Monte Carlo methods for effective theories and lattice nuclei

Lorenzo Contessi

Alessandro Lovato

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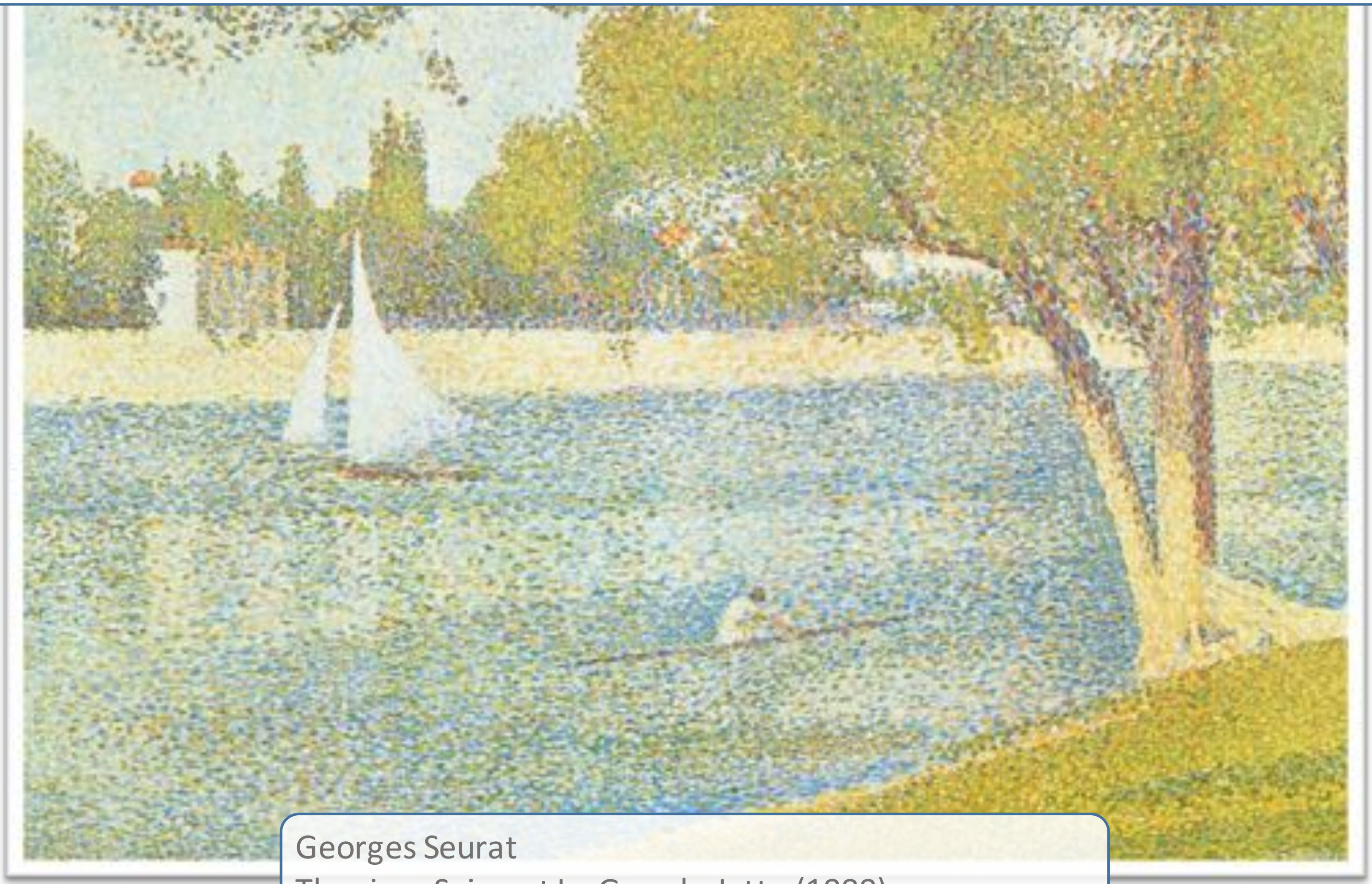
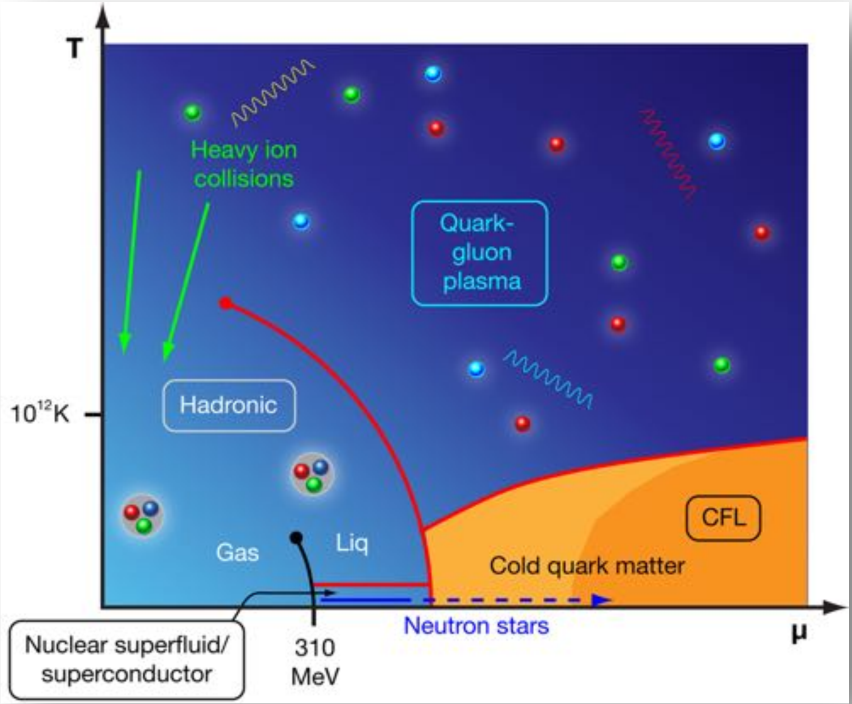
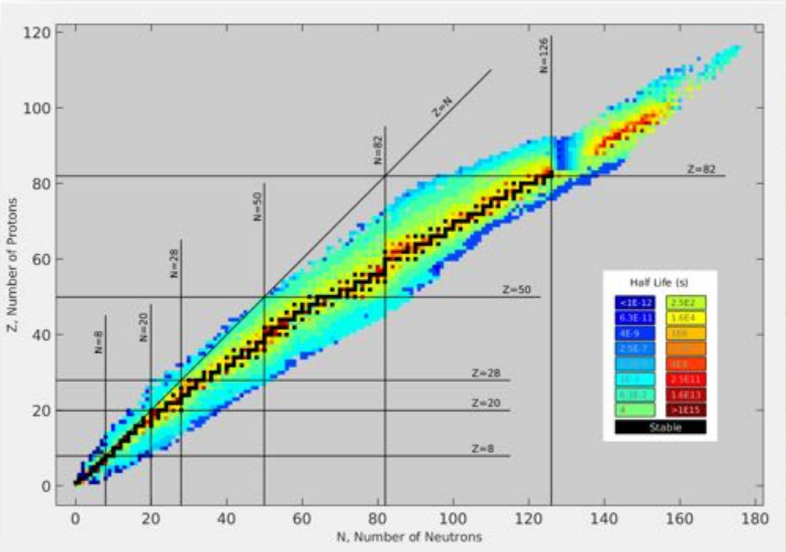
Theoretical introduction to contact EFT



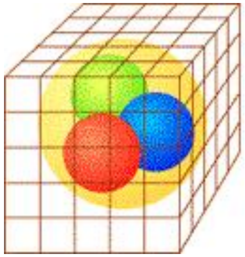
Georges Seurat
The river Seine at La Grande-Jatte (1888)

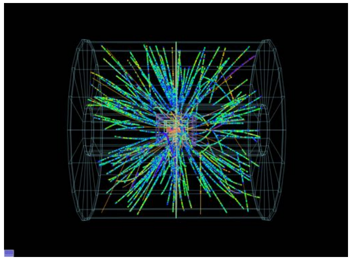
connect energy scales



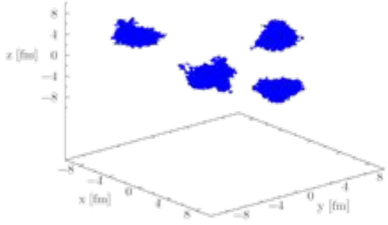


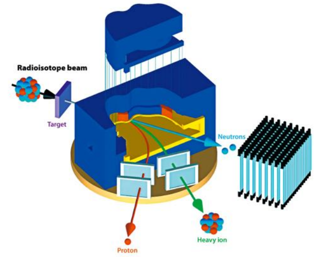
Lattice QCD and experiments





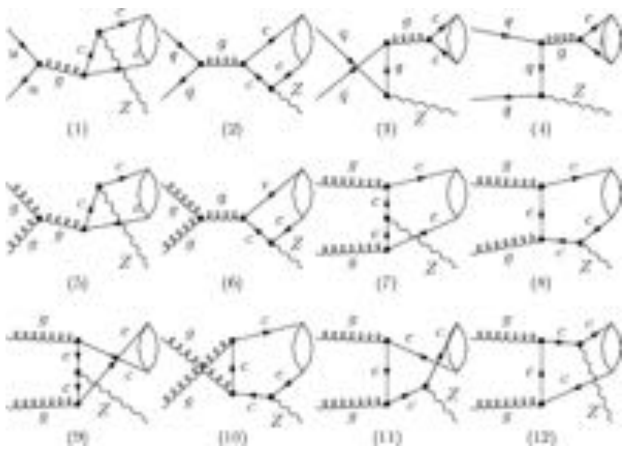
Experiments and many body methods





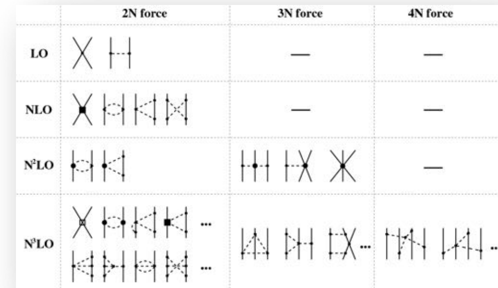
connect energy scales

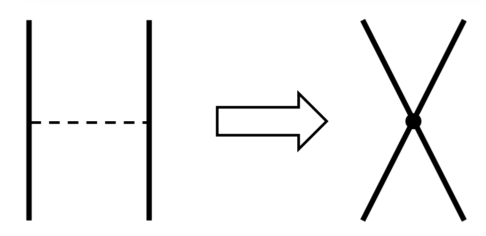
QCD



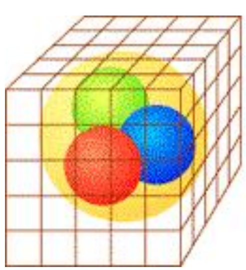
$$m_\pi = 800, 450, 140\ \text{MeV}$$

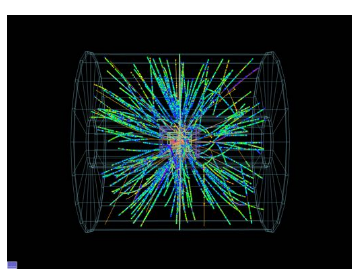
Nuclear interaction



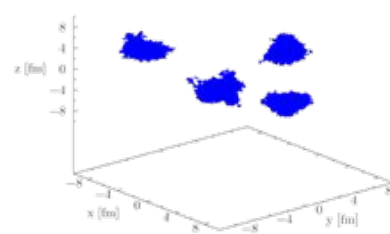


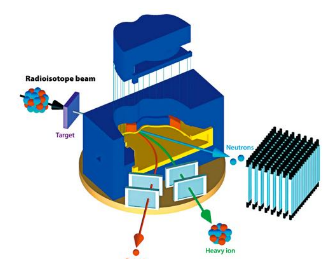
Lattice QCD and experiments





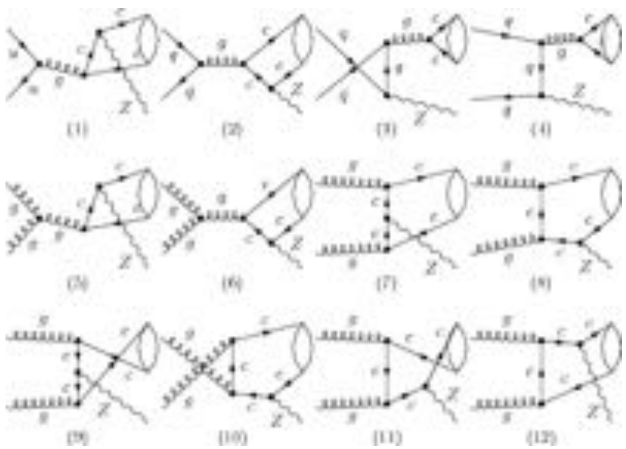
Experiments and many body methods





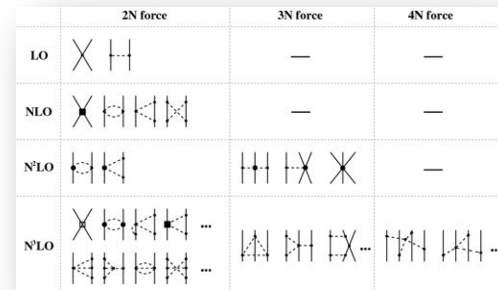
connect energy scales

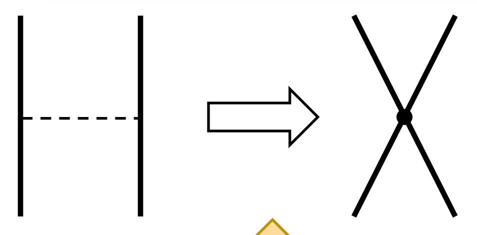
QCD



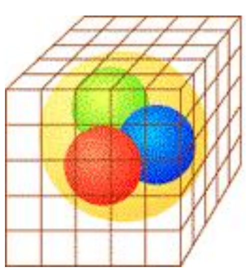
$$m_\pi = 800, 450, 140 \text{ MeV}$$

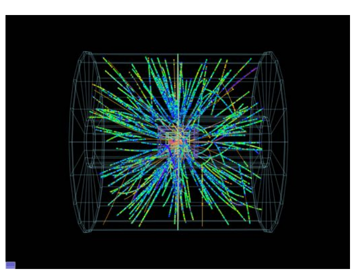
Nuclear interaction



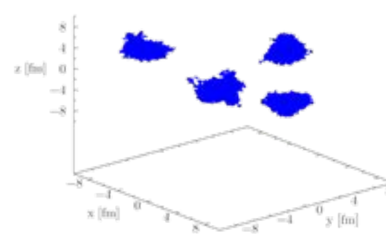


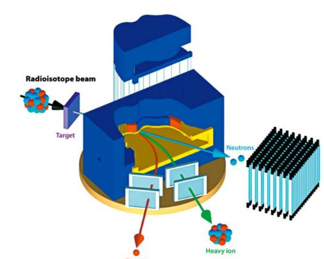
Lattice QCD and experiments





Experiments and many body methods



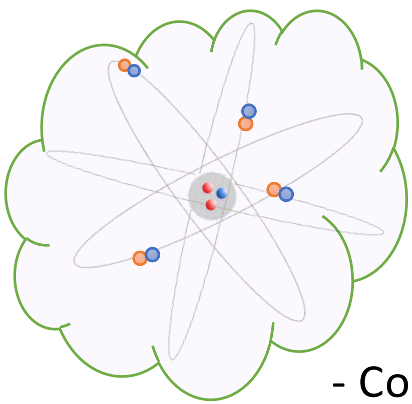


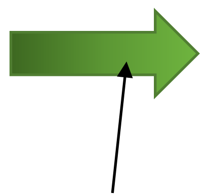
Separation of scales

- Many particles.
- Cloud of quarks around the nucleus.

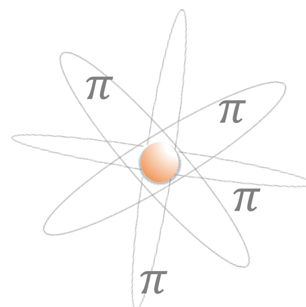
- Fewer particles
- Pion cloud

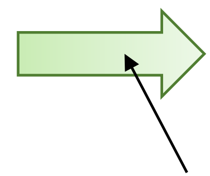
- Nucleons are the only DoFs.
- Only contact interactions



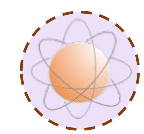


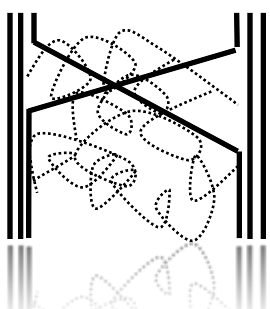
- Color confinement



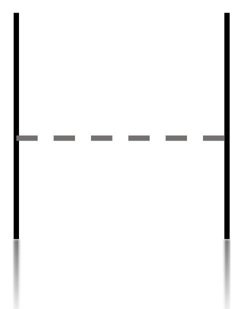


- Low exchanged momentum
- Large pion mass

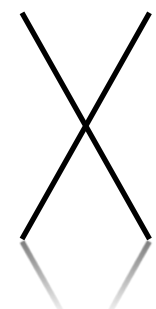




QCD



χEFT



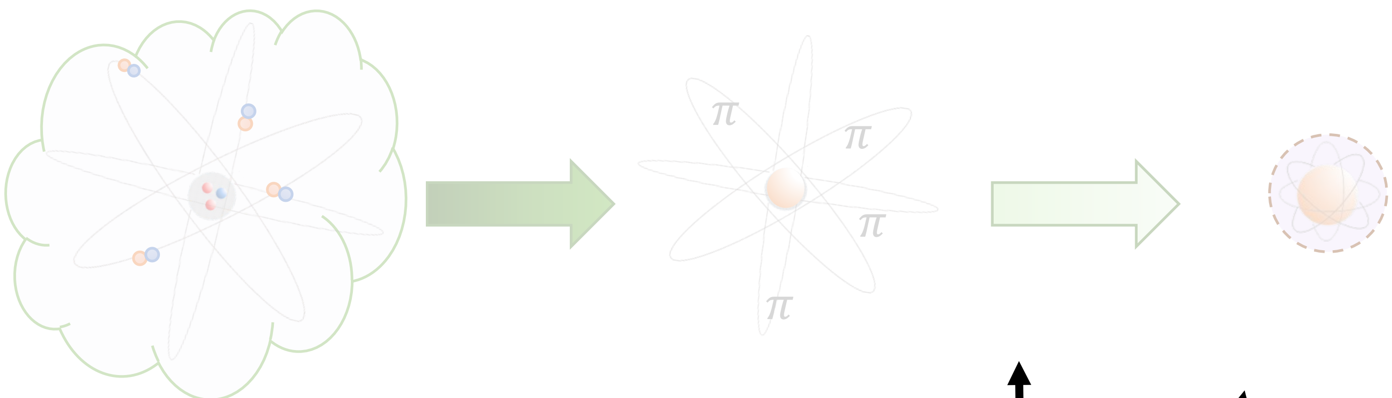
Contact EFT

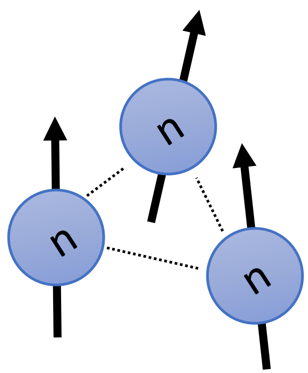
Separation of scales

- Many particles
- Cloud of quarks around the nucleus

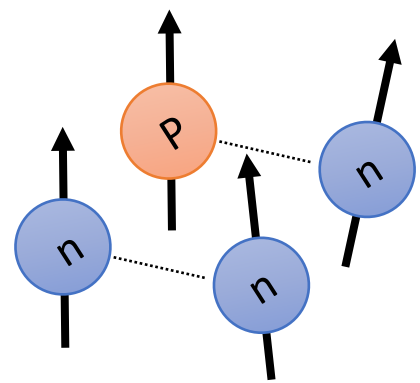
- Fewer particles
- Pion cloud

- Nucleons are the only DoFs





Three body forces



Spin, Isospin and Momentum dependence. (magnitude and angular)

Few technicalities of contact EFT

$\boldsymbol{r}_{ij} = \boldsymbol{r}_i\text{-}\boldsymbol{r}_j$

An **EFT is an expansion of operators** with the **relevant symmetries** of the underlying theory.

- Expansion of the Baryon-Baryon interaction in $\{\boldsymbol{\delta}, \boldsymbol{\nabla}^2\boldsymbol{\delta} \dots\}$

- $\boldsymbol{\pi}$ **- EFT** is an expansion in orders of $\left(\frac{\boldsymbol{Q}}{\boldsymbol{M}}\right)^{\boldsymbol{n}}$ valid for low exchanged-momentum $\boldsymbol{Q}$.

- **Leading Order** has one degree of freedom for each possible two- and three-body S-wave state (**2 two-body and 1 three-body**).

- Contact interaction need to be **regularized/renormalized** introducing a cut-off Λ Result are cut-off independent for $\Lambda \to \infty$.

$$\delta(r_{ij}) = e^{-\frac{1}{2}|r_{ij}|^2\Lambda^2}$$

Interaction in coordinate space

$$\delta_\Lambda^{ij} = e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2}$$

Free parameters to be fitted on "experimental" data
($\mathrm{N} - \mathrm{N}$ **scattering lenghts** or **boundstates**)

$$V^{LO} = \sum_{i<j} [C_0(\Lambda) + C_1(\Lambda)(\vec{\sigma_i} \cdot \vec{\sigma_j})]\, \delta_\Lambda^{ij}$$

$$+ D_0(\Lambda) \sum_{(i<j)\neq k} [\delta_\Lambda^{ij}\delta_\Lambda^{ik} + \delta_\Lambda^{ij}\delta_\Lambda^{jk} + \delta_\Lambda^{ik}\delta_\Lambda^{jk}]$$

$^3\mathrm{H}$ **boundstate**

van Kolck, U. Nucl.Phys. A645 (1999) 273-302
Barnea, N. et al. Phys.Rev.Lett. 114 (2015) no.5

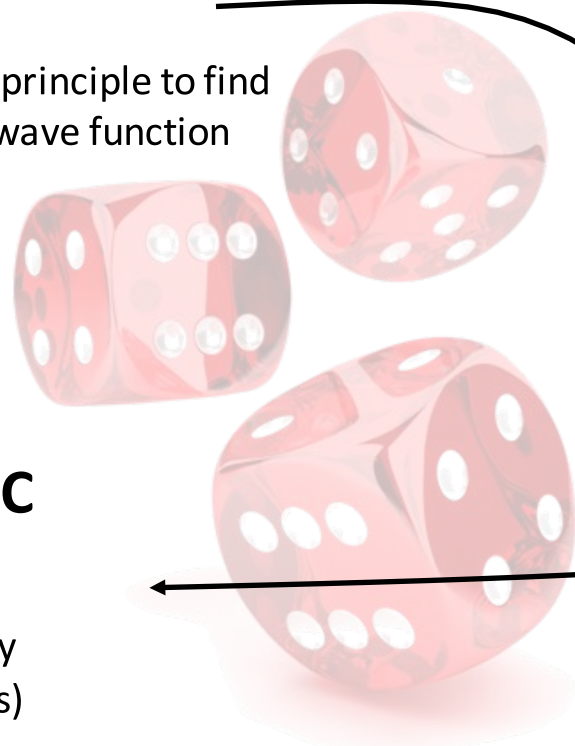
Monte Carlo

Quantum Monte carlo in coordinate space

Quantum Monte Carlo is a class of ab initio, numerical, stochastic many-body methods able to solve the Schrödinger equation with improvable uncertainties.

Variational Monte Carlo

- Exploits the variational principle to find the best parameterized wave function



Diffusion in imaginary time

- Excited states contributions exponentially suppressed
- Need some approximation to keep the sign problem under control

Unconstrained MC

- Unbiased estimators.
- (results only affected by stochastic uncertainties)

Quantum VMC

Hastings, W.K. Biometrika 57 (1970) 97-109

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

Variational Monte Carlo:

$$E_T = \langle \psi_T | H | \psi_T \rangle = \int \psi_T^*(\boldsymbol{X}) H \psi_T(\boldsymbol{X}) d\boldsymbol{X} = \int |\psi_T(\boldsymbol{X})|^2 \frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})} d\boldsymbol{X}$$

$$E_T^n = \frac{1}{n} \sum_{\boldsymbol{X} \in |\psi_T|^2} \frac{H\psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})}$$

T. Skyrme Nucl.Phys. 9 (1959) 615-634

J. Toulouse, C. J. Umrigar Journal of Chemical Physics 126, 084102 (2007)

Trial wave function:

$$\psi_T = \left[\prod_{i=2}^{n} U_i(\boldsymbol{X}) \right] \phi^A(\boldsymbol{X})$$

Before

2-body Schröedinger equation solution

$U_3^{ijk} = U_2^{ij} + U_2^{ik} + U_2^{jj}$

Skyrme wave functions Slater determinant

After

Spline functions

Linear Method optimization automatically finds the best wave function.

Quantum VMC

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J. Toulouse, C. J. Umrigar Journal of Chemical Physics 126, 084102 (2007)

Trial wave function:

$$\psi_T = \left[\prod_{i=2}^{n} U_i(\boldsymbol{X}) \right] \phi^A(\boldsymbol{X})$$

Physical guess

- 2-body Schrödinger equation solution
- $U_3^{ijk} = U_2^{ij} + U_2^{ik} + U_2^{jj}$
- Skyrme wave functions Slater determinant

General assumption

Spline functions

Linear Method optimization automatically finds the best wave function.

"Linear Method" optimization

J. Toulouse and C. J. Umrigar, J. Chem. Phys. **126**, 084102 (2007)

Considering a ψ_T dependent from a **set of parameters** $\{p_1, \ldots, p_k\}$:

$$|\bar{\psi}_T(\boldsymbol{p})\rangle = \frac{|\psi_T(\boldsymbol{p})\rangle}{\sqrt{\langle\psi(\boldsymbol{p})|\psi(\boldsymbol{p})\rangle}}$$

$$\{\bar{H}\}_{ij} = \left\langle \bar{\psi}_T^i(\boldsymbol{p}) | H | \bar{\psi}_T^j(\boldsymbol{p}) \right\rangle$$

$$\{\bar{S}\}_{ij} = \left\langle \bar{\psi}_T^i(\boldsymbol{p}) \mid \bar{\psi}_T^j(\boldsymbol{p}) \right\rangle$$

It can be **expanded**

$$|\bar{\psi}_T^{lin}(\boldsymbol{p})\rangle = |\bar{\psi}_T(\boldsymbol{p}^0)\rangle = \sum_{i=1}^{N_p} \Delta p_i |\bar{\psi}_T^i(\boldsymbol{p}^0)\rangle$$

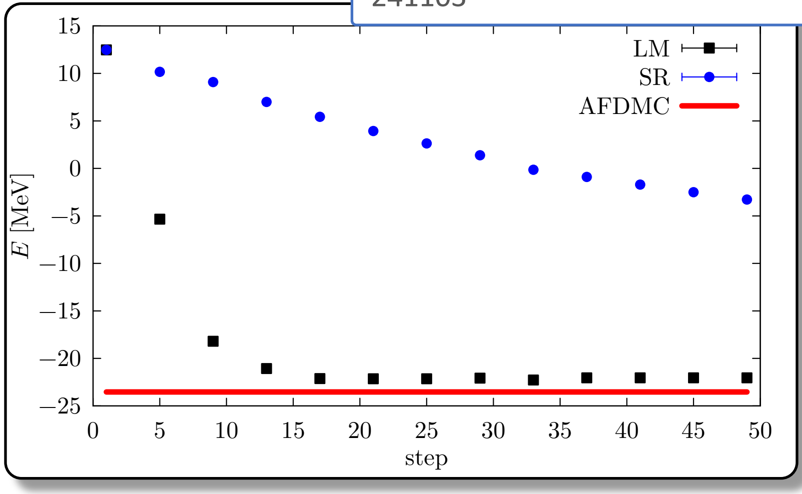
The first variation $\Delta\boldsymbol{p}$ that minimizes the energy

$$E_{lin}(\boldsymbol{p}) = \frac{\langle\bar{\psi}_T^{lin}(\boldsymbol{p})|H|\bar{\psi}_T^{lin}(\boldsymbol{p})\rangle}{\langle\bar{\psi}_T^{lin}(\boldsymbol{p})|\bar{\psi}_T^{lin}(\boldsymbol{p})\rangle}$$

Can be found solving the linear equation

$$\bar{H}\,\Delta\boldsymbol{p} = \Delta E\,\bar{S}\,\Delta\boldsymbol{p}$$

S. Sorella, Phys. Rev. B 71 (2005) 241103



Quantum DMC

D. Ceperley and B. Alder, Science 231, 555–560 (1986)

M. Kalos and P. Whitlock, Monte Carlo methods (Wilei 2008)

Diffusion Monte Carlo:

Trial wave function

Estimator

$$E_0 = \frac{\langle \psi_0 | H | \psi_T \rangle}{\langle \psi_0 | \psi_T \rangle} = \frac{\int \psi_0^*(\boldsymbol{X}) H \psi_T(\boldsymbol{X}) \, d\boldsymbol{X}}{\int \psi_0^*(\boldsymbol{X}) \psi_T(\boldsymbol{X}) \, d\boldsymbol{X}} = \frac{\int \left(\psi_0^*(\boldsymbol{X}) \psi_T(\boldsymbol{X}) \right) \frac{H \psi_T(\boldsymbol{X})}{\psi_T(\boldsymbol{X})} \, d\boldsymbol{X}}{\int \psi_0^*(\boldsymbol{X}) \psi_T(\boldsymbol{X}) \, d\boldsymbol{X}}$$

Ground state is calculated **evolving in the imaginary time**:

$$|\psi_0\rangle = e^{-(H - E_0)\tau} |\psi\rangle = c_0 |\psi_0\rangle + \sum_{n=1}^{\infty} c_n \, e^{-(E_n - E_0)\tau} |\psi_n\rangle \to^{\tau \to \infty} |\psi_0\rangle$$

Symmetric wave functions have the smallest energy → **Sign problem.**

Fixed node /
Fixed phase /
Constrained path approximation:

→ Alleviates the **sign problem**.
→ Introduces a **systematic error** (reduce the available Hilbert space).

Spin / Isospin degrees of freedom

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 $\rightarrow$ $\mathbf{2}^{\boldsymbol{N}}$ components.

Spin / Isospin degrees of freedom

Spin/Isospin:

Using an **Hubbard-Stratonovich** transformation:

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

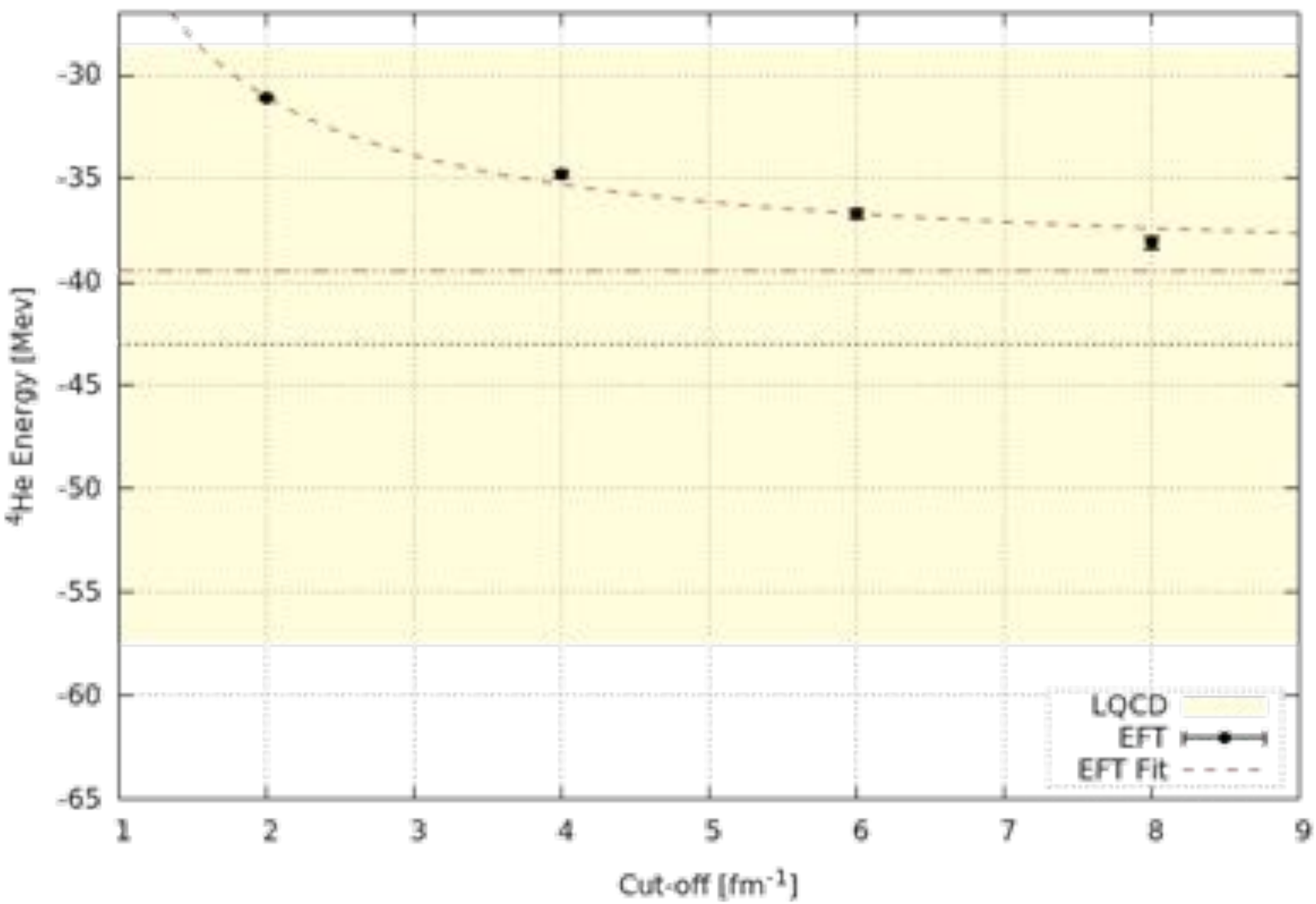
A quadratic operator can be transformed in a linear one,
at the price of an **integral** (per operator).

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

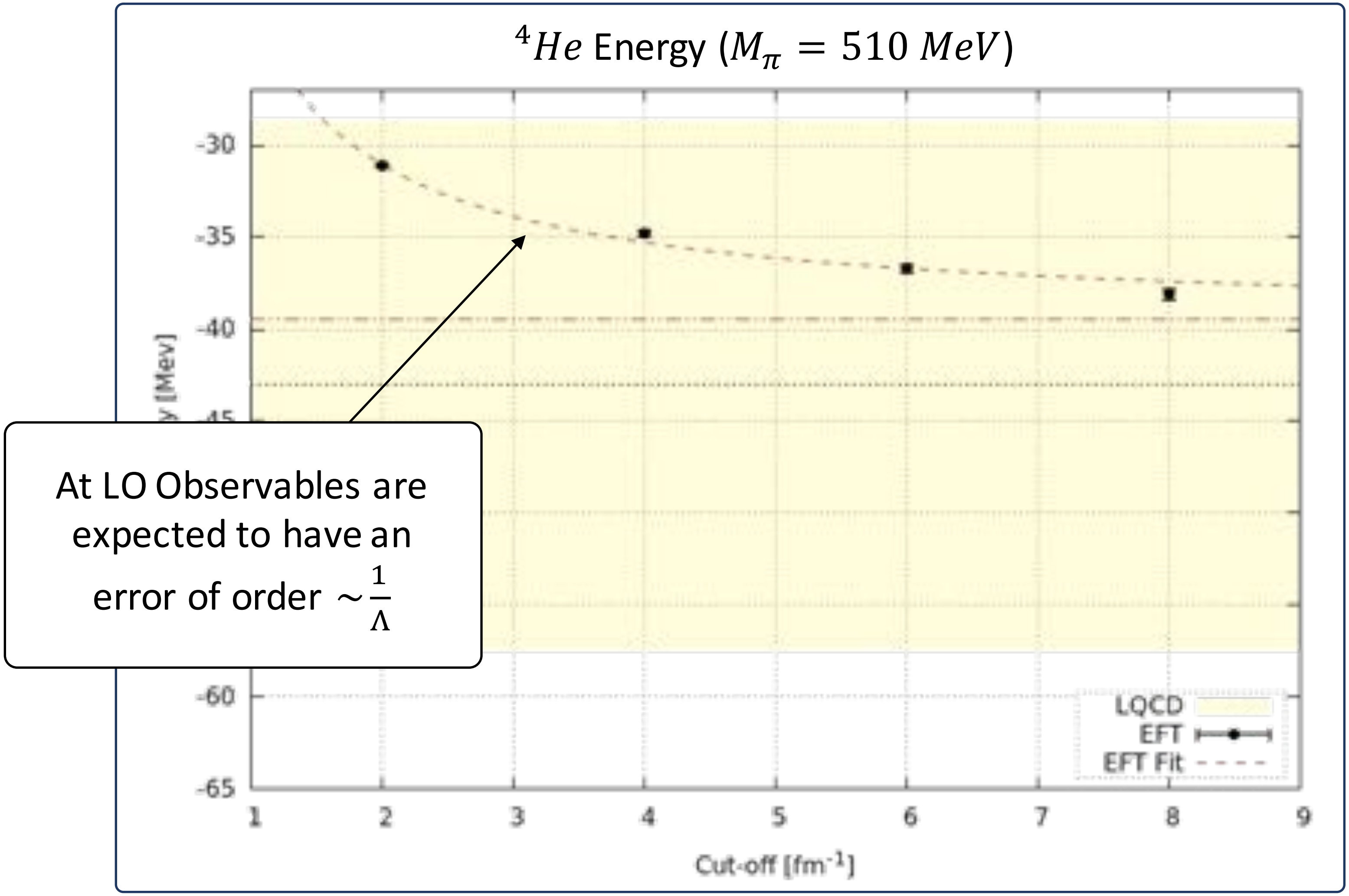
New scaling is $4\mathrm{N}$ instead of 4^{N}

contact EFT

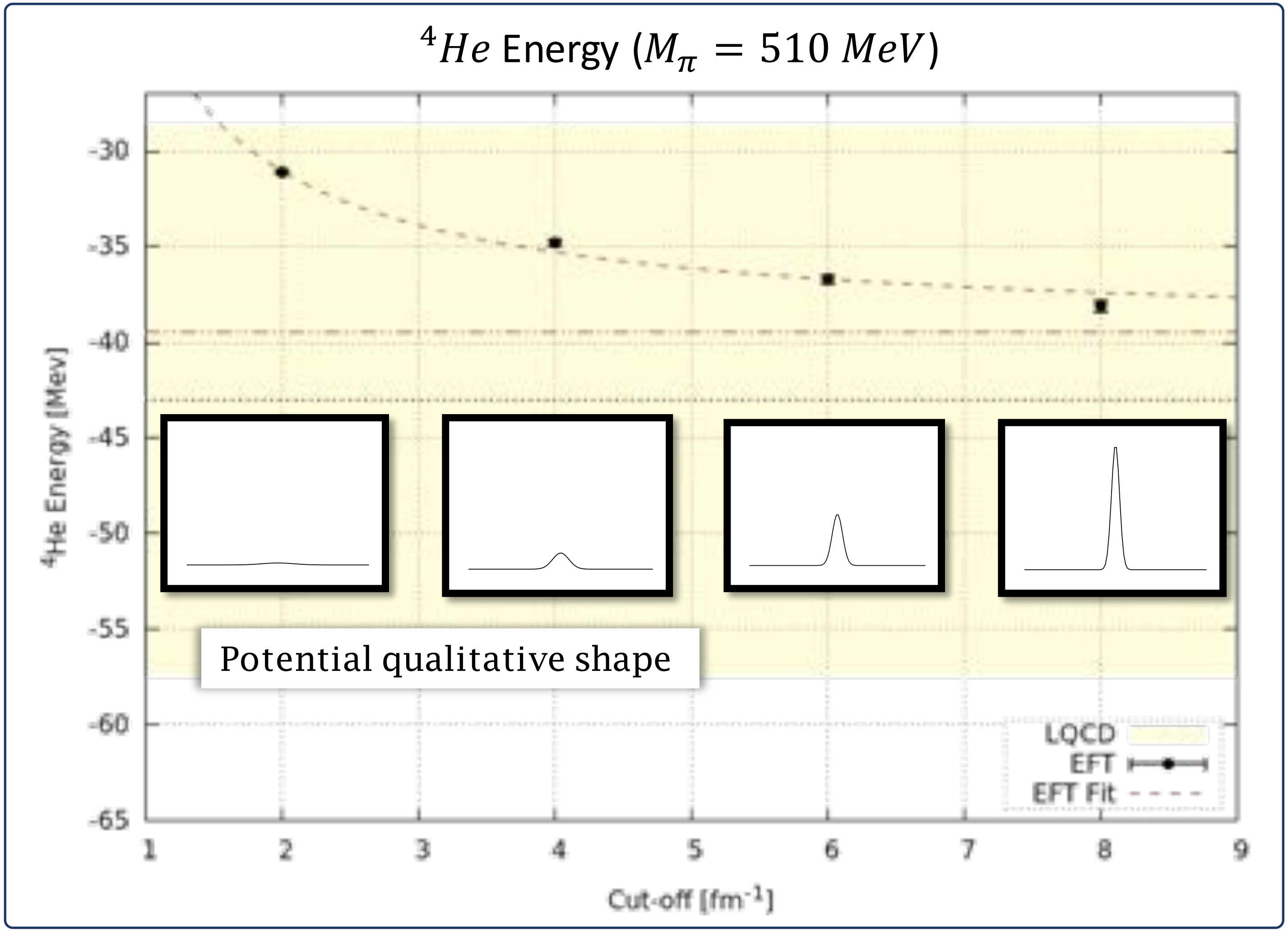
^4He Energy ($M_\pi = 510\ MeV$)



contact EFT


^4He Energy ($M_\pi = 510\ MeV$)
-30
-35
-40
-45
-60
-65
1
2
3
4
5
6
7
8
9
Cut-off [fm^{-1}]
LQCD
EFT
EFT Fit
At LO Observables are expected to have an error of order $\sim\frac{1}{\Lambda}$

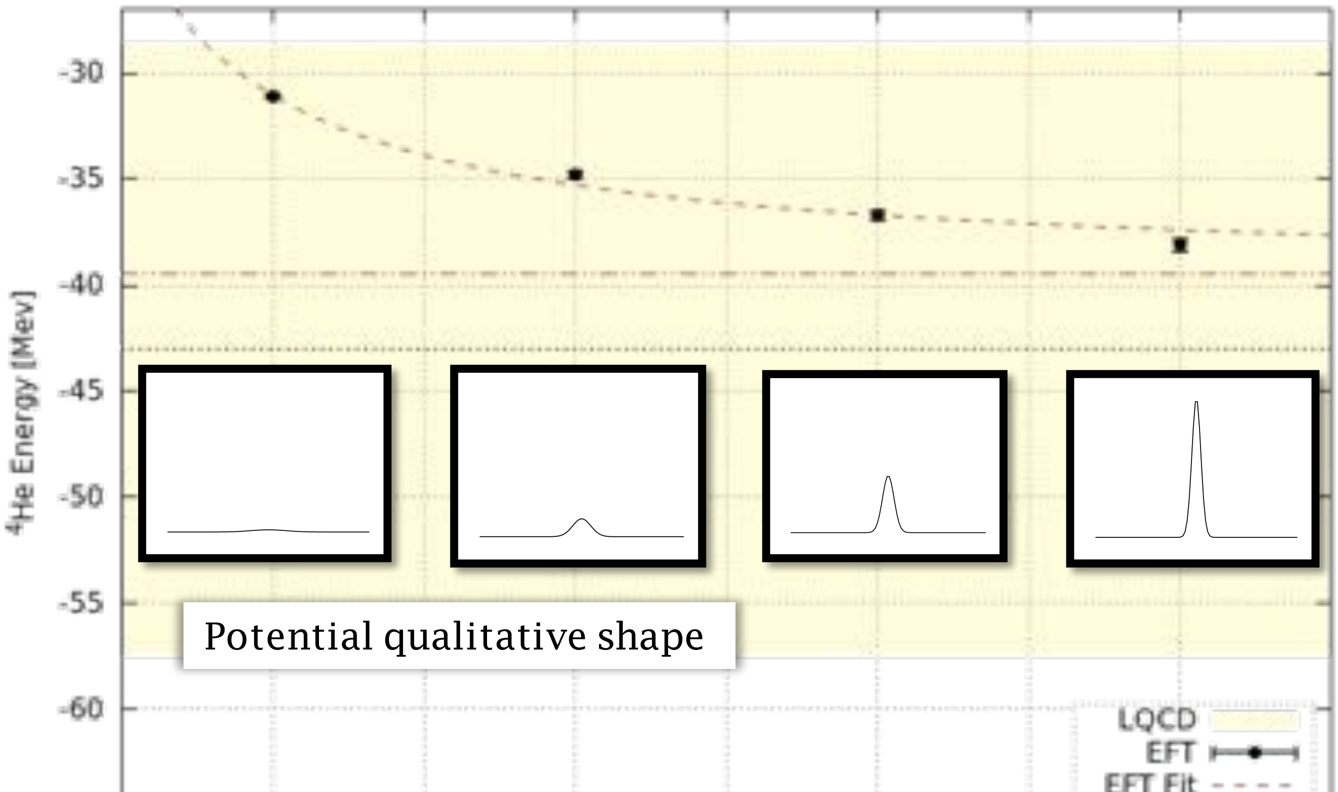
contact EFT



^4He 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}]
Potential qualitative shape
LQCD
EFT
EFT Fit

contact EFT

^4He Energy ($M_\pi = 510\ MeV$)



Large cancellation between 2-, 3-body forces and kinetic energy.

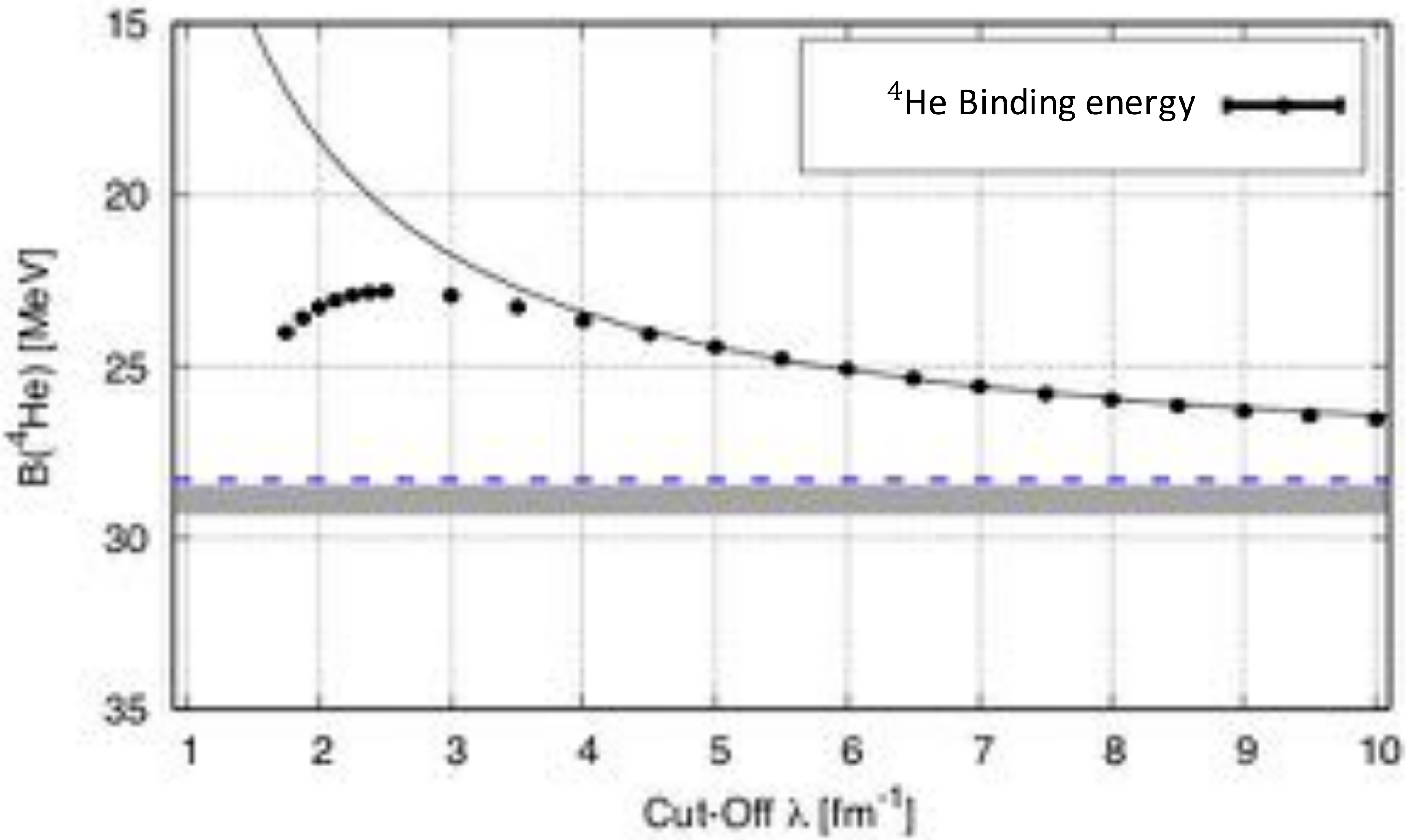

<<
<<
<< RESULTS :

^{4}He

$m_\pi = 140\ MeV$		$m_\pi = 510\ MeV$		$m_\pi = 805\ MeV$	
Λ $[\mathrm{fm}^{-1}]$	^{4}He Energy [MeV]	Λ $[\mathrm{fm}^{-1}]$	^{4}He Energy [MeV]	Λ $[\mathrm{fm}^{-1}]$	^{4}He Energy [MeV]
2	-23.17(2)	2	-31.15(2)	2	-87.9(2)
4	-23.63(3)	4	-34.8(83)	4	-91.3(3)
6	-24.06(2)	6	-36.89(2)	6	-96.4(4)
8	-26.04(5)	8	-37.65(3)	8	-101.3(5)
∞	$-30^{0.3(sys)}_{2.0(stat)}$	∞	$-39^{1(sys)}_{2(stat)}$	∞	$-124^{3(sys)}_{1(stat)}$
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 $\Lambda = 2\ \mathrm{fm}^{-1}$.
- All the errors shown are statistical errors from Monte Carlo method and extrapolation errors.
- Physical m_π LECs have been fitted using BE(d), a(p - n) and BE(^{3}H)

Results: ^{4}He



^{4}He Binding energy
15
20
25
30
35
B(^{4}He) [MeV]
1
2
3
4
5
6
7
8
9
10
Cut-Off λ [fm^{-1}]

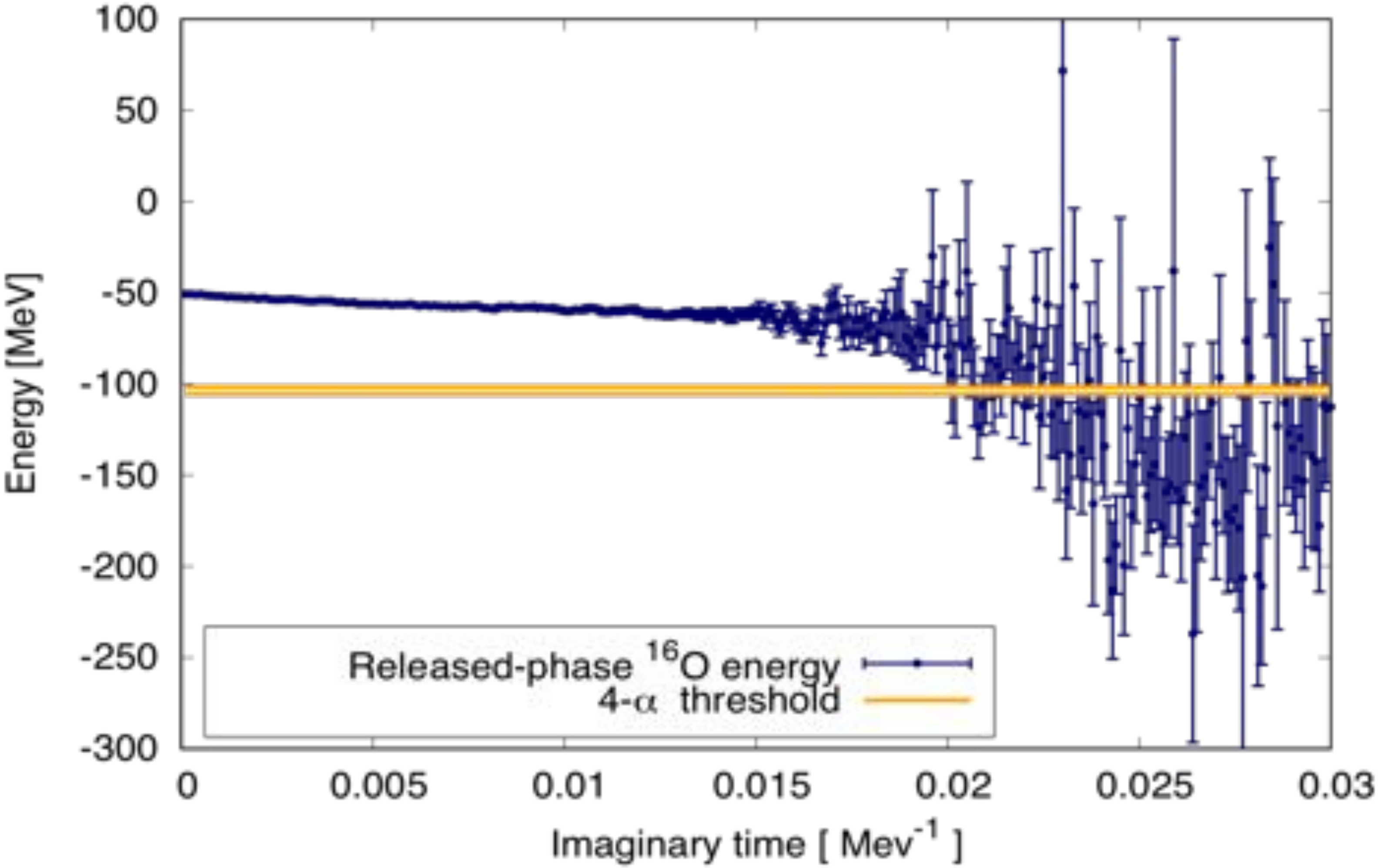
^{16}O - Physical motivated wave function

$m_\pi = 140$ 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)	-92.68(8)	2	-114.6(2)	-124.6(1)	2	-347(1)	-352.36(4)
4	-58(1)	-94.52(9)	4	-113.8(2)	-139.5(1)	4	-335(1)	-365.6(1)
6	-50(1)	-100.24(8)	6	-109.7(1)	-147.6(1)	6	-326(1)	-387.88(4)
8	-52(1)	-104.2(2)	8	-105.7(5)	-150.6(1)	8	-315(1)	-406.9(1)

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

Unconstrained Monte carlo

$m_\pi = 140$ MeV $\Lambda = 8$ fm $^{-1}$



^{16}O - Linear Minimized (LM) + Spline

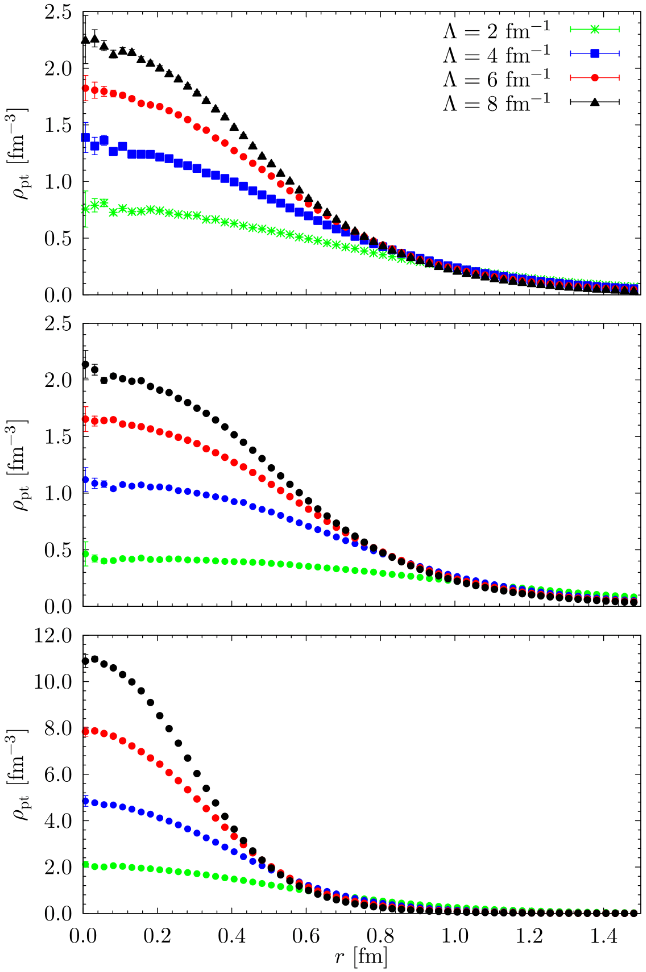
$m_\pi = 140$ MeV			$m_\pi = 510$ MeV			$m_\pi = 805$ MeV		
Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]	Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]	Λ [fm^{-1}]	^{16}O Energy [MeV]	4α treshold [MeV]
2	-97.19(6)	-92.68(8)	2	-116.59(8)	-124.6(1)	2	-350.69(5)	-352.36(4)
4	-92.23(14)	-94.52(9)	4	-137.15(15)	-139.5(1)	4	-362.92(7)	-365.6(1)
6	-97.51(14)	-100.24(8)	6	-143.84(17)	-147.6(1)	6	-382.17(25)	-387.88(4)
8	-100.97(20)	-104.2(2)	8	-146.37(27)	-150.6(1)	8	-402.24(39)	-406.9(1)
∞	$-115^{1(sys)}_{8(stat)}$	$-120^{1(sys)}_{8(stat)}$	∞	$-151^{2(sys)}_{10(stat)}$	$-156^{4(sys)}_{8(stat)}$	∞	$-504^{20(sys)}_{12(stat)}$	$-496^{9(sys)}_{4(stat)}$

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

Be(^{16}O) ~ 127 MeV
Be(4α) ~ 113 MeV
It is only 10% of difference!

Radial density

^{4}He radial density

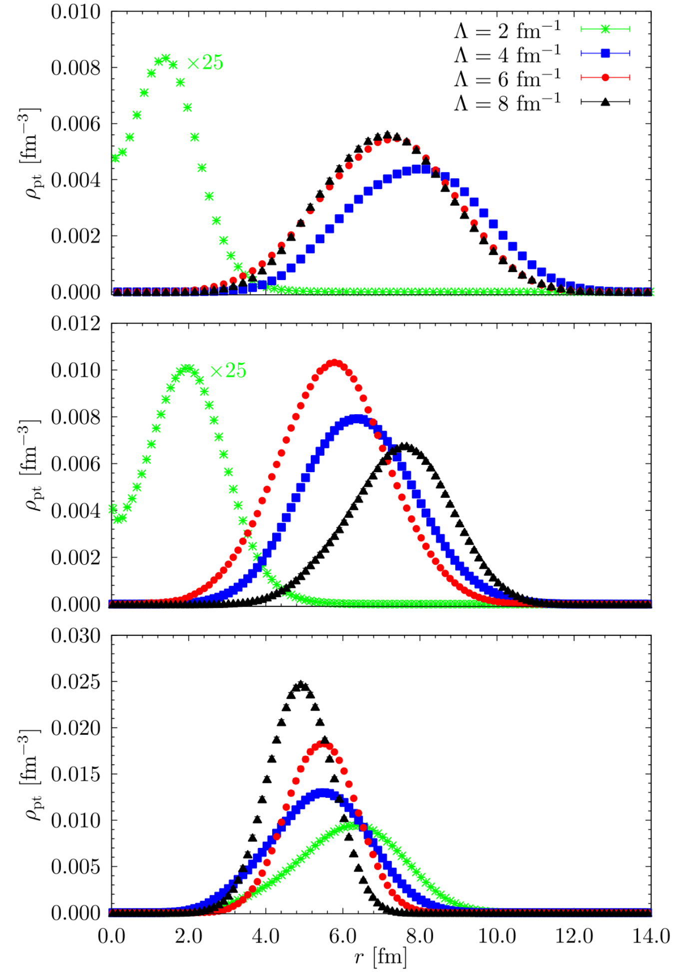


$m_\pi = 140$ MeV

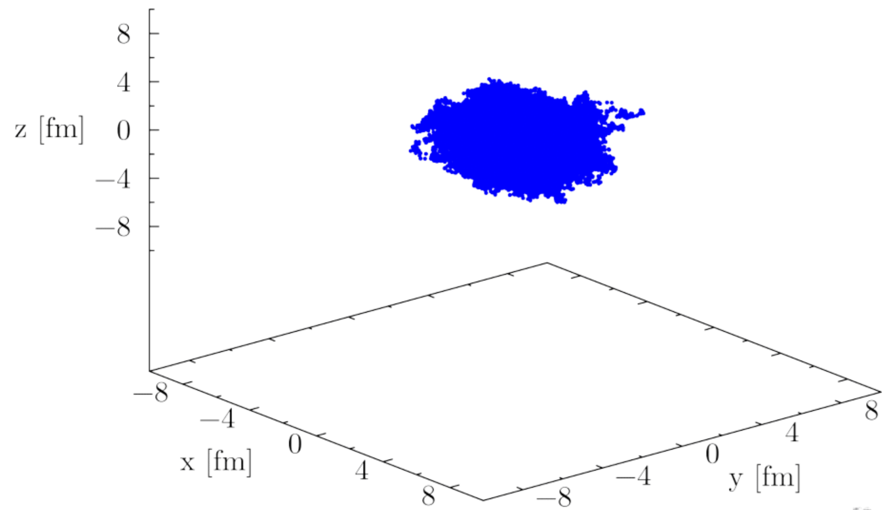
$m_\pi = 510$ MeV

$m_\pi = 805$ MeV

^{16}O radial density

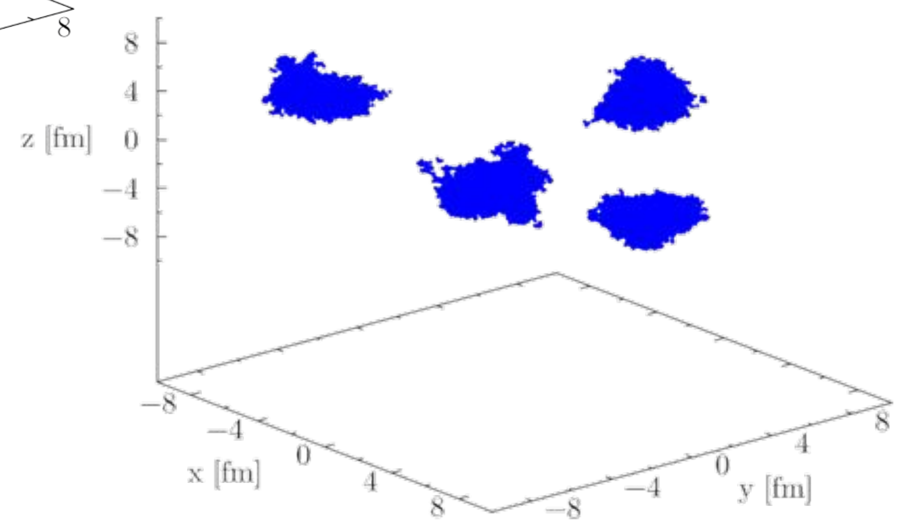


Oxygen density ($m_\pi = 140$ MeV)



$\Lambda = 2\ \mathrm{fm}^{-1}$

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



Mixed estimators:

VMC $$\mathcal{O}_{VMC} = \frac{\langle \psi_T | \mathcal{O} | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

DMC $$\mathcal{O}_{DMC} = \frac{\langle \psi_0 | \mathcal{O} | \psi_T \rangle}{\langle \psi_0 | \psi_T \rangle}$$

$\mathcal{O}_{DMC}$=$\mathcal{O}_{gs}$ only if $\mathcal{O}$ is Hermitian

corrected estimators:

$|\psi_T\rangle = |\psi_{gs} + \delta\psi\rangle$

$\langle \psi_{gs} | \psi_{gs} \rangle = 1$

O is real

$$2\,\mathcal{O}_{DMC} - \mathcal{O}_{VMC} = \langle \psi_0 | \mathcal{O} | \psi_o \rangle + O(\delta^2)$$

$$\frac{\mathcal{O}_{DMC}^2}{\mathcal{O}_{VMC}} = \langle \psi_0 | \mathcal{O} | \psi_o \rangle + O(\delta) = \langle \psi_0 | \mathcal{O} | \psi_o \rangle + O(\delta)$$

Next to leading order:

$$\delta_\Lambda^{ij} = e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2}$$

$$V^{NLO} = \sum_{i<j} \left[\left(E_0(\Lambda) + \boldsymbol{r^2}\, E_1(\Lambda) \right) + \left(E_2(\Lambda) + \boldsymbol{r^2}\, E_3(\Lambda) \right) \left(\vec{\sigma_i} \cdot \vec{\sigma_j} \right) \right] \delta_\Lambda^{ij}$$
$$+ F_0(\Lambda) \sum_{(i<j)\neq k} \left[\delta_\Lambda^{ij}\delta_\Lambda^{ik} + \delta_\Lambda^{ij}\delta_\Lambda^{jk} + \delta_\Lambda^{ik}\delta_\Lambda^{jk} \right]$$

NLO should be treated in **first order perturbation theory** (NOT ITERATED) !

$$E^{NLO} = \langle \psi_{gs} | H_{LO} | \psi_{gs} \rangle + \langle \psi_{gs} | V^{NLO} | \psi_{gs} \rangle$$

It require a **precise knowledge** of the ground state **wave function**!

Next to leading order:

$$\delta_\Lambda^{ij} = e^{-\frac{1}{2}|r_{ij}|^2 \Lambda^2}$$

System	$(E_0 + E_2\ \sigma\sigma)\ \delta_\Lambda^{ij}$	$r^2\ (E_0 + E_2\ \sigma\sigma)\ \delta_\Lambda^{ij}$	3 - body	$< VMC >$	$< DMC >$	MC Corrected estimator	Expected (SVM)
$^3\mathrm{H}_{1200}$	881.38	-938.77	57.39	5.17(2)	2.42(6)	-0.32(87)	0.
$^4\mathrm{He}_{600}$	1661.13	-1862.63	192.57	-9.10(9)	-10.15(14)	-11.2(2)	-11.24

All the energies are measured in MeV

⇧

Large cancellation that depend on the knowledge of the **wavefunction.**

conclusions:

- **EFT($\boldsymbol{\not\pi}$)** is used to **<u>connect</u>** high- and low- energy theories.
  - The theory is relatively simple

    (contains **central**, $\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}$ and **three body forces)**.
  - $\mathrm{Be}(^4\mathrm{He})$ **agreement** with experiments and LQCD prediction ($m_\pi = 140, 510, 805$ MeV).
  - Oxygen is **unstable with respect 4$\boldsymbol{\alpha}$** for $m_\pi = 140, 510$ and 805 MeV.

- **Quantum Monte Carlo** fulfill greatly the task of bridging the theories.
  - **Auxiliary Field** allows to perform calculations in medium and large nuclei.
  - **Linear Minimization** algorithm is **crucial** in investigate systems with unexpected symmetries.
  - **Mixed estimators** need special care and a precise variational wave function.

    (Especially in presence of large cancellations)

Thanks for your attention

Cat that guards a door
in Jerusalem (old city).