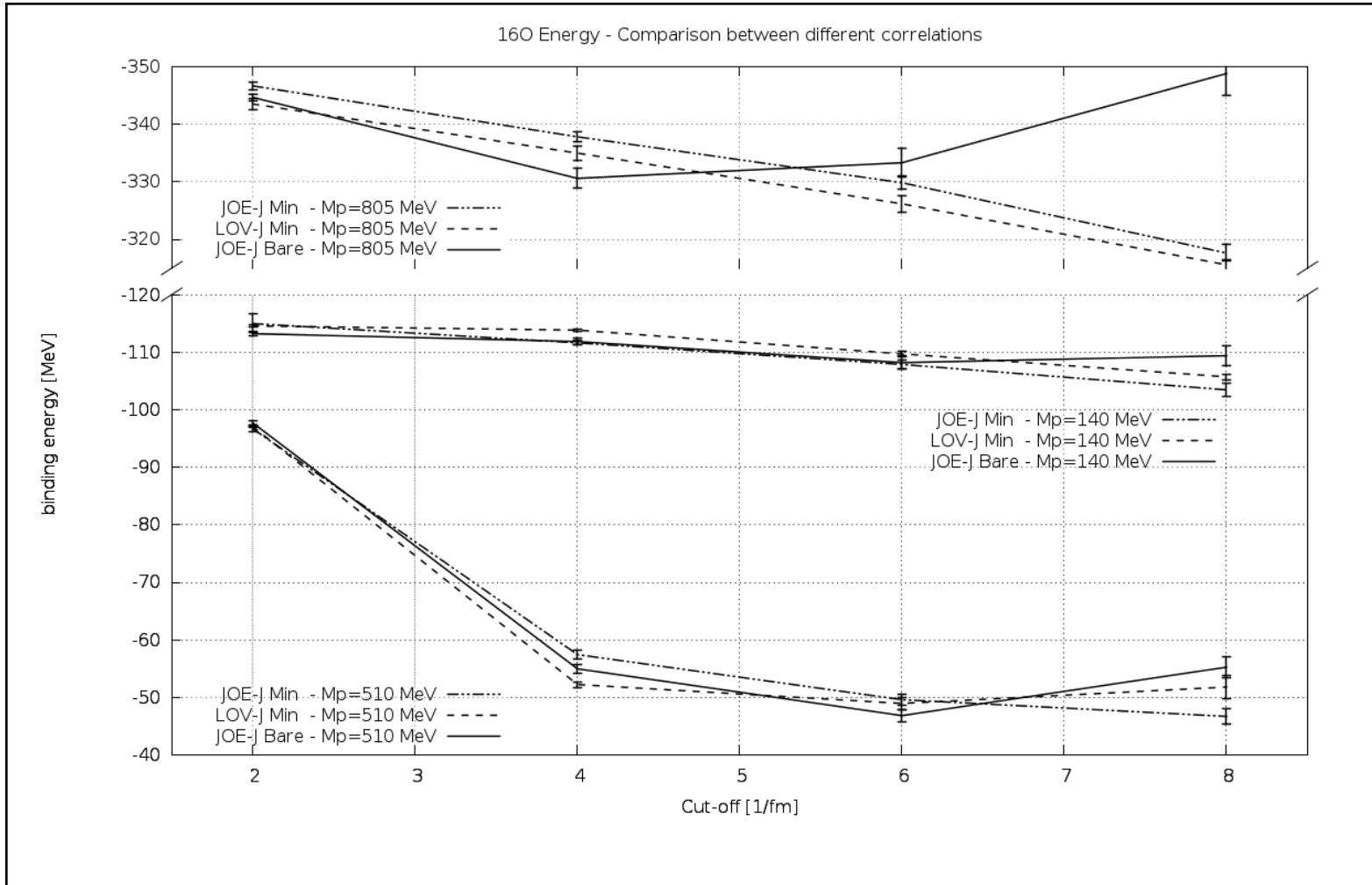
$$V_{Lo} = \sum_{ij} [C_0 + C_1(\sigma_1 \cdot \sigma_2)] \delta_{r_i, r_j} + \sum_{ijk} D_0 \delta_{r_i, r_j, r_k}$$

$n - p$
scattering lenght
and binding energy

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



Different correlations in AFDMC



^{40}Ca

$m_\pi = 510 \text{ MeV}$		
Λ [fm $^{-1}$]	$^{40}\text{Ca Energy}$ [MeV]	10α threshold [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		
	-	-