Quantum Monte Carlo Calculations With Chiral Effective Field Theory Interactions

Nuclear Theory in the Supercomputing Era - 2016

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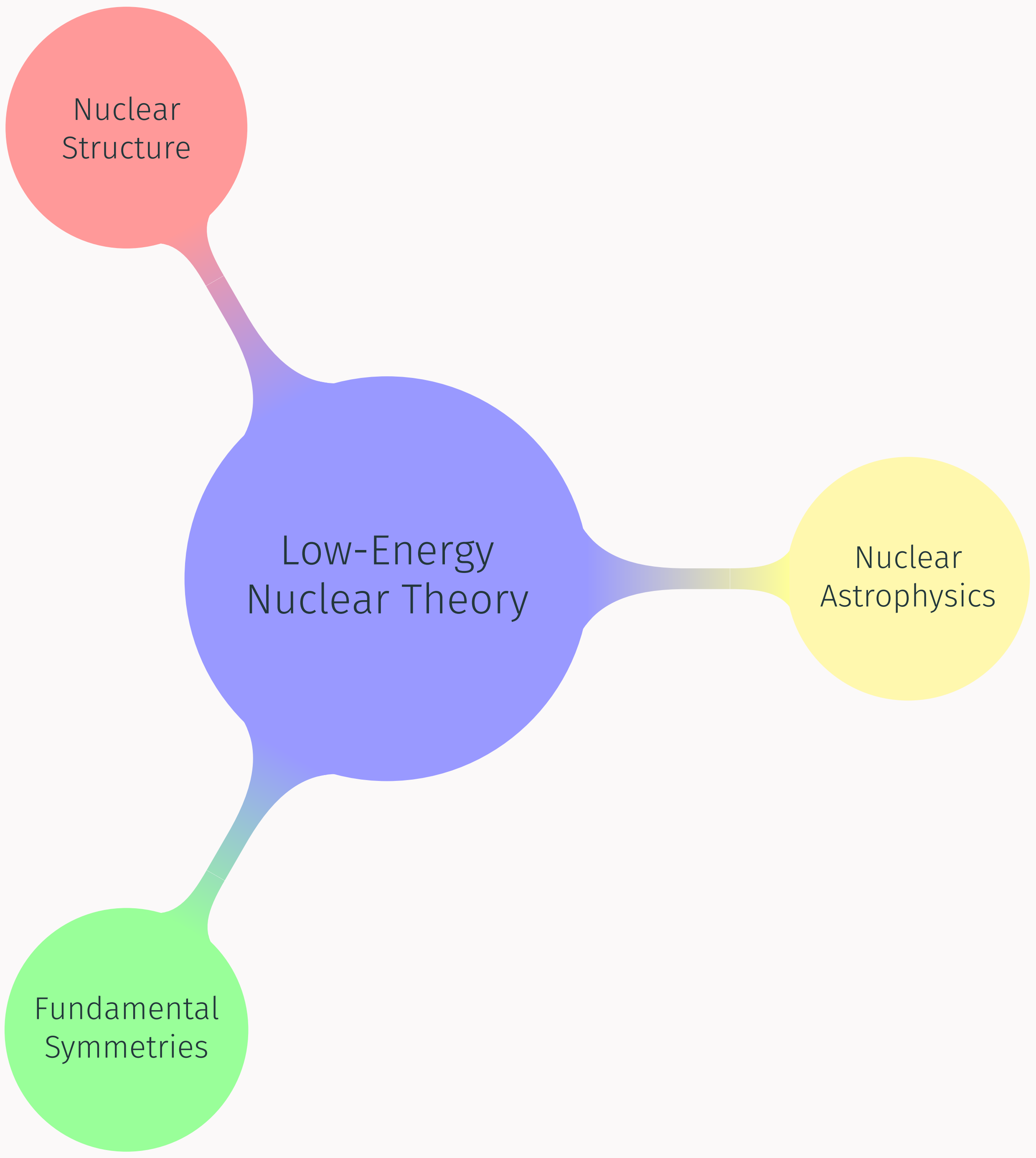
Motivation - Be **Bold!** Ask Big Questions

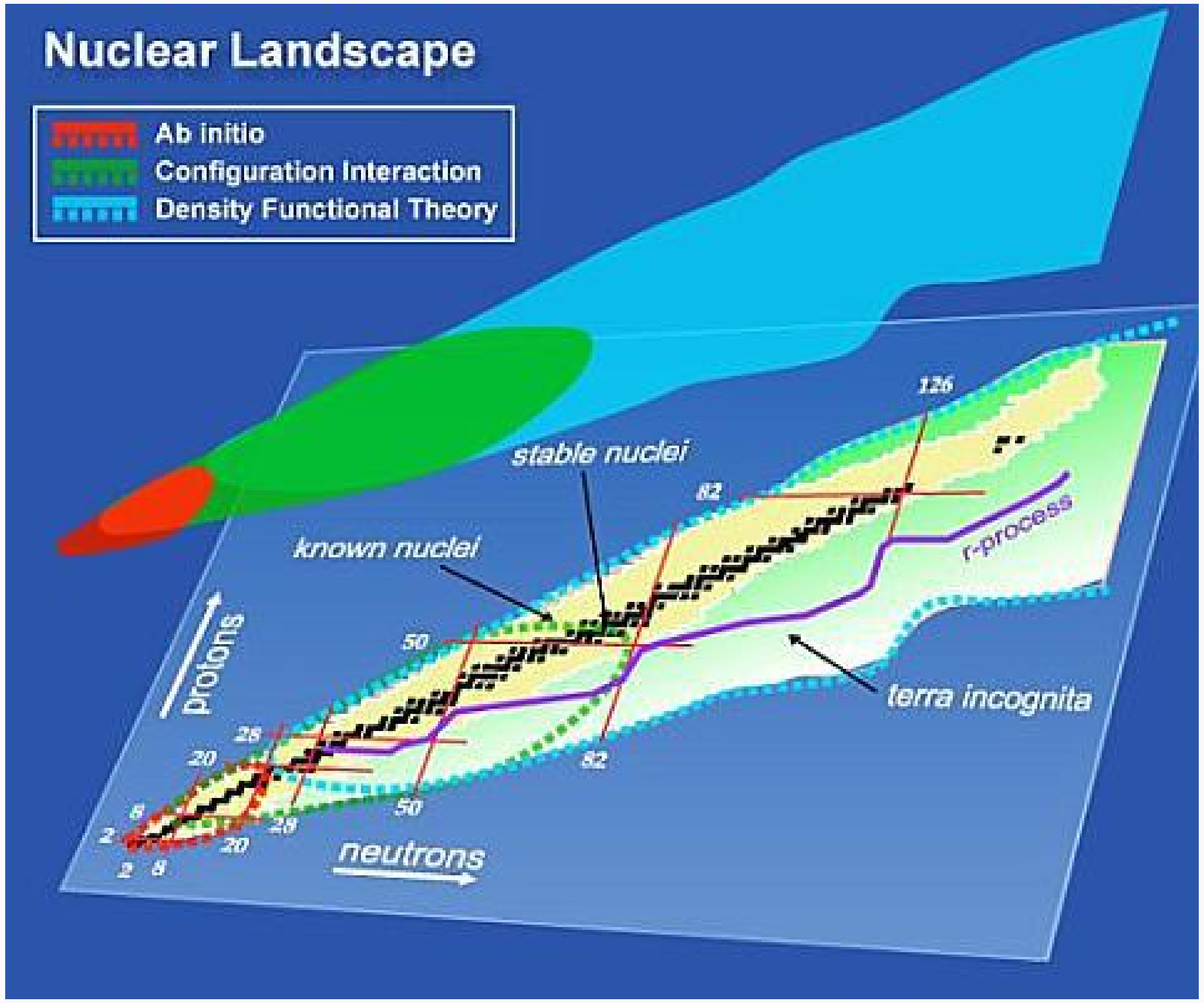
Motivation

Low-energy nuclear theory sits in a privileged position, connecting many research areas.



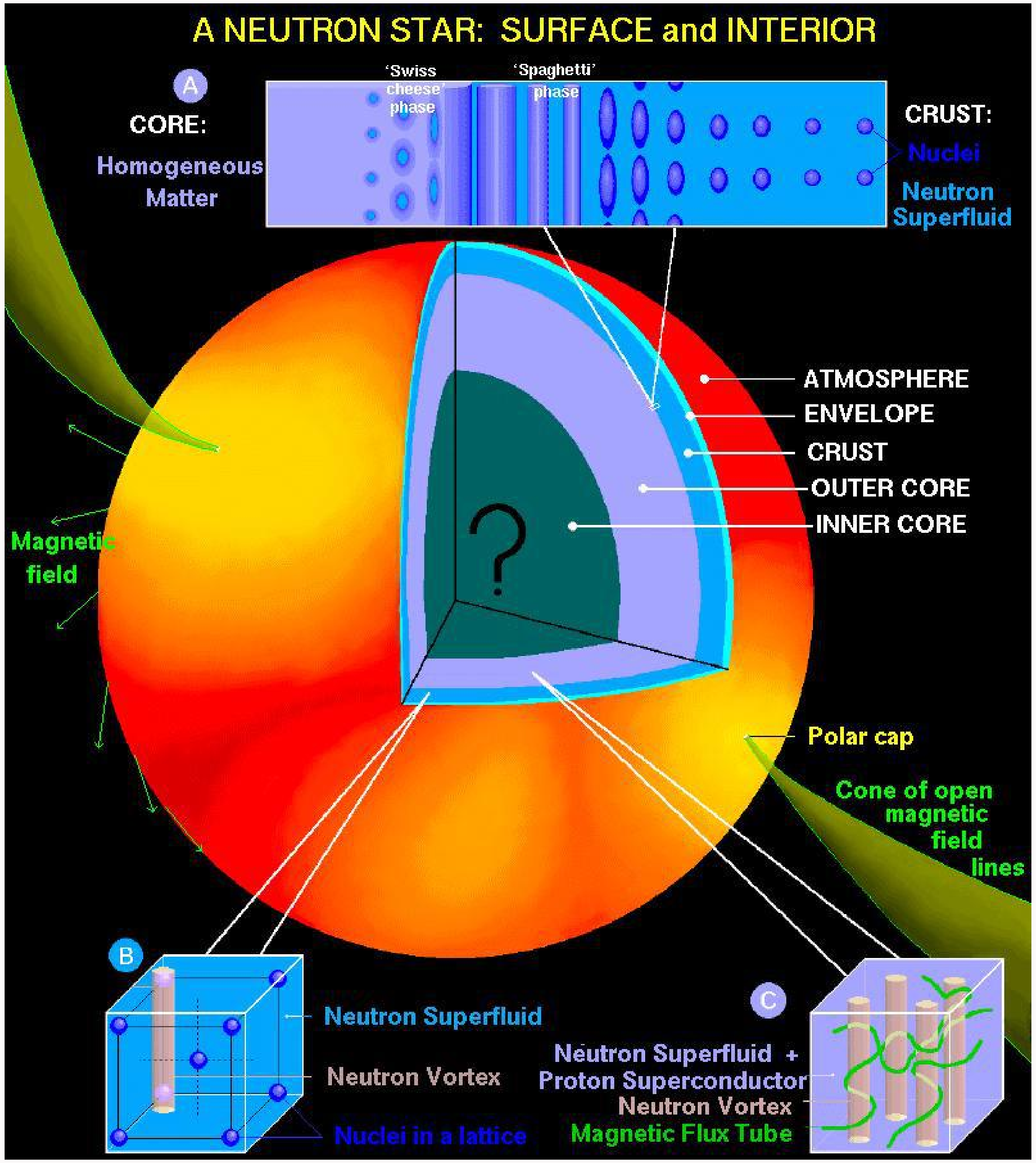
Motivation - Nuclear Structure

- What are the limits of nuclear existence?
- How far can we push *ab initio* calculations?
- How can we build a coherent framework for describing, nuclei, nuclear matter, and nuclear reactions?



Motivation - Nuclear Astrophysics

- How did the elements come into existence?
- What is the structure of neutron stars and how do their properties depend on the nuclear Hamiltonian?
- What role does pairing play in properties of neutron stars?

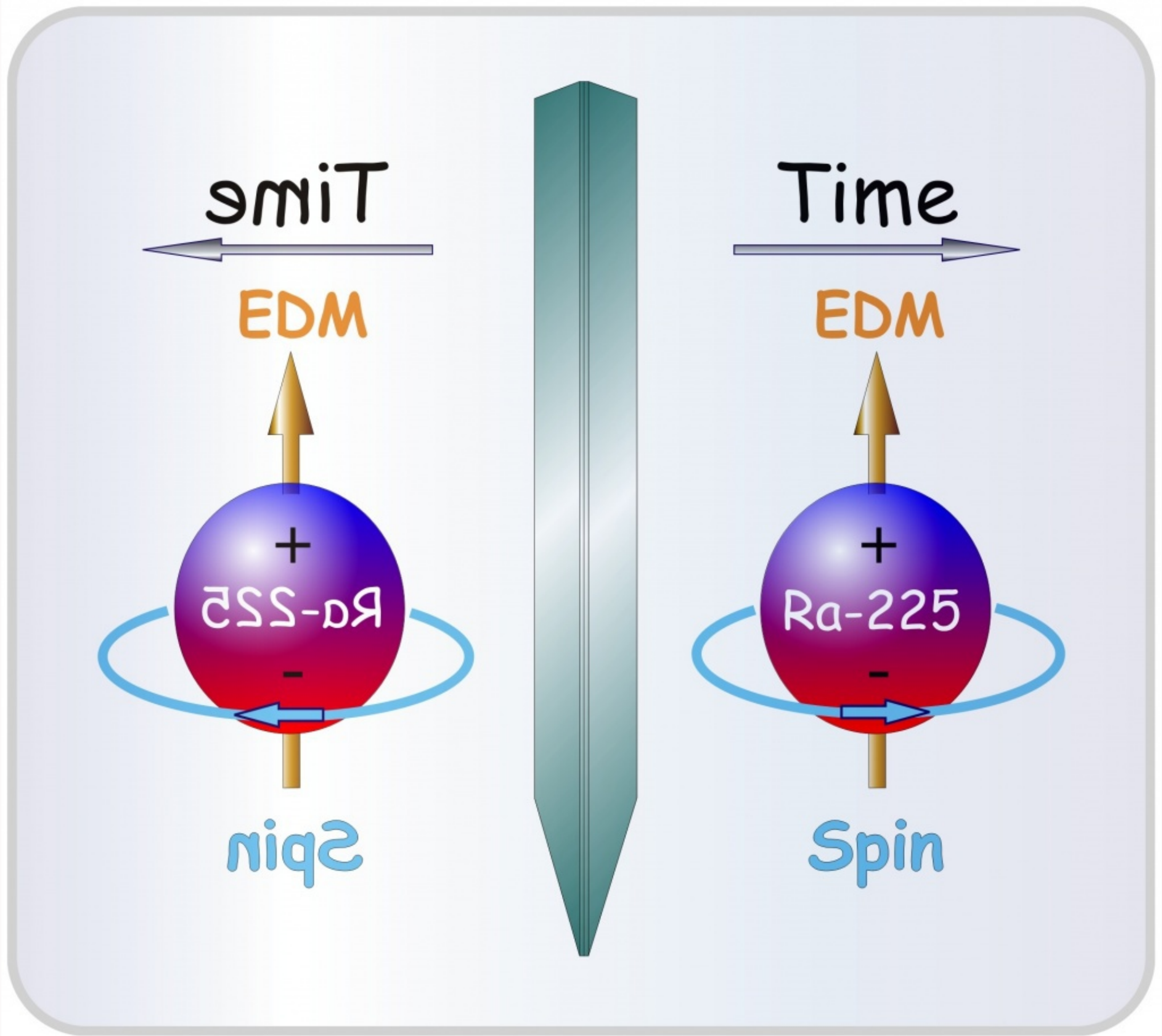


Motivation - Fundamental Symmetries

- What explains the dominance of matter over antimatter in the universe?

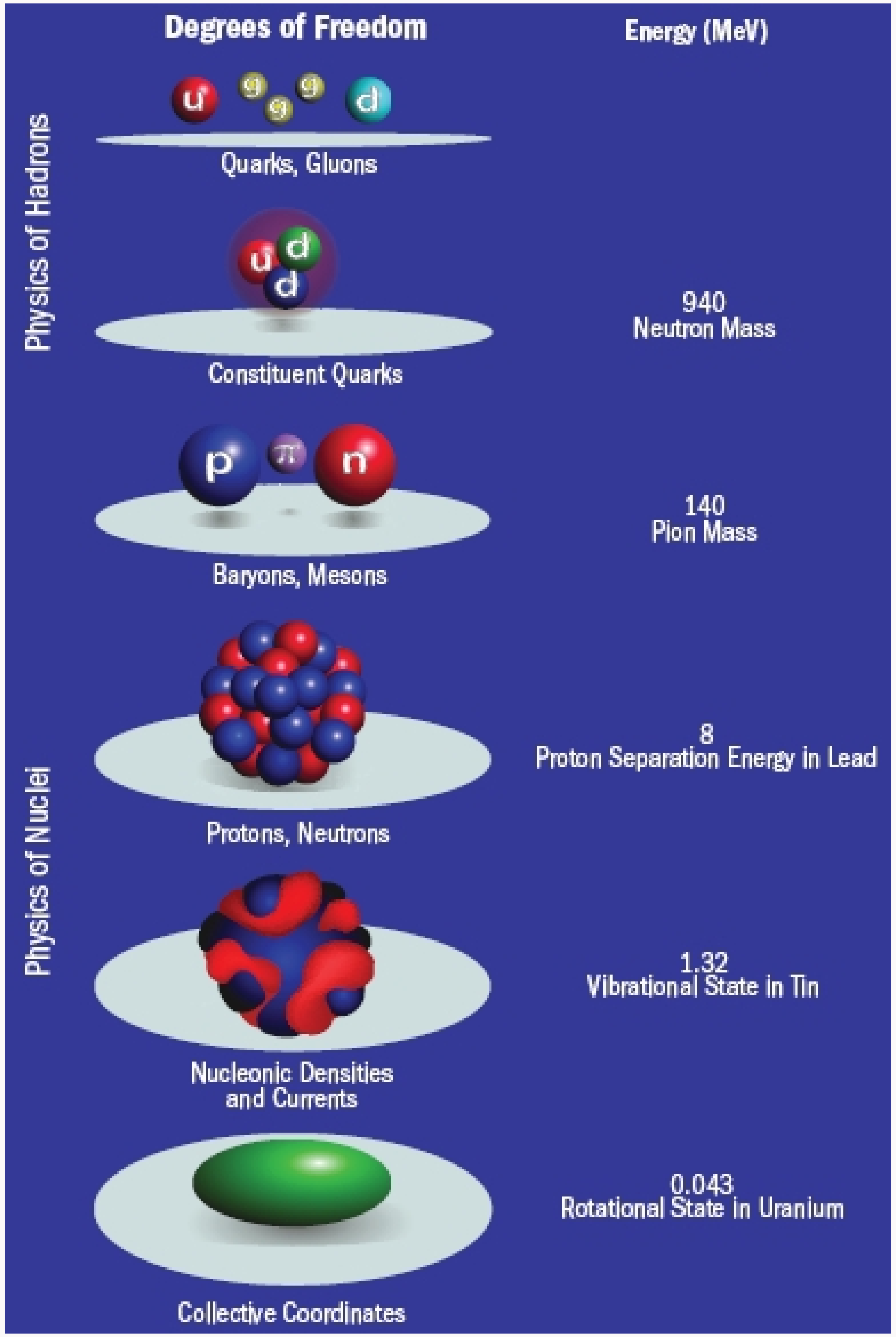
- What is the nature of neutrinos and how do they interact with nuclei?

- Electric dipole moments of light nuclei?



Motivation - Framework

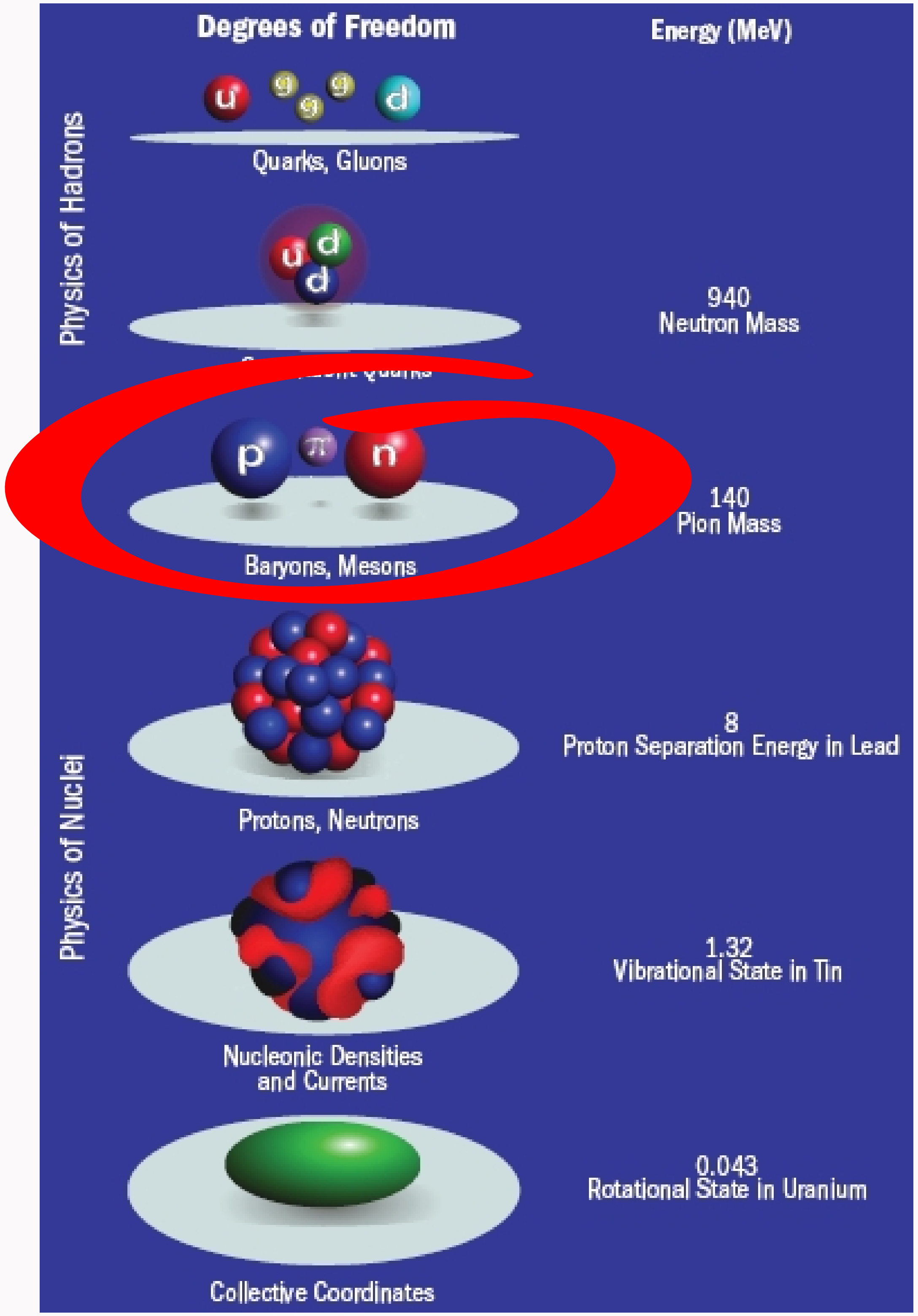
Quantum chromodynamics (QCD) is ultimately responsible for strong interactions.



Motivation - Framework

Quantum chromodynamics (QCD) is ultimately responsible for strong interactions.

Nucleons are the relevant degrees of freedom for low-energy nuclear physics.



Motivation - A Hard Problem!

Nuclei are strongly interacting many-body systems.

1. **How do we solve the many-body Schrödinger equation?**

$$H|\Psi\rangle = E|\Psi\rangle$$

$2^A\binom{A}{Z}$ coupled differential equations in $3A-3$ variables.

^{4}He $\rightarrow$ 96 equations in 9 variables
^{12}C $\rightarrow$ 3 784 704 equations in 33 variables

2. **What is the Hamiltonian?**

Motivation - A Hard Problem!

Nuclei are strongly interacting many-body systems.

1. **How do we solve the many-body Schrödinger equation? QMC methods!**

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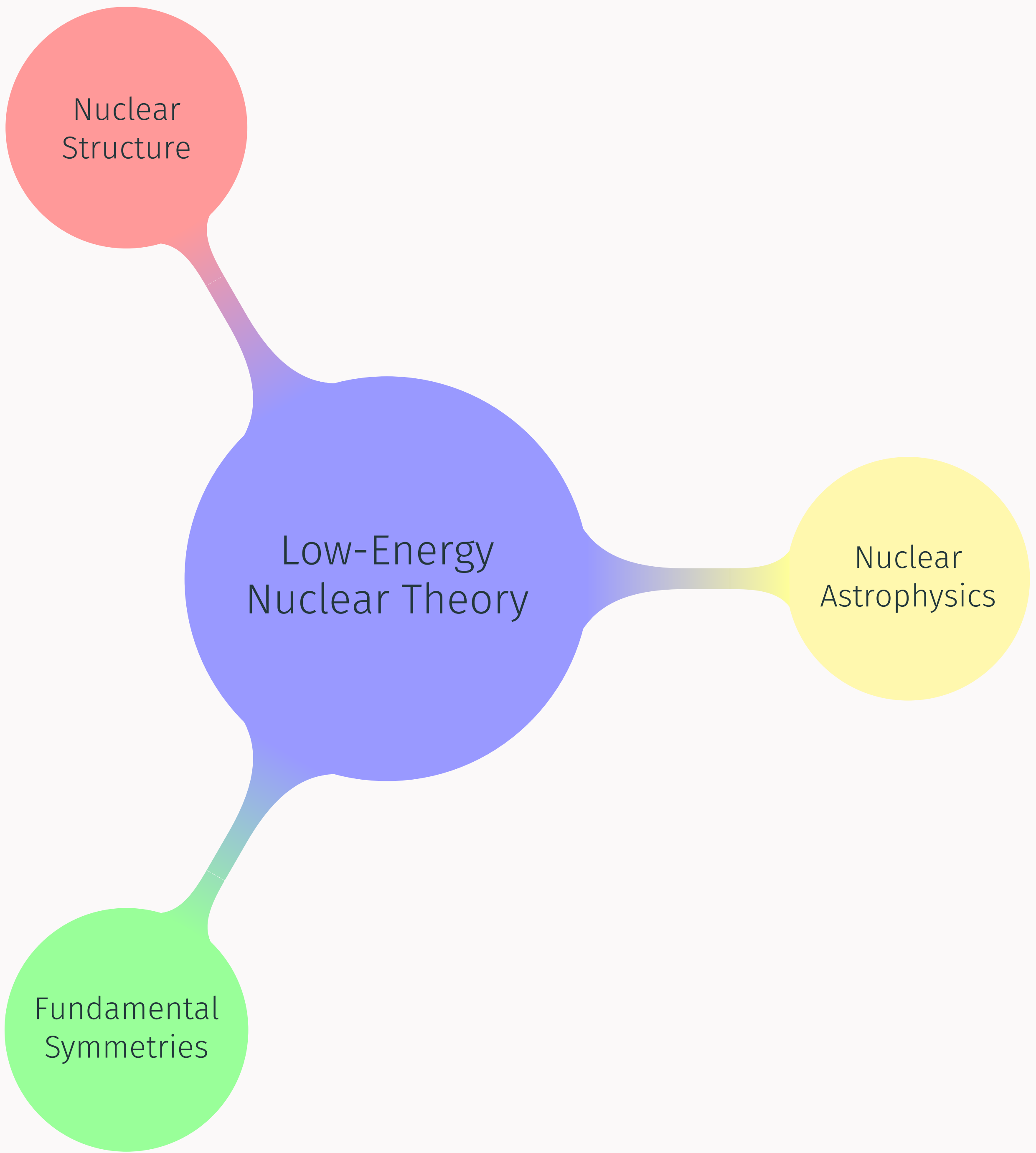
$$^{12}\text{C} \rightarrow 3\,784\,704 \text{ equations in } 33 \text{ variables}$$

2. **What is the Hamiltonian?** $\rightarrow$ **Chiral EFT!**

Motivation

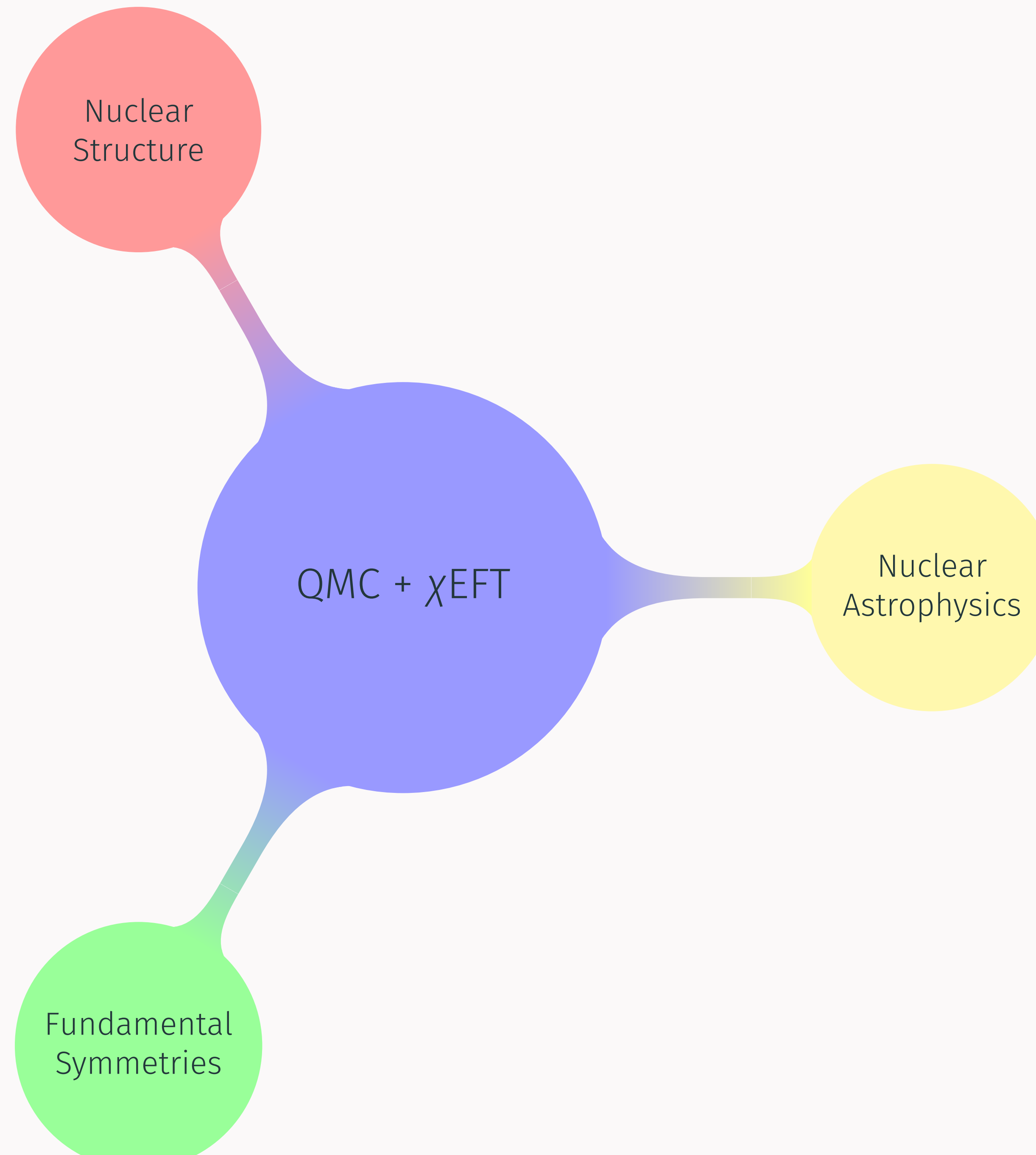
Low-energy nuclear theory sits in a privileged position, connecting many research areas.



Motivation

Low-energy nuclear theory sits in a privileged position, connecting many research areas.

QMC + χEFT is a compelling piece of the puzzle.



Outline

- Quantum Monte Carlo Methods
- Chiral EFT
    - Three-Nucleon Interactions
    - Fits and Results
- An Application

Quantum Monte Carlo (QMC) Methods

QMC METHODS

QMC methods in two lines:

$$H|\Psi\rangle = E|\Psi\rangle$$

$$\lim_{\tau\to\infty} e^{-H\tau}|\Psi_T\rangle \to |\Psi_0\rangle$$

QMC methods in more than two lines:

J. Carlson et al, RMP **87**, 1067 (2015).

QMC Methods - Variational Monte Carlo (VMC) Method

1. Guess a trial wave function Ψ_T and generate a random position: $\mathrm{R} = \mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_A$.

2. Use the Metropolis algorithm to generate new positions R' based on the probability $P = \frac{|\Psi_T(\mathrm{R}')|^2}{|\Psi_T(\mathrm{R})|^2}$. (Yields a set of "walkers" distributed according to $|\Psi_T|^2$).

3. Invoke the variational principle: $E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} > E_0$.

QMC Methods - Diffusion Monte Carlo Method

- The wave function is imperfect: $|\Psi_T\rangle = \sum_{i=0}^{\infty} \alpha_i |\Psi_i\rangle$.
- Propagate in imaginary time to project out the ground state $|\Psi_0\rangle$.

$$
\begin{aligned}
|\Psi(\tau)\rangle &= e^{-(H-E_T)\tau} |\Psi_T\rangle \\
&= e^{-(E_0-E_T)\tau}[\alpha_0 |\Psi_0\rangle + \sum_{i\neq 0} \alpha_i e^{-(E_i-E_0)\tau} |\Psi_i\rangle].
\end{aligned}
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\end{aligned}
$$

$$
|\Psi(\tau)\rangle \xrightarrow{\tau\to\infty} |\Psi_0\rangle .
$$

QMC Methods - An Example

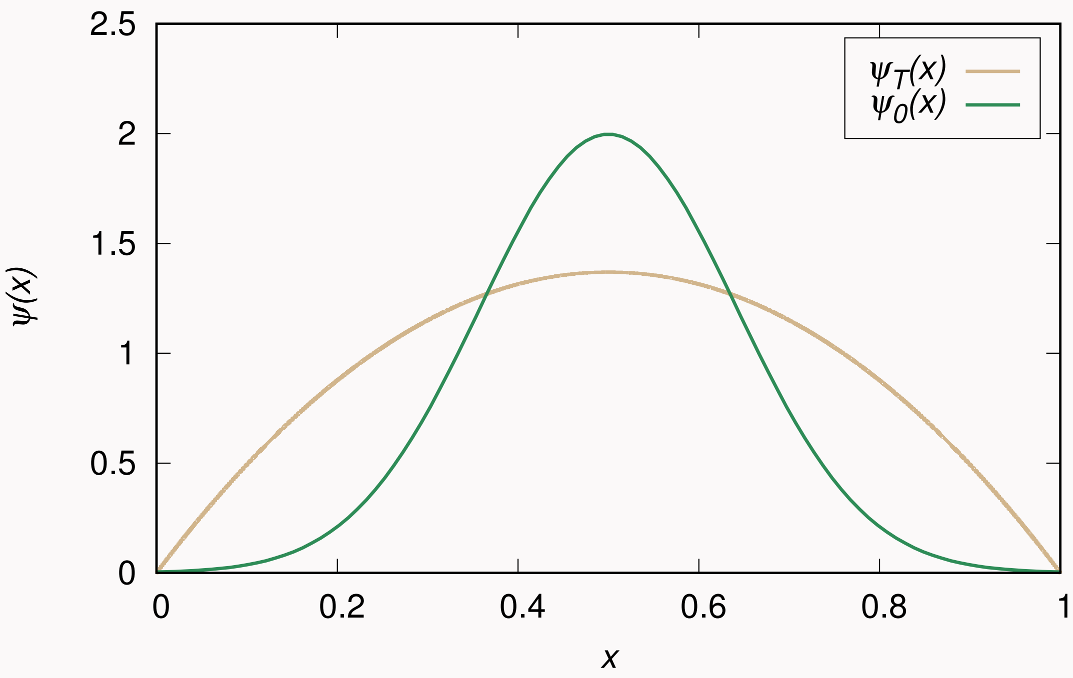
$$H = \frac{p_x^2}{2m} + V(x),\ V(x) = \frac{1}{2}m\omega^2x^2$$

$$\hbar = m = 1$$

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega x^2/2} H_n(\sqrt{\omega}x)$$

Trial wave function; e.g.

$$\Psi_T(x) = \sqrt{30}x(1-x).$$

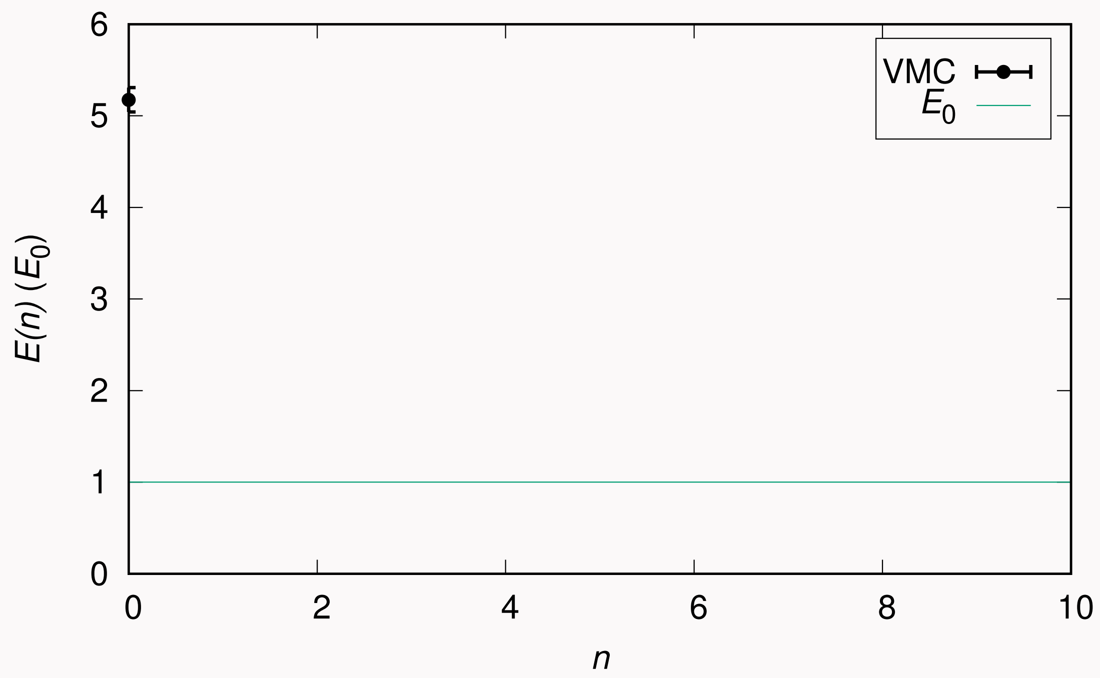


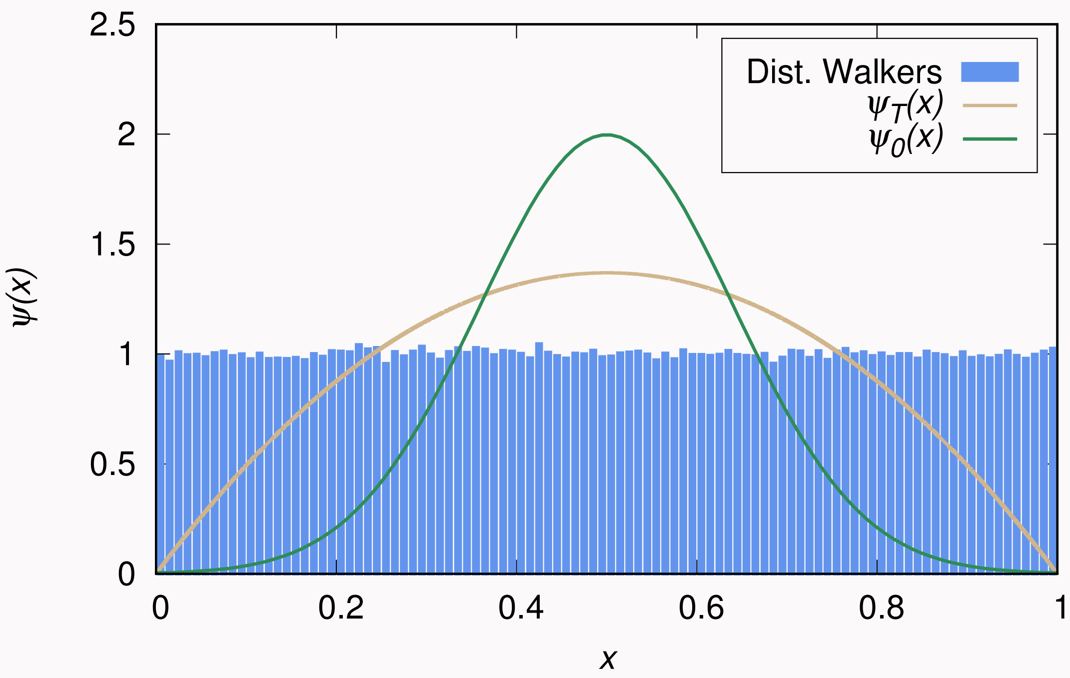
QMC Methods - An Example

First, VMC equilibration:

$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step $n = 0$





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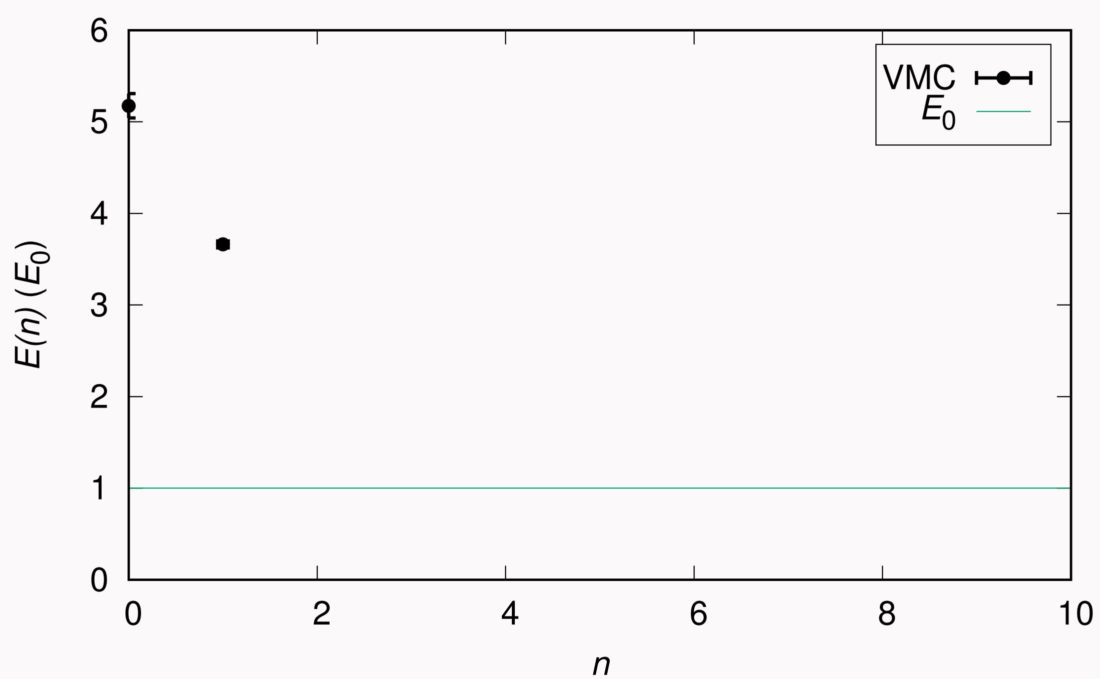
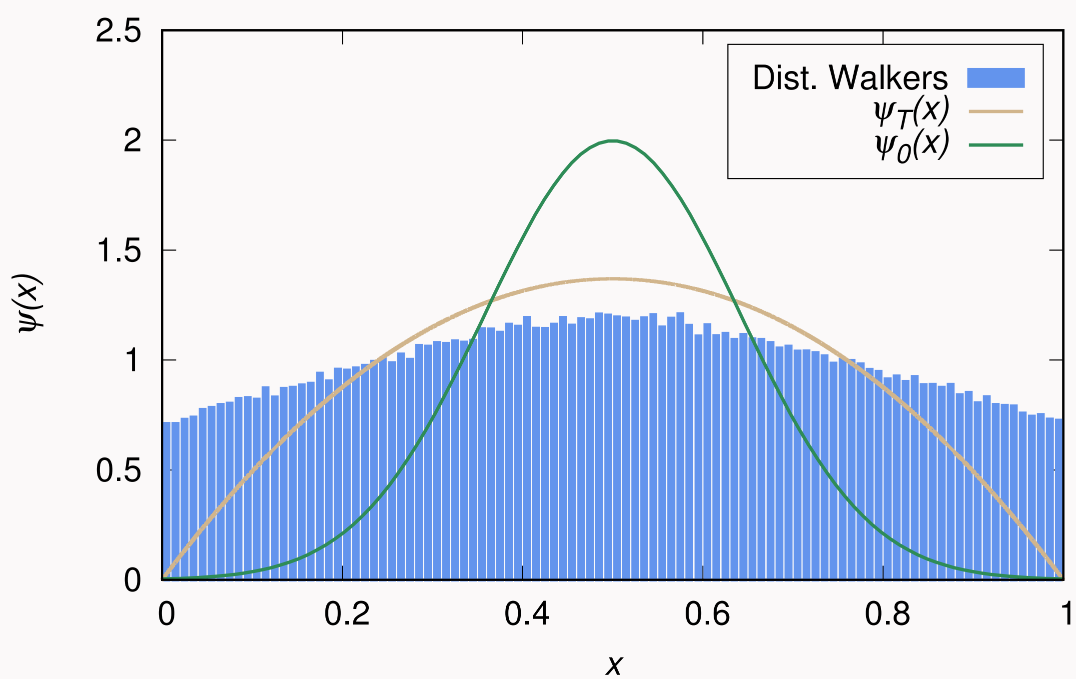
Metropolis step $n = 1$





QMC Methods - An Example

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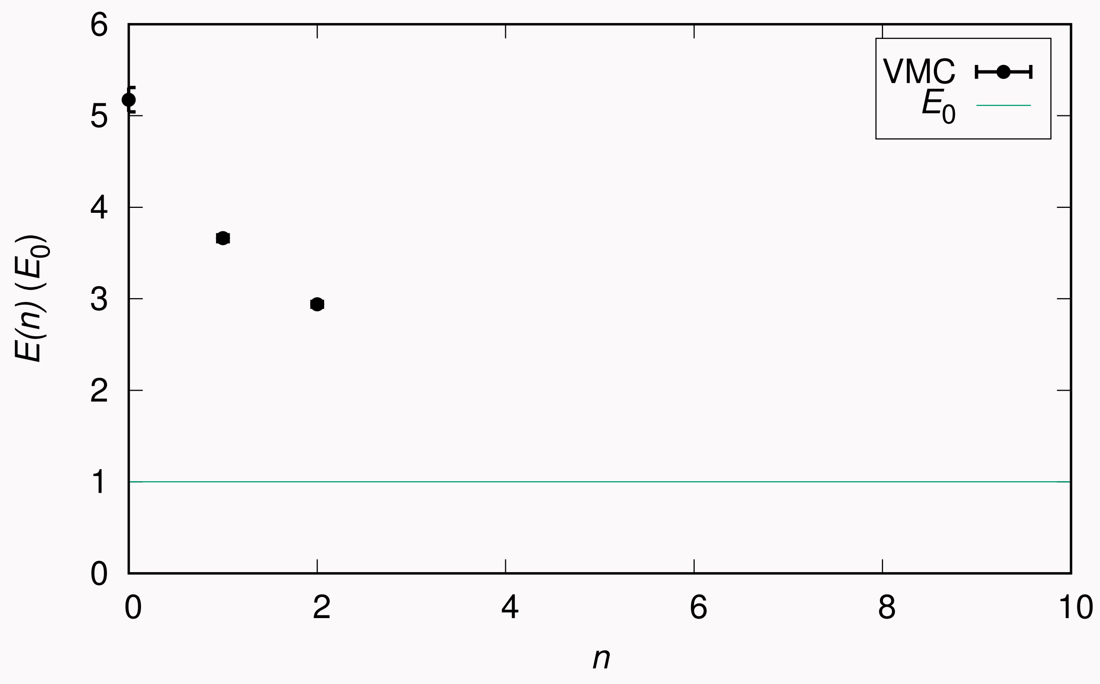
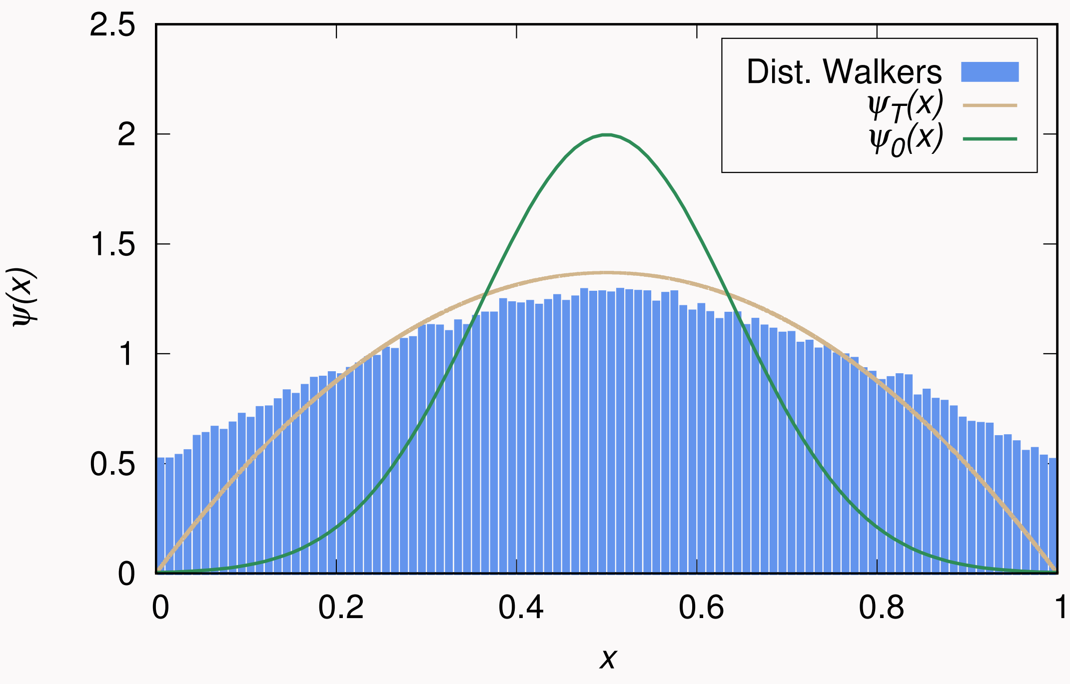
Metropolis step $n = 2$



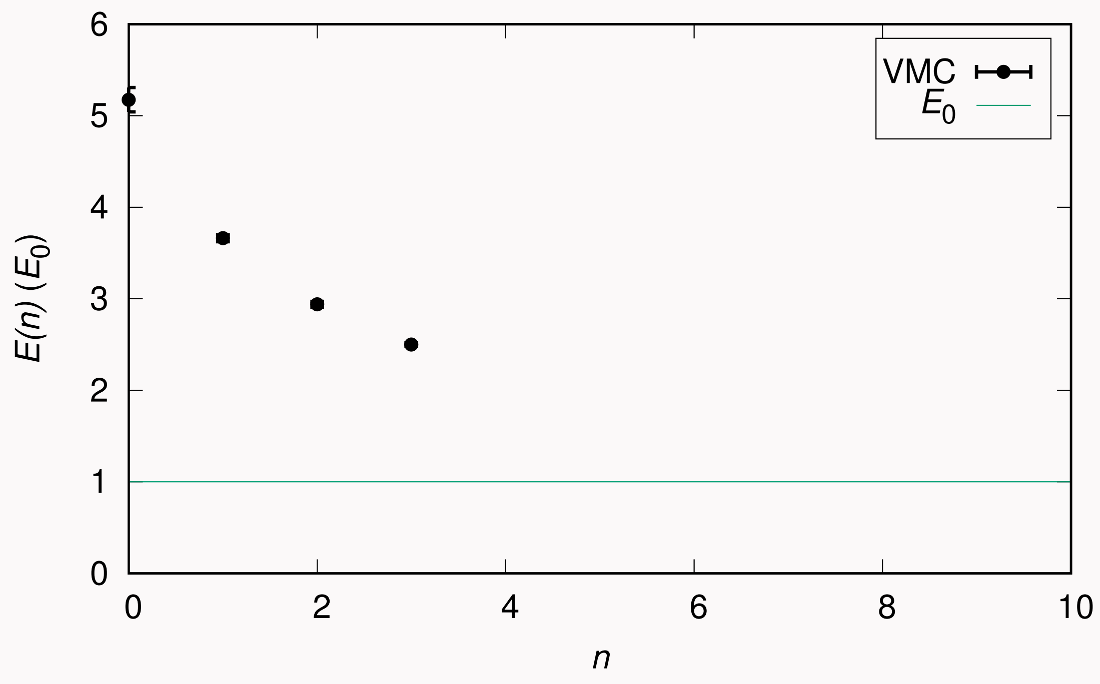


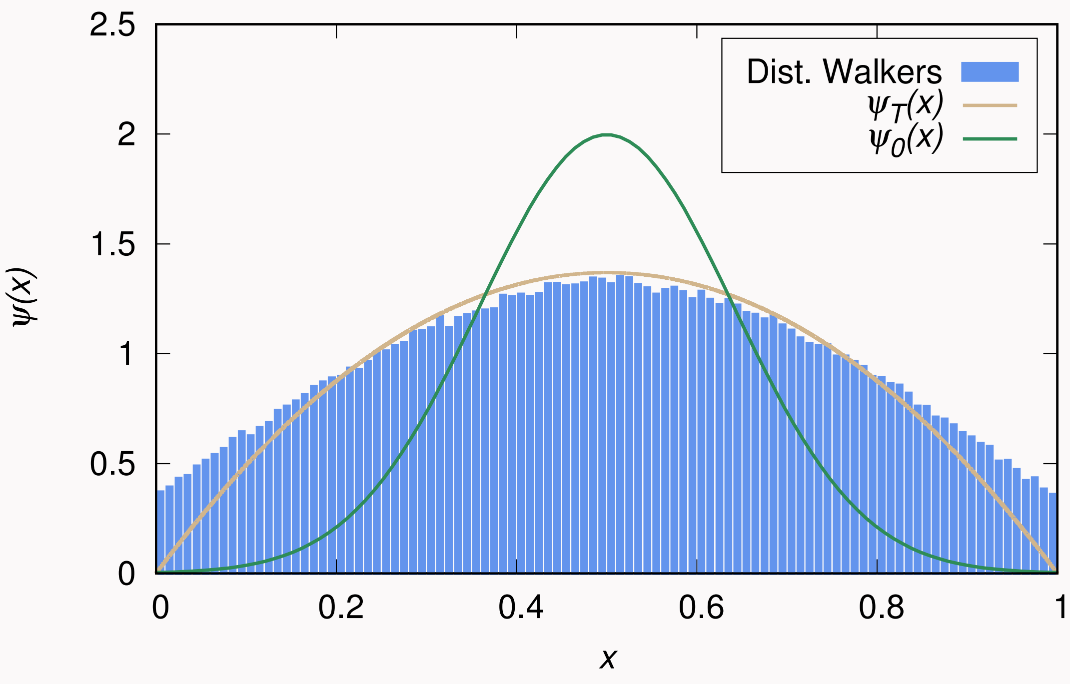
QMC Methods - An Example

First, VMC equilibration:

$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step $n = 3$



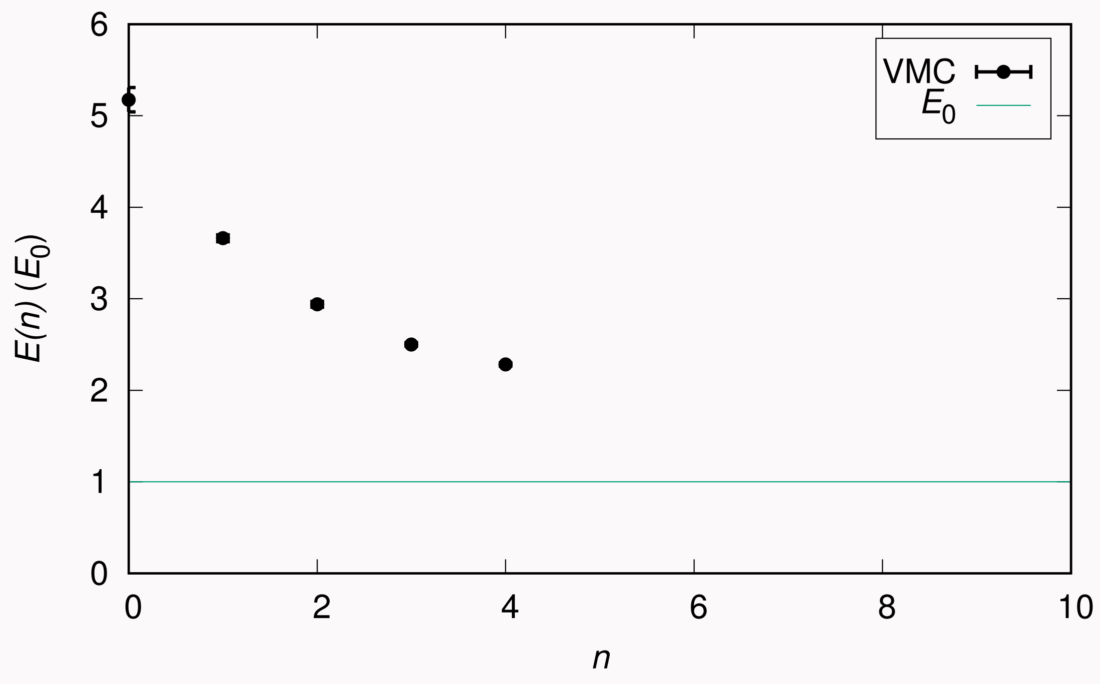


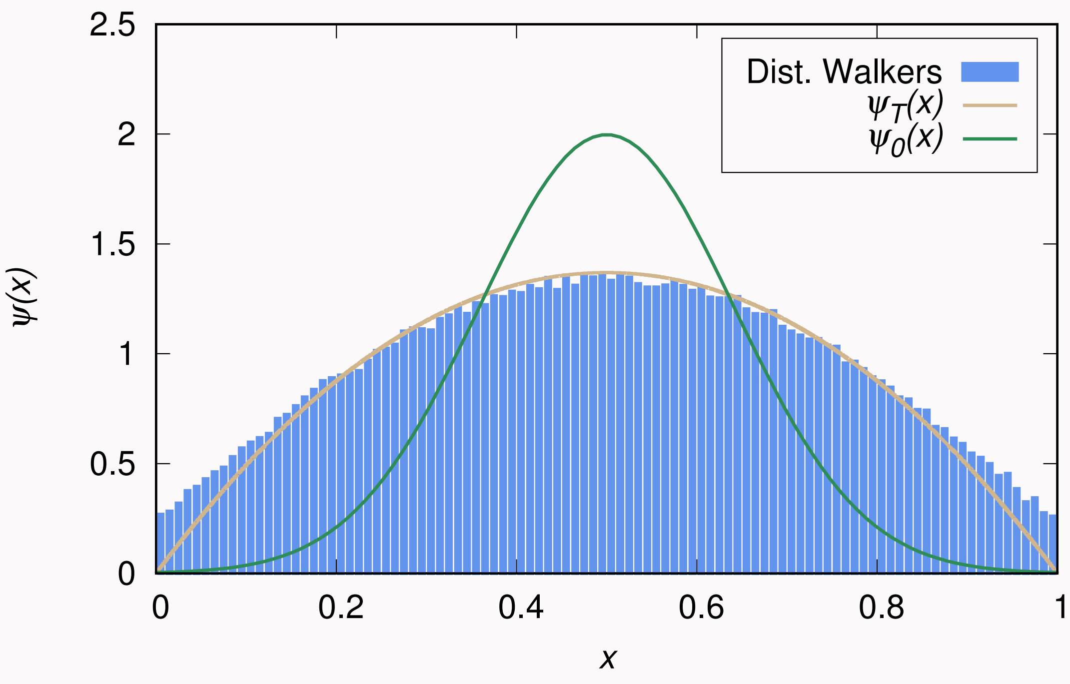
QMC Methods - An Example

First, VMC equilibration:

$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step $n = 4$



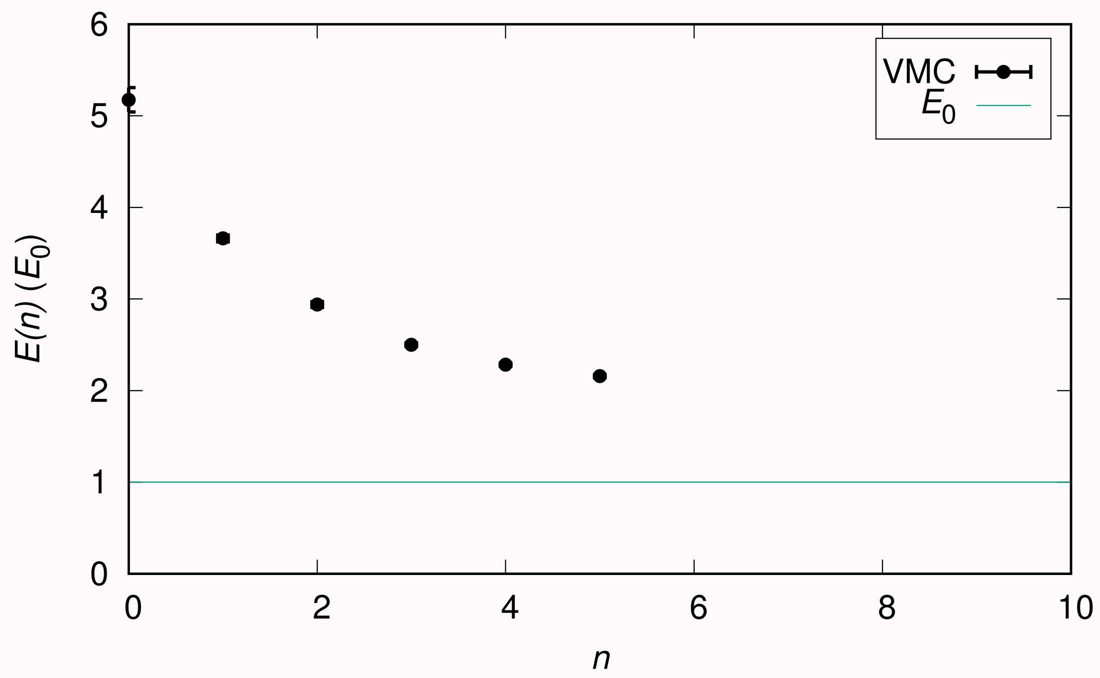


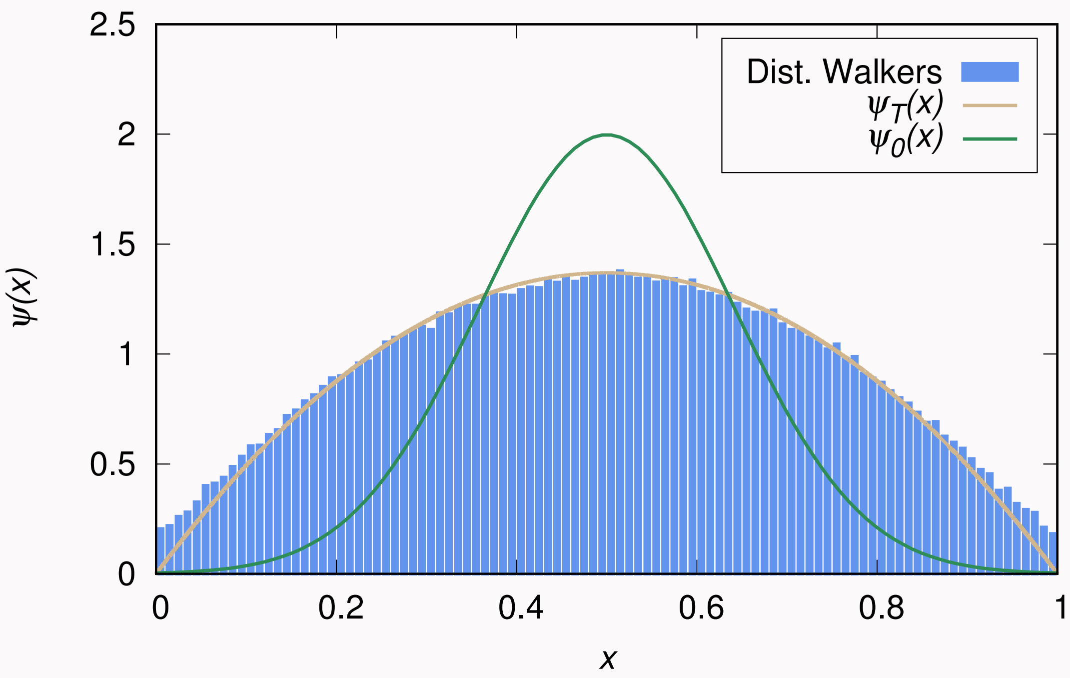
QMC Methods - An Example

First, VMC equilibration:

$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step $n = 5$





QMC Methods - An Example

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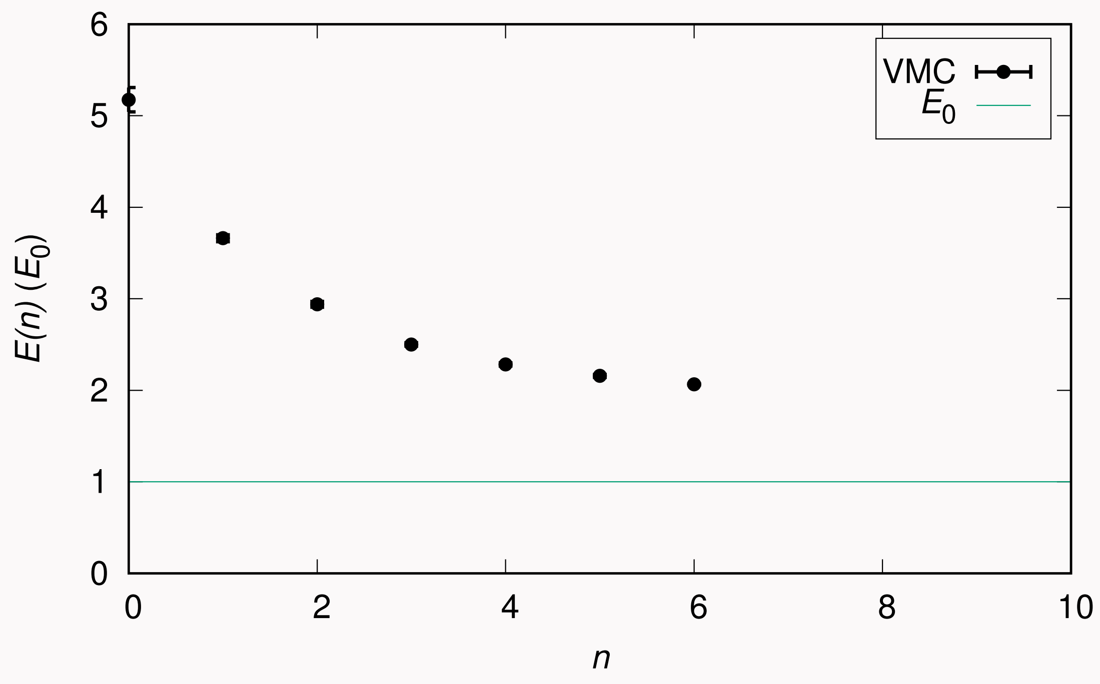
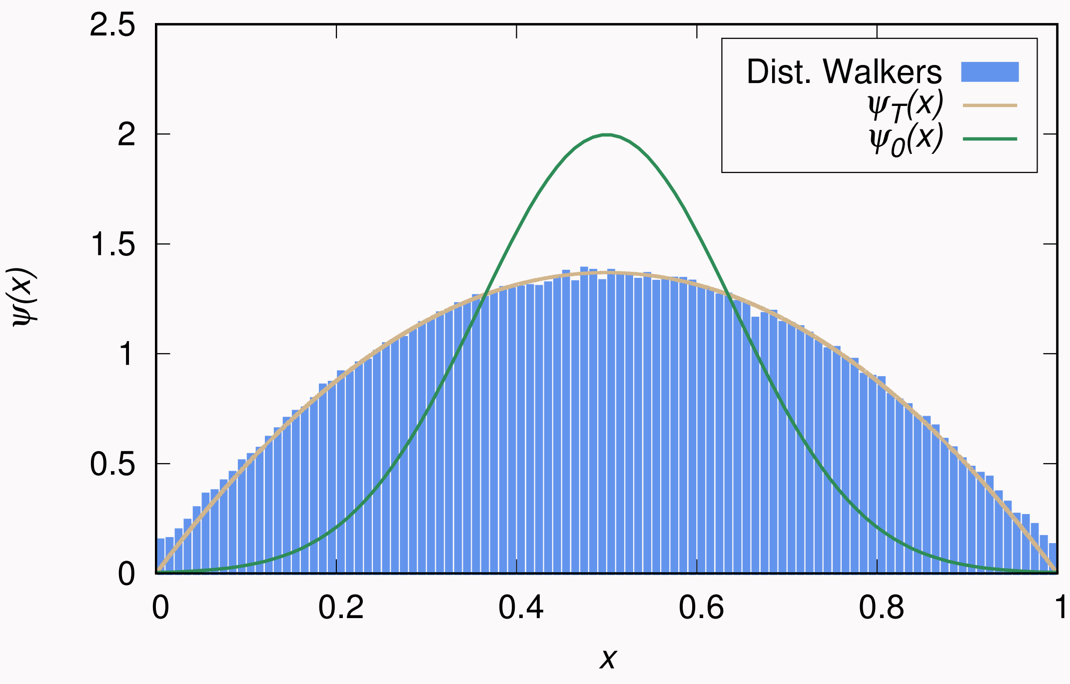
$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step $n = 6$





QMC Methods - An Example

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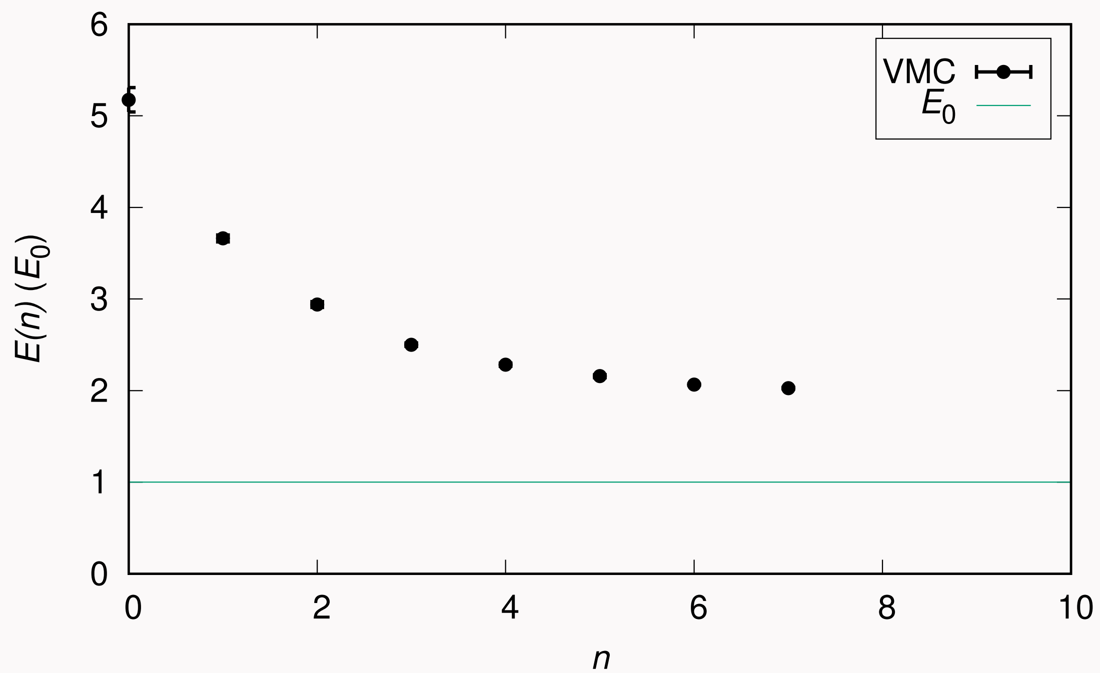
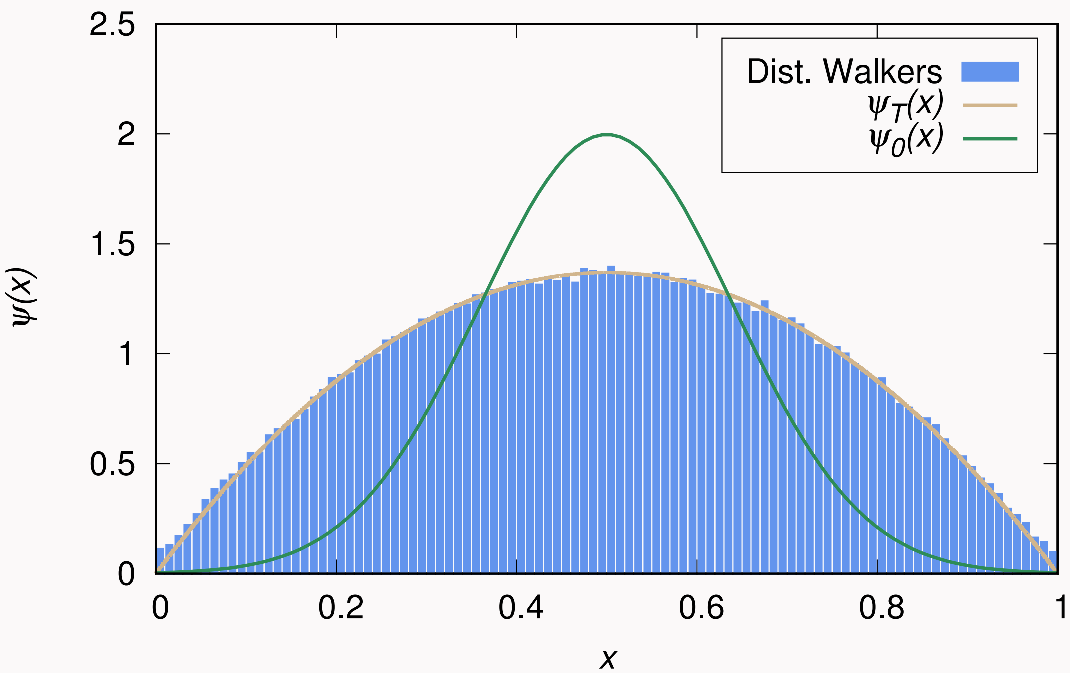
Metropolis step $n = 7$





QMC Methods - An Example

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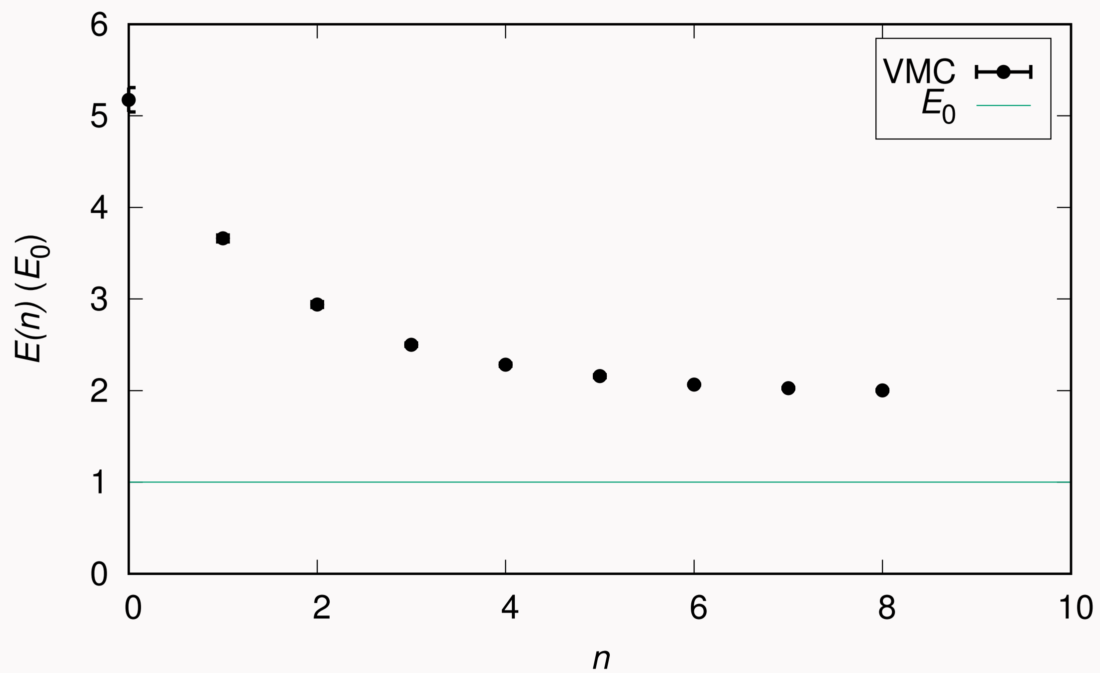
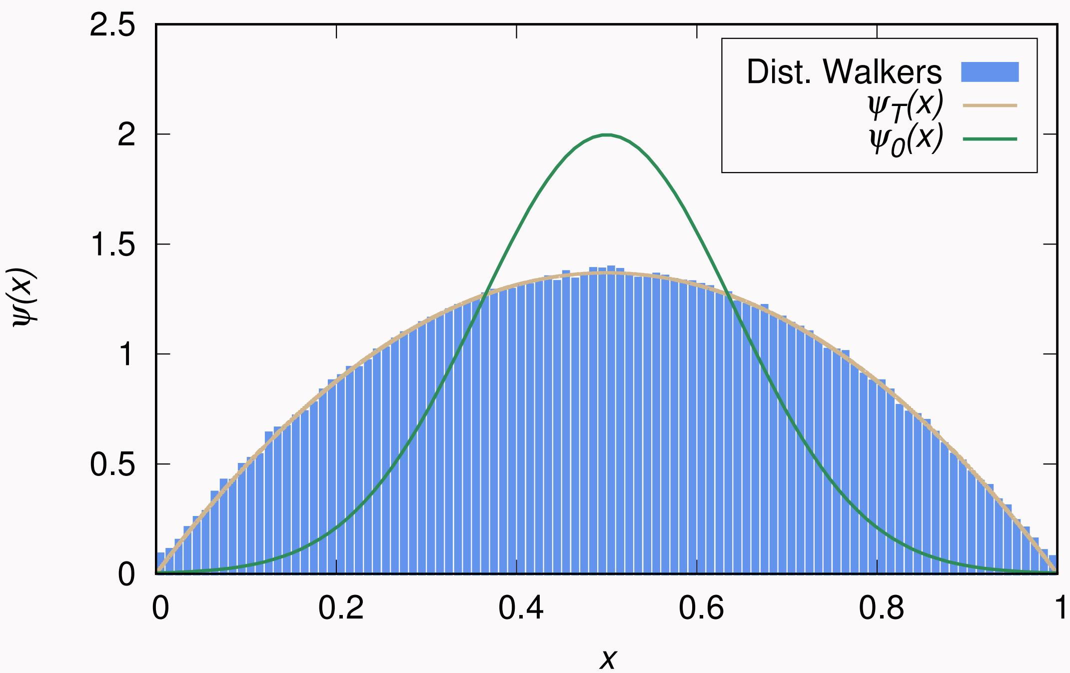
$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step $n = 8$





QMC Methods - An Example

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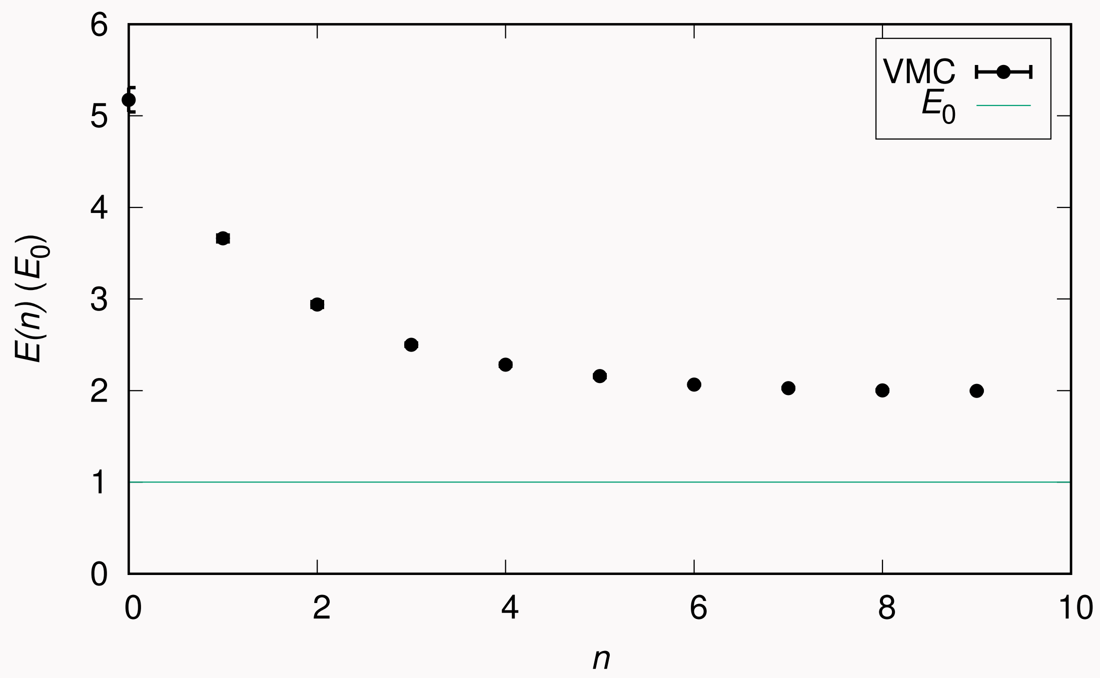
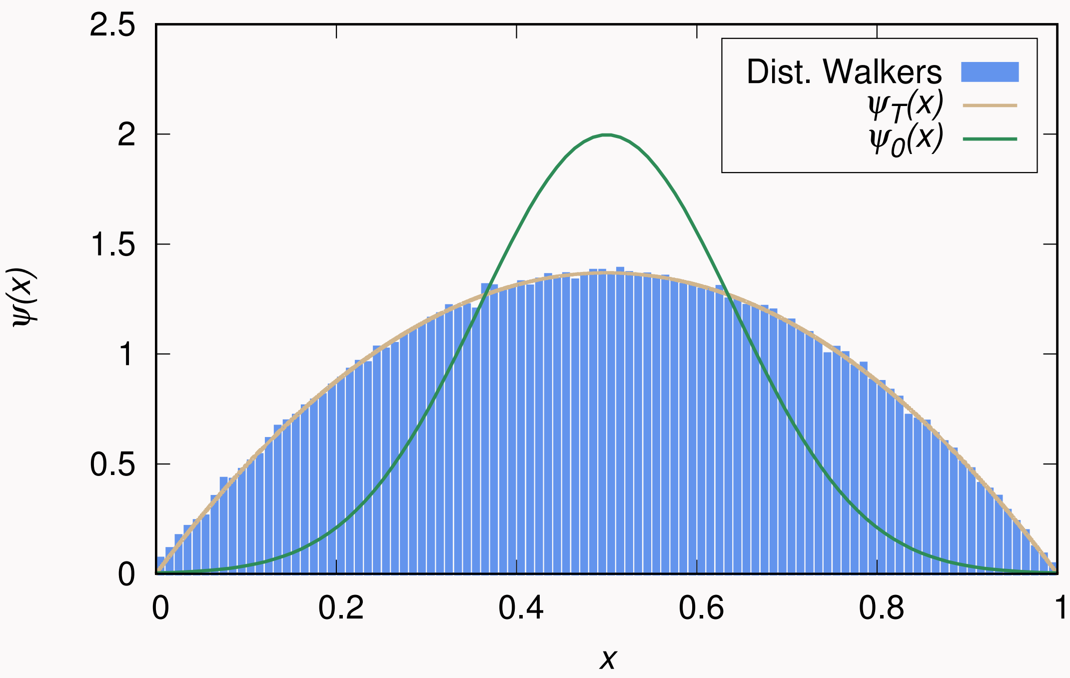
Metropolis step $n = 9$





QMC Methods - An Example

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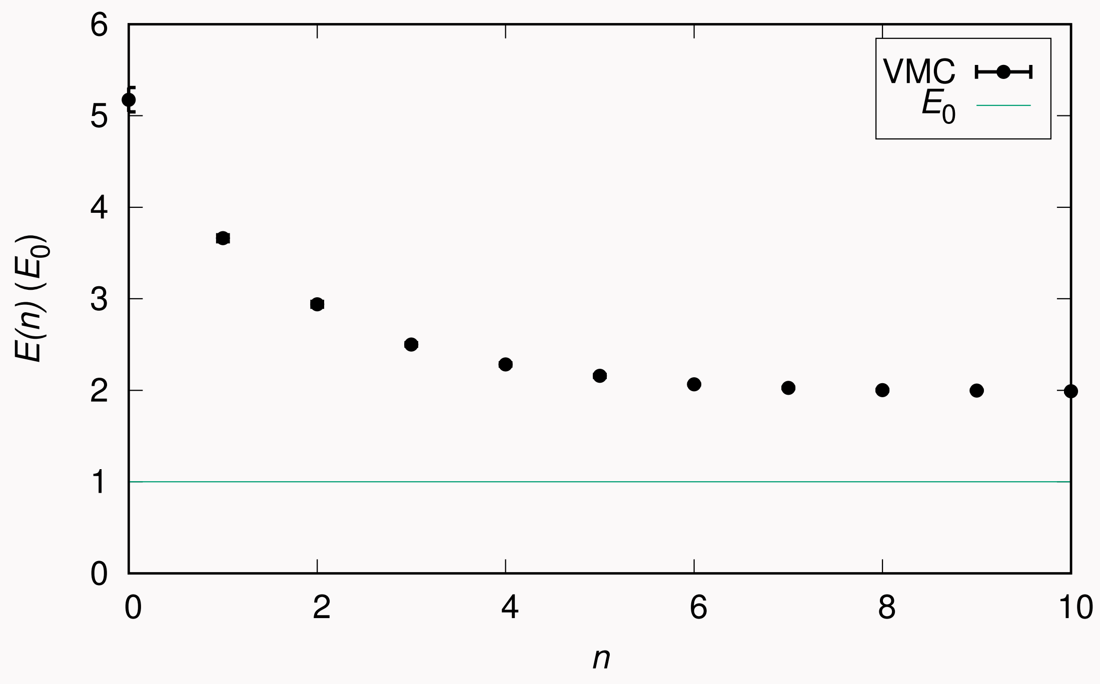
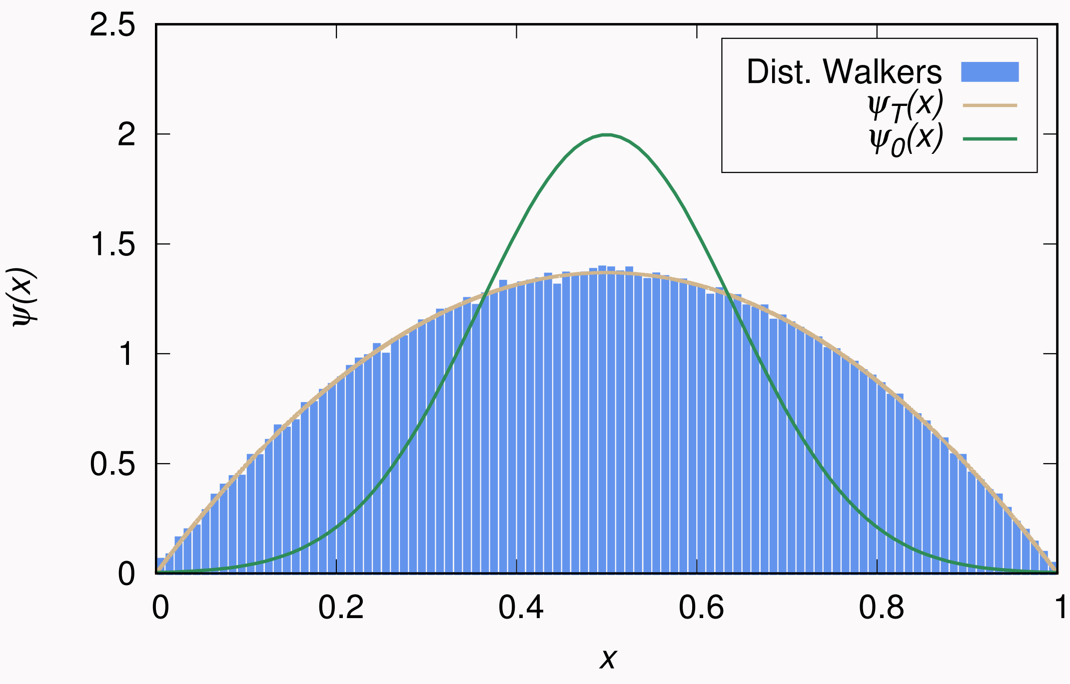
$$\frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

Metropolis step n =10



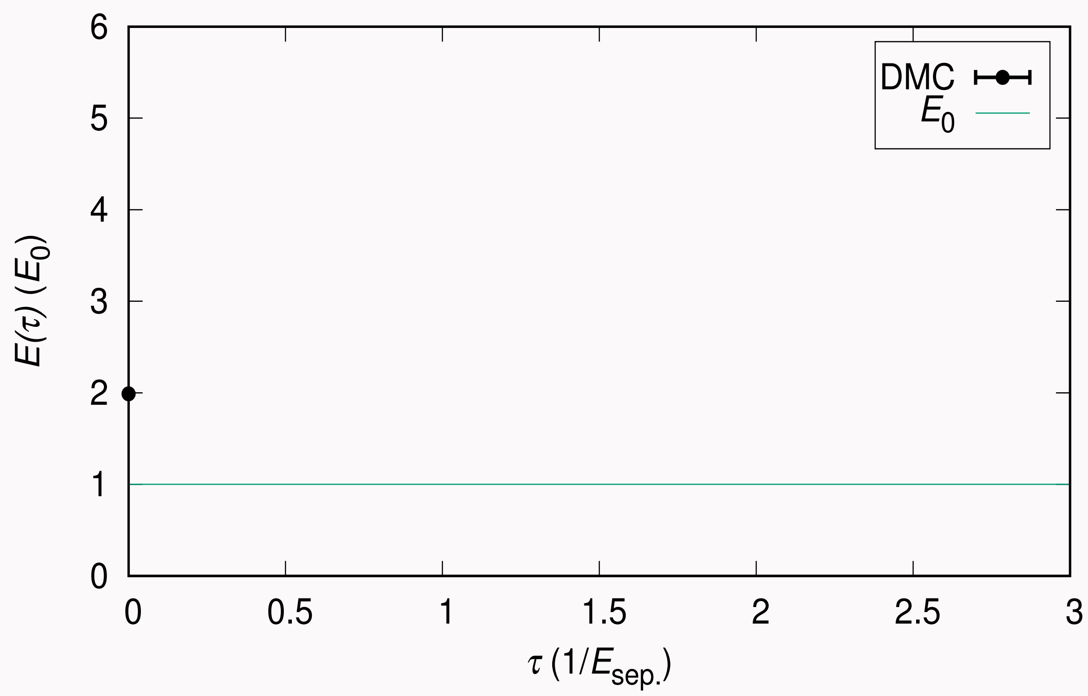


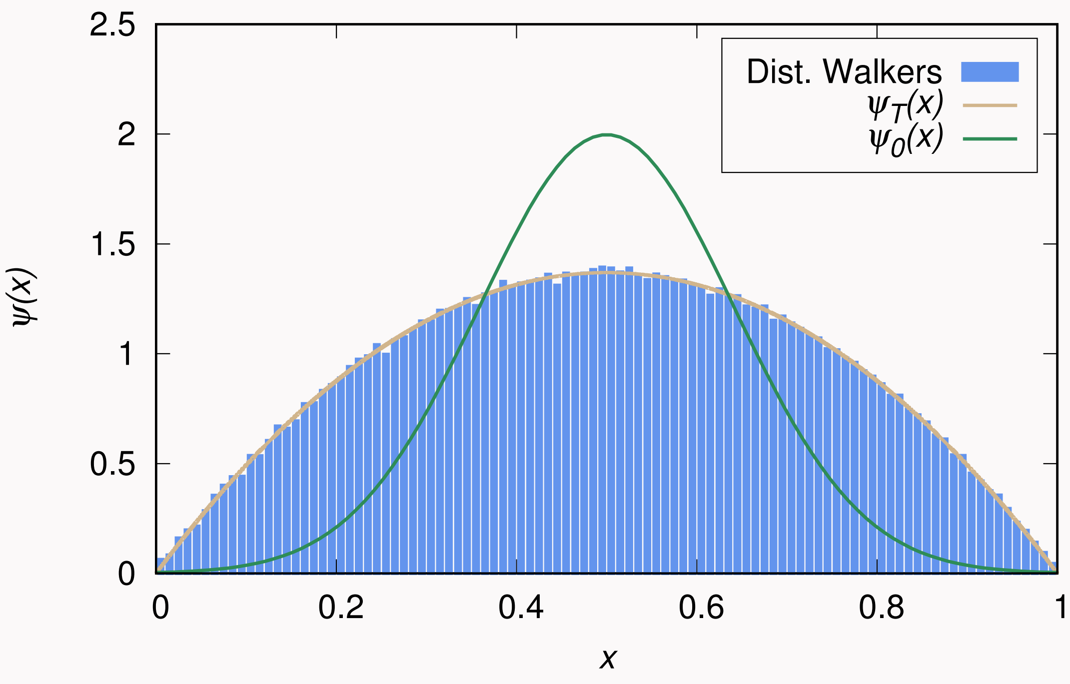
QMC Methods - An Example

Now, imaginary-time evolution:

$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

$$\tau = 0.00(1/E_{\rm sep})$$





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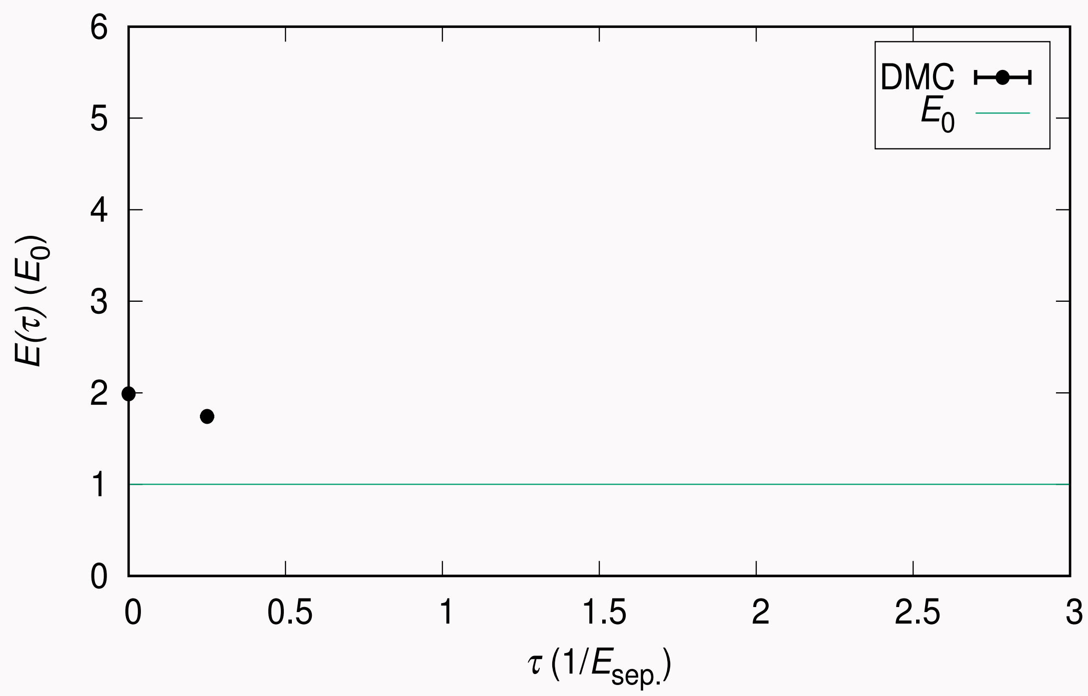
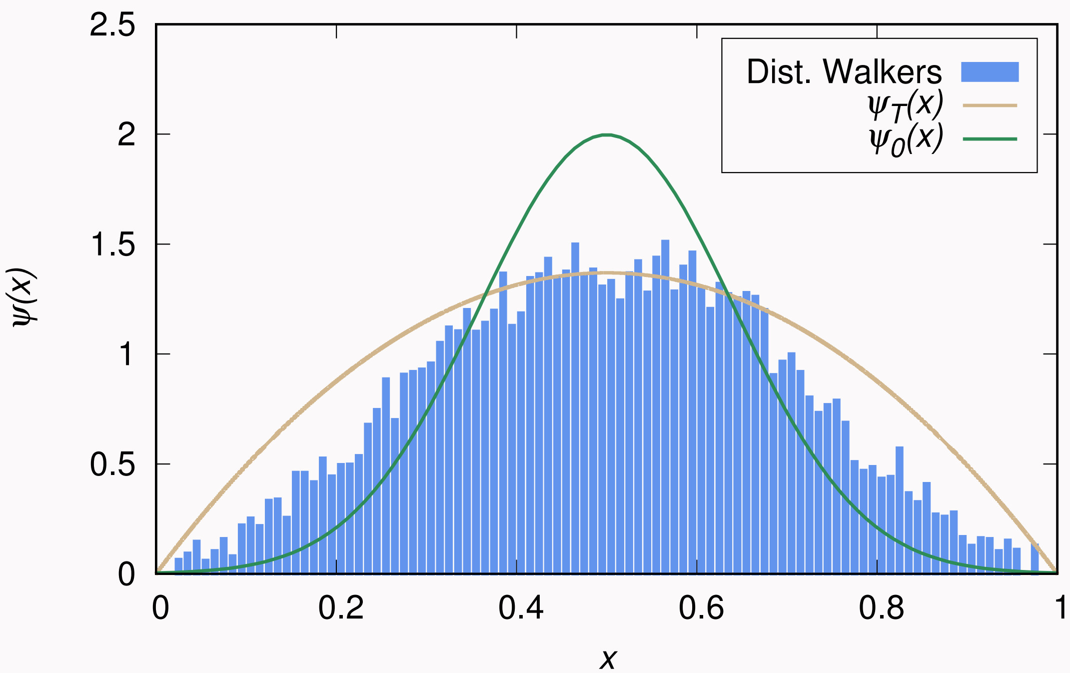
$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

$$\tau = 0.25\,(1/E_{\text{sep}})$$





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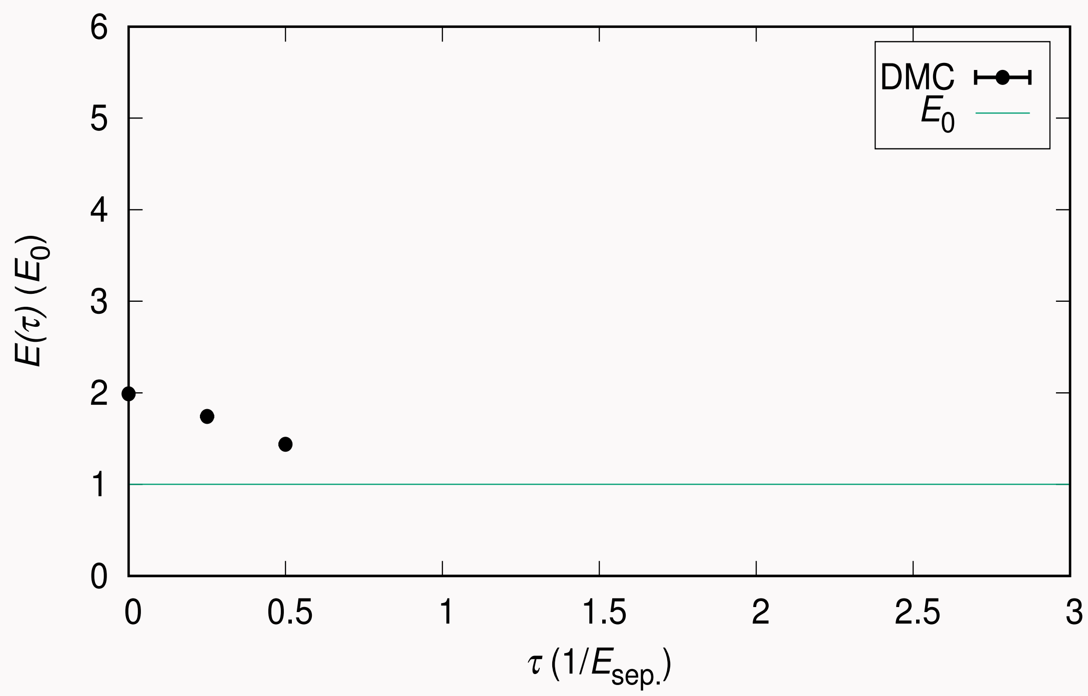
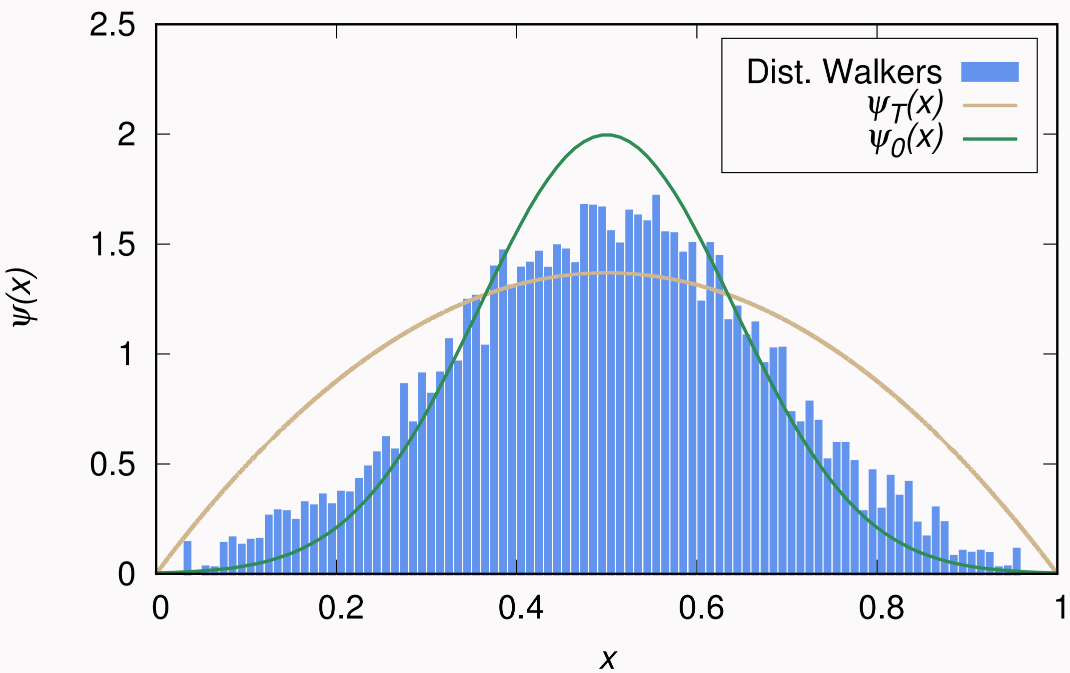
$$\tau = 0.50\,(1/E_{\rm sep})$$





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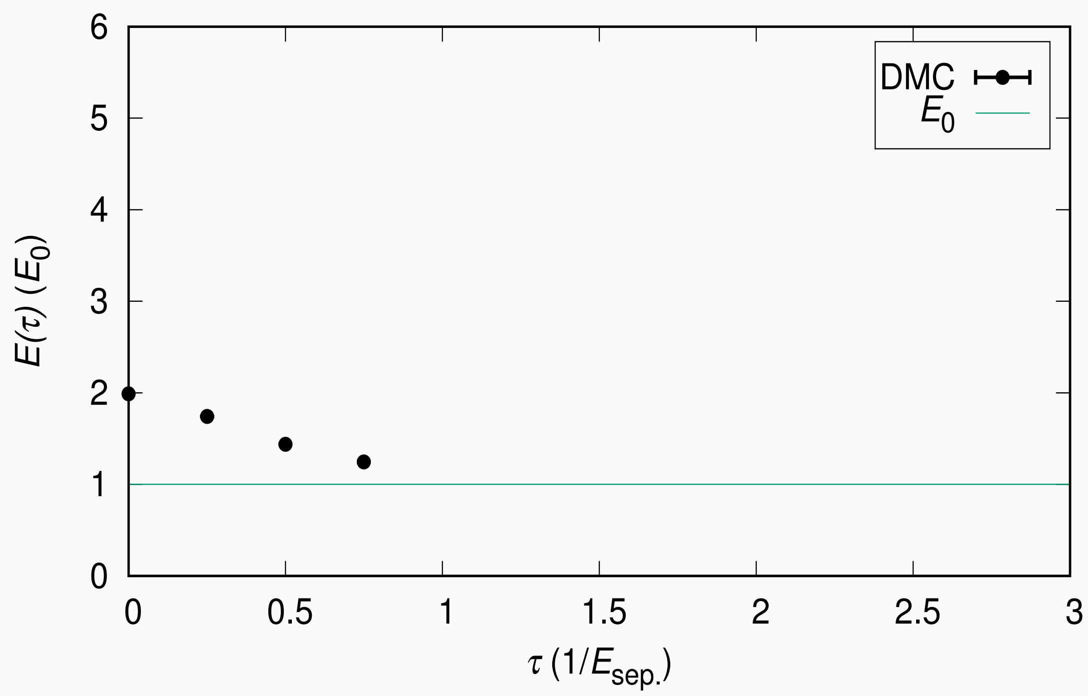
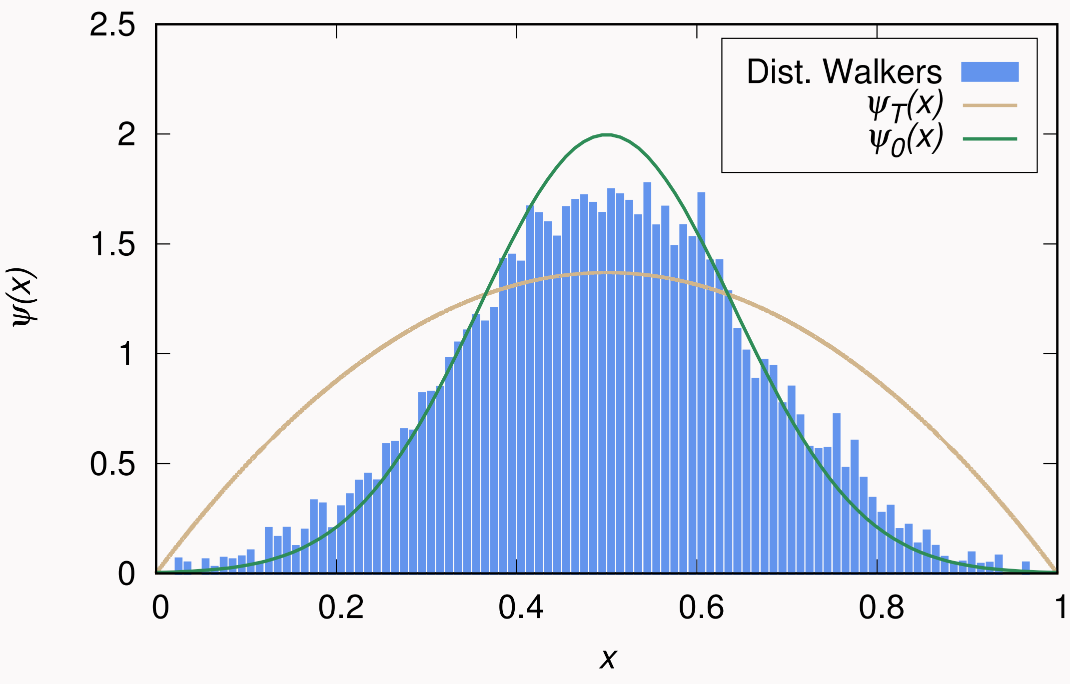
$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

$$\tau = 0.75\ (1/E_{\mathrm{sep}})$$





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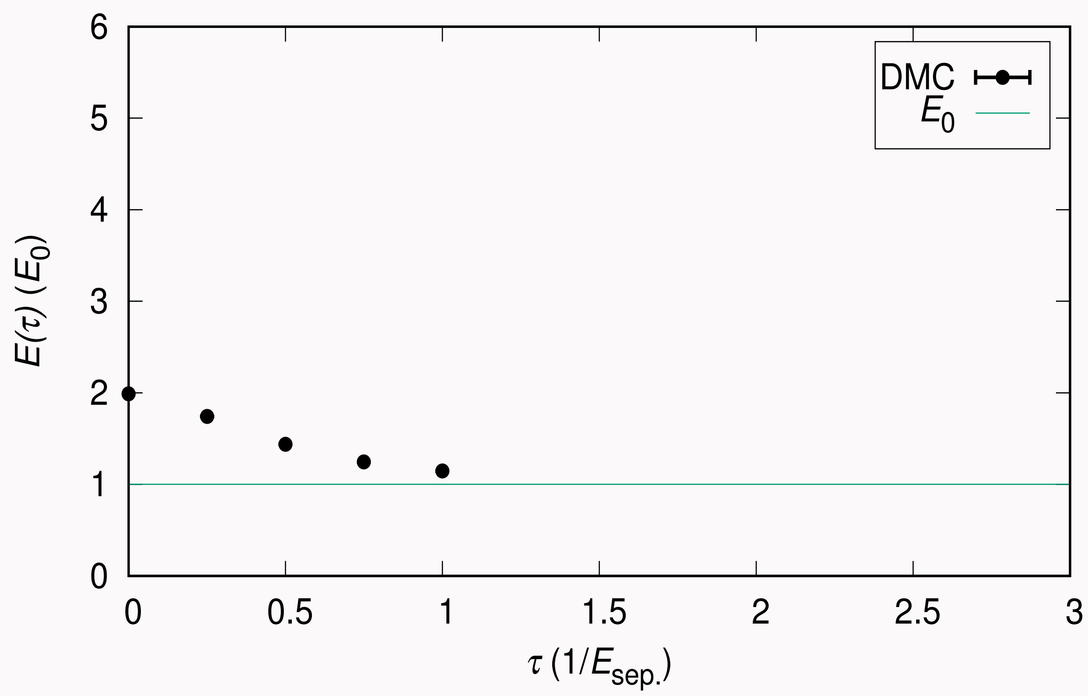
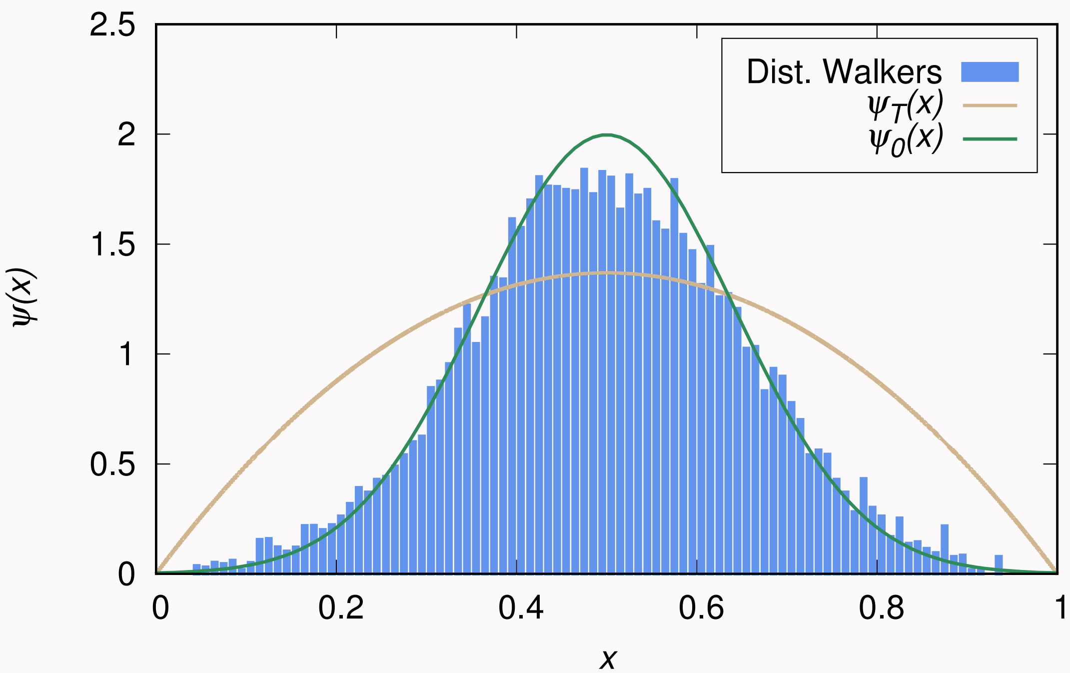
$$\tau = 1.00(1/E_{\text{sep}})$$





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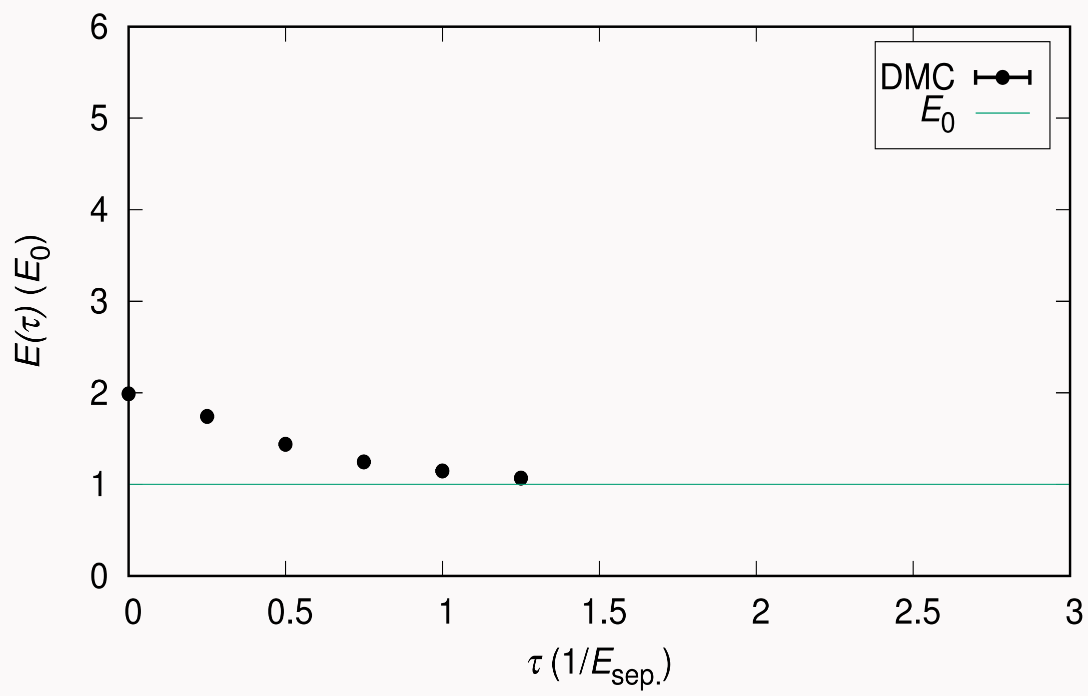

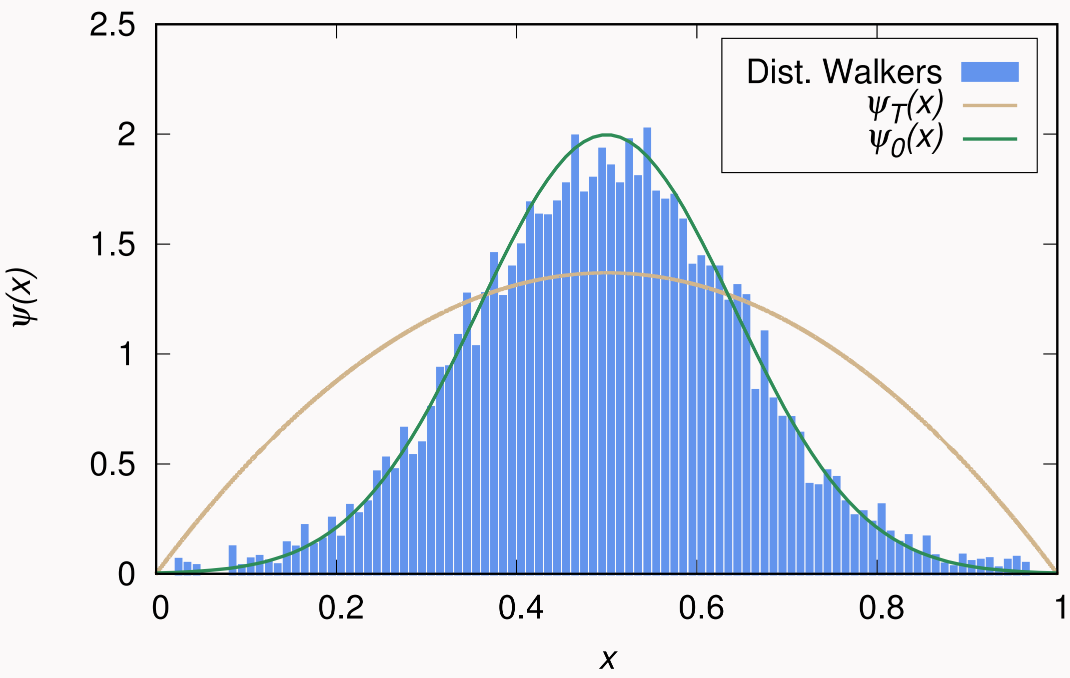

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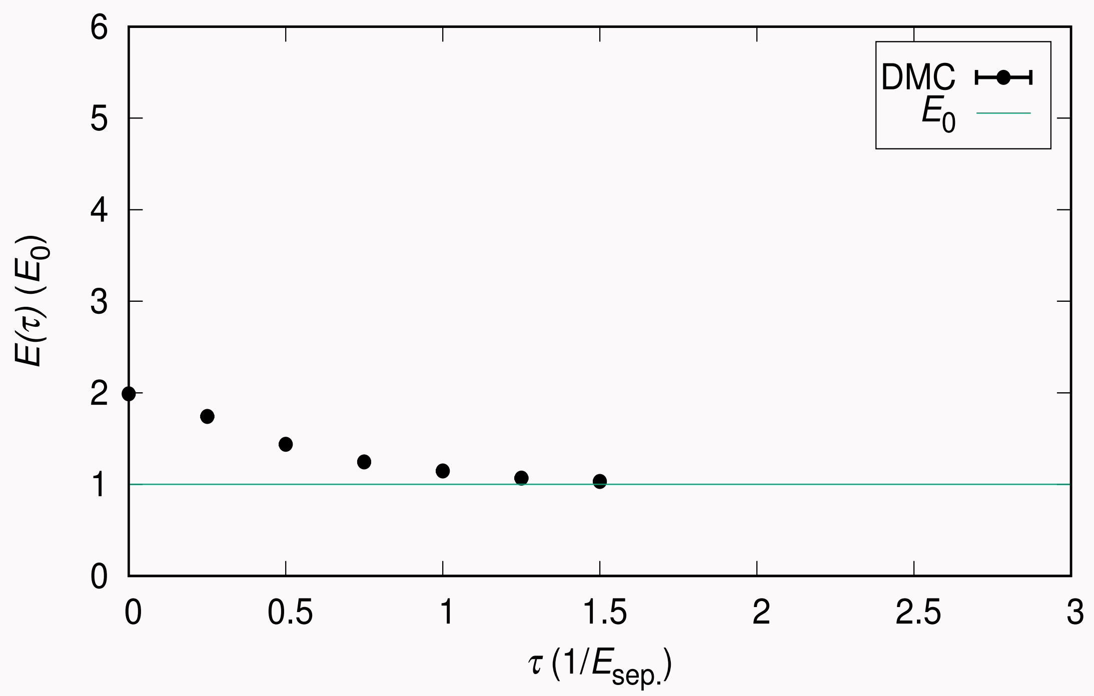

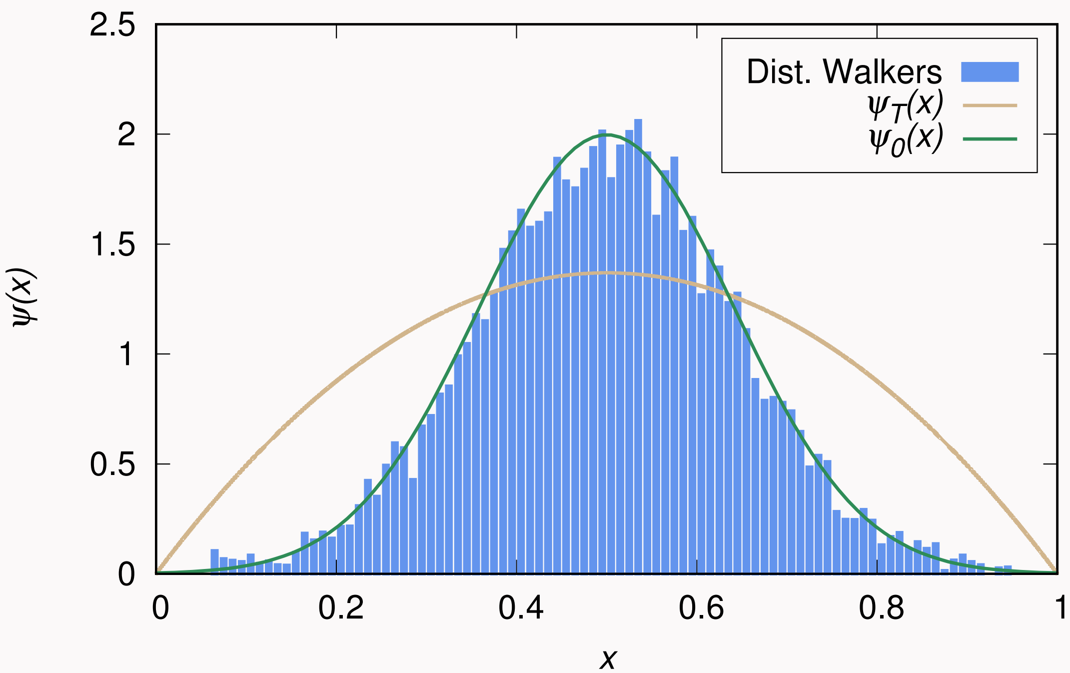

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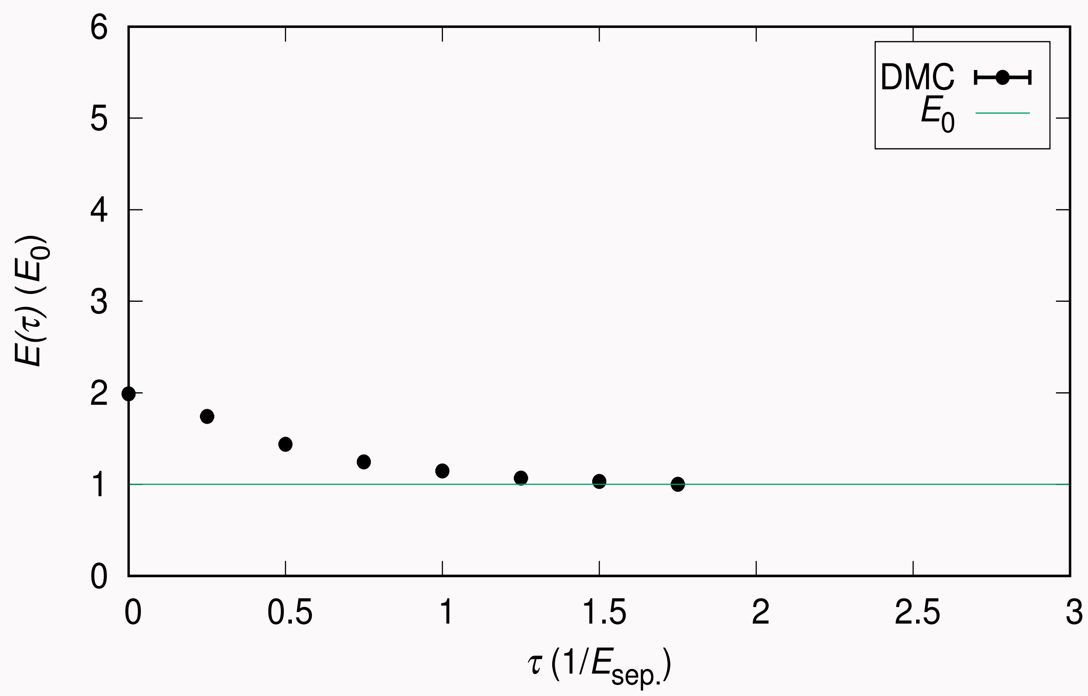

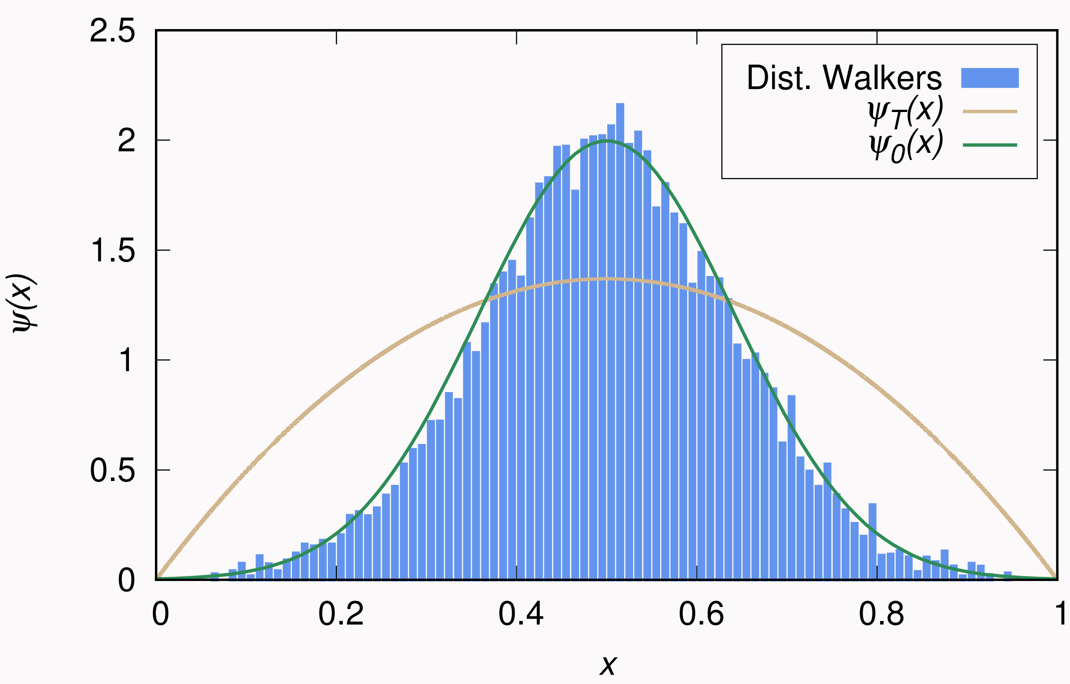

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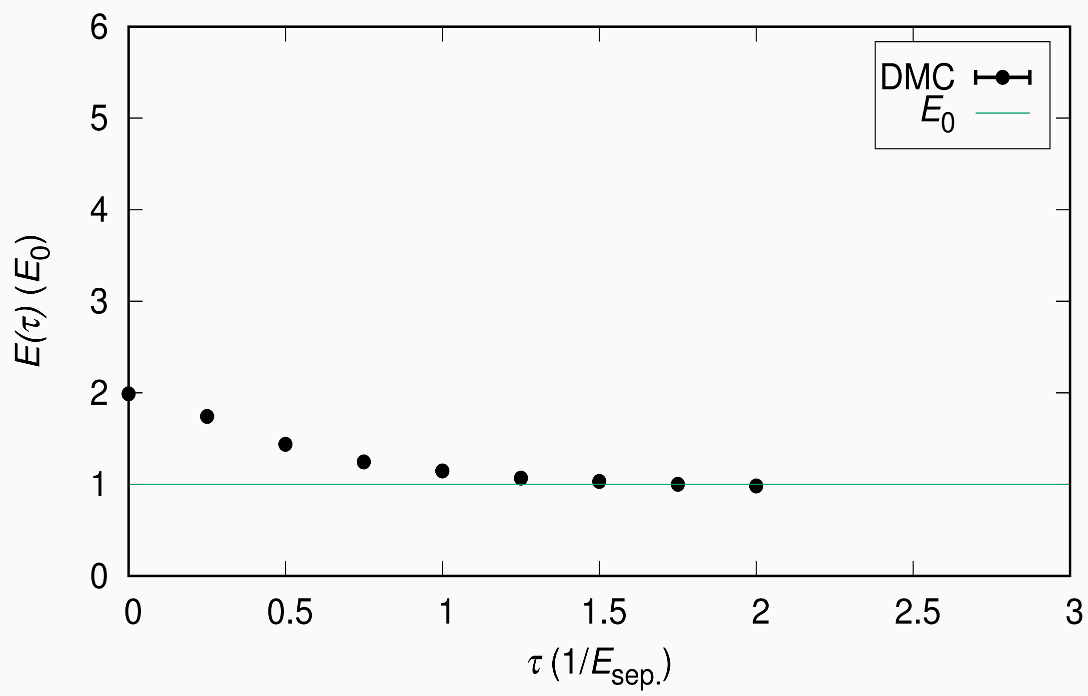
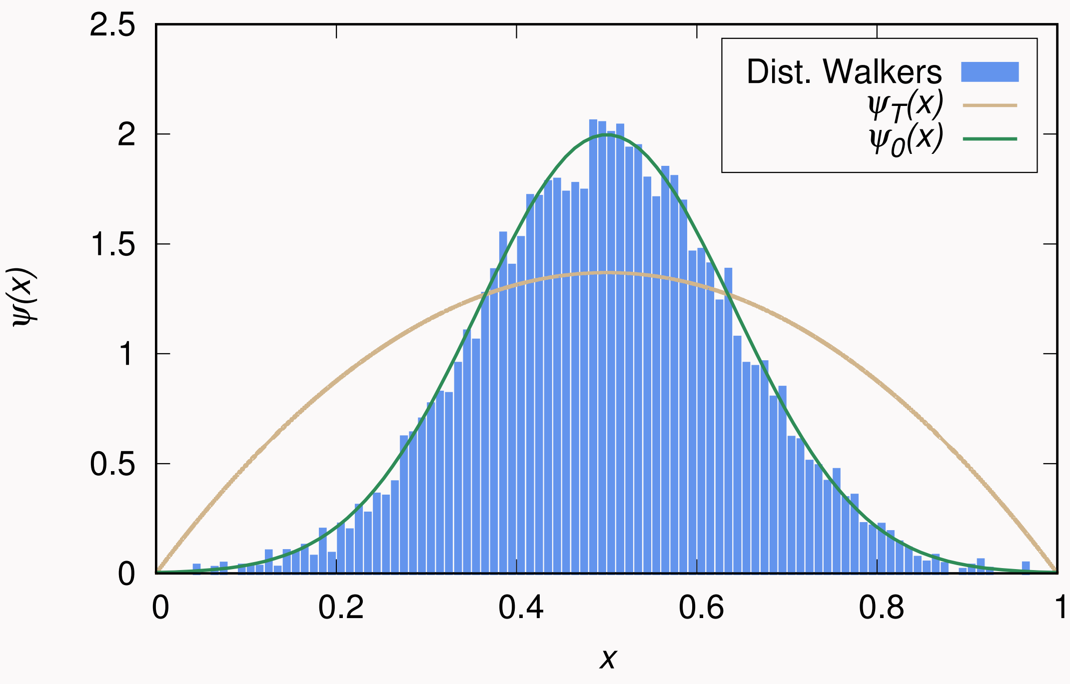
$$\tau = 2.00(1/E_{\mathrm{sep}})$$





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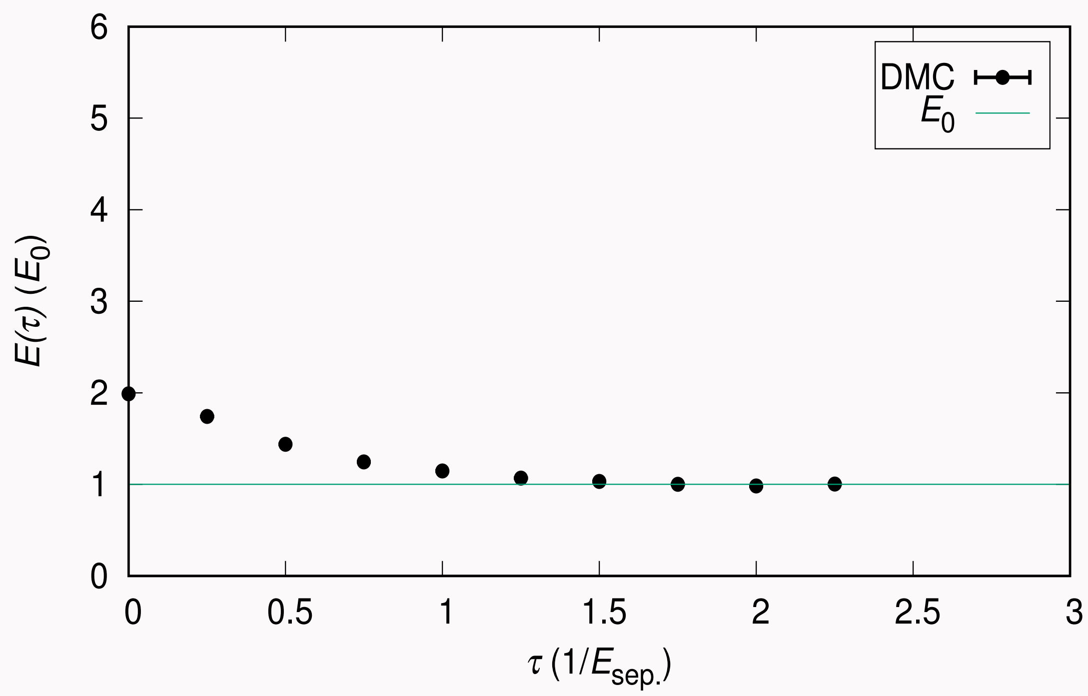
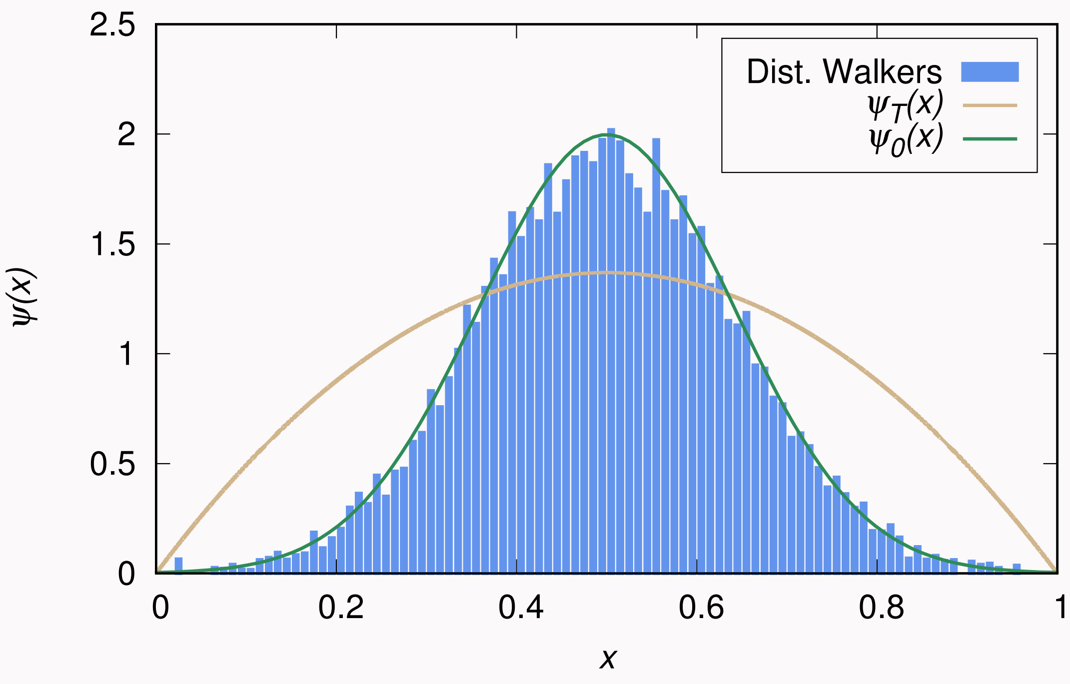
$$\tau = 2.25\,(1/E_{\text{sep}})$$



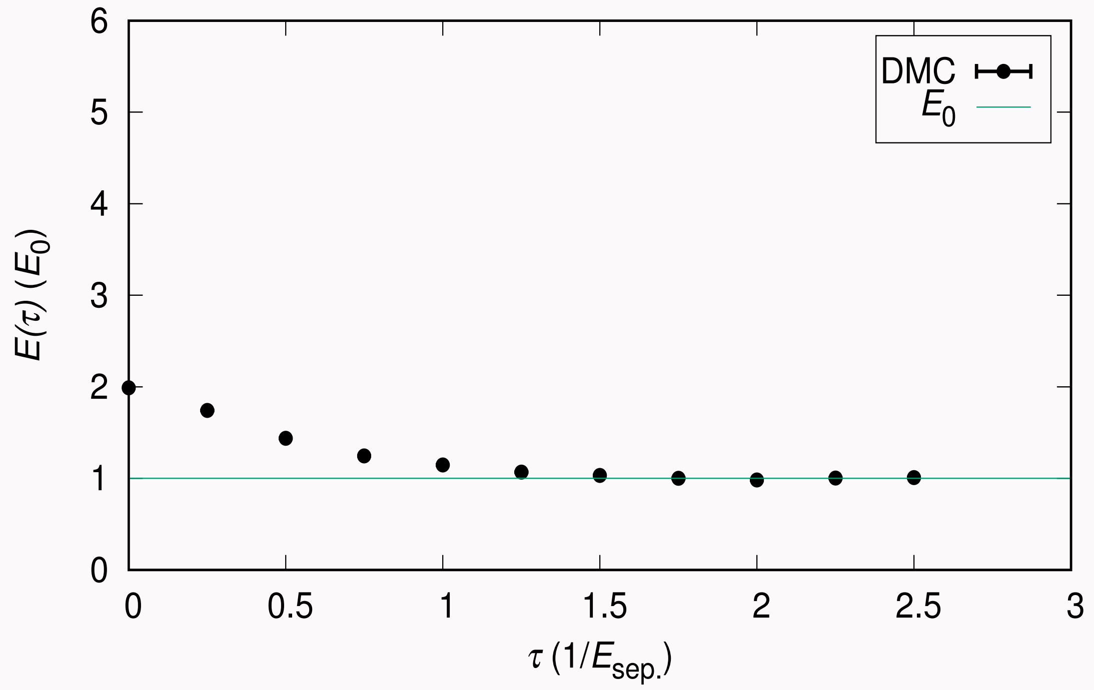


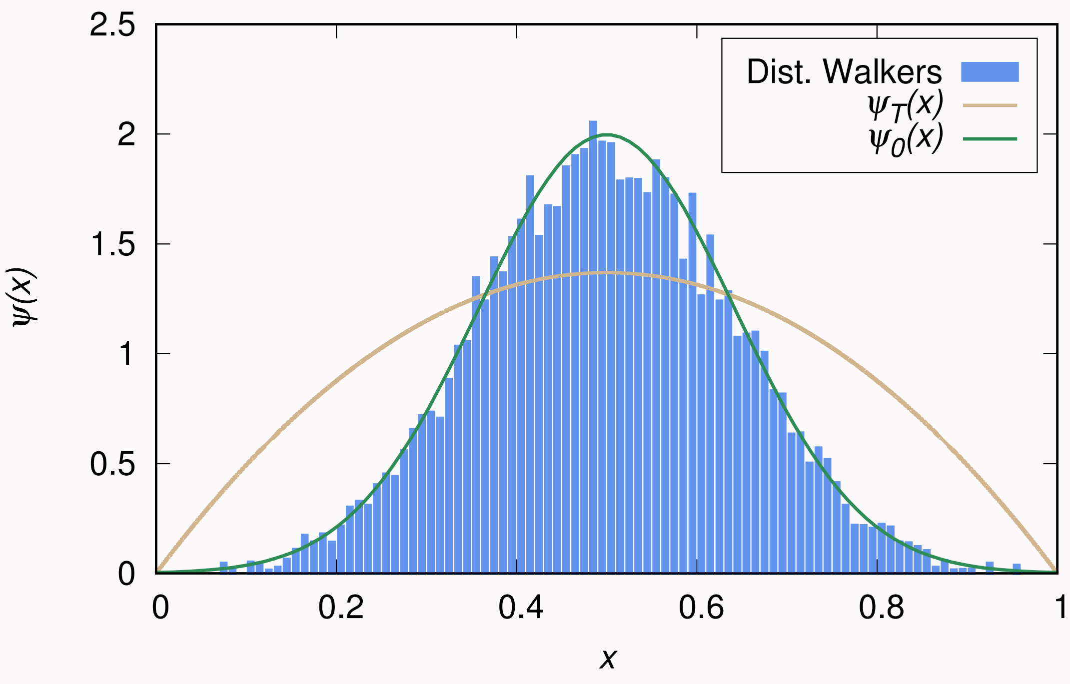
QMC Methods - An Example

Now, imaginary-time evolution:

$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

$$\tau = 2.50\,(1/E_{\text{sep}})$$



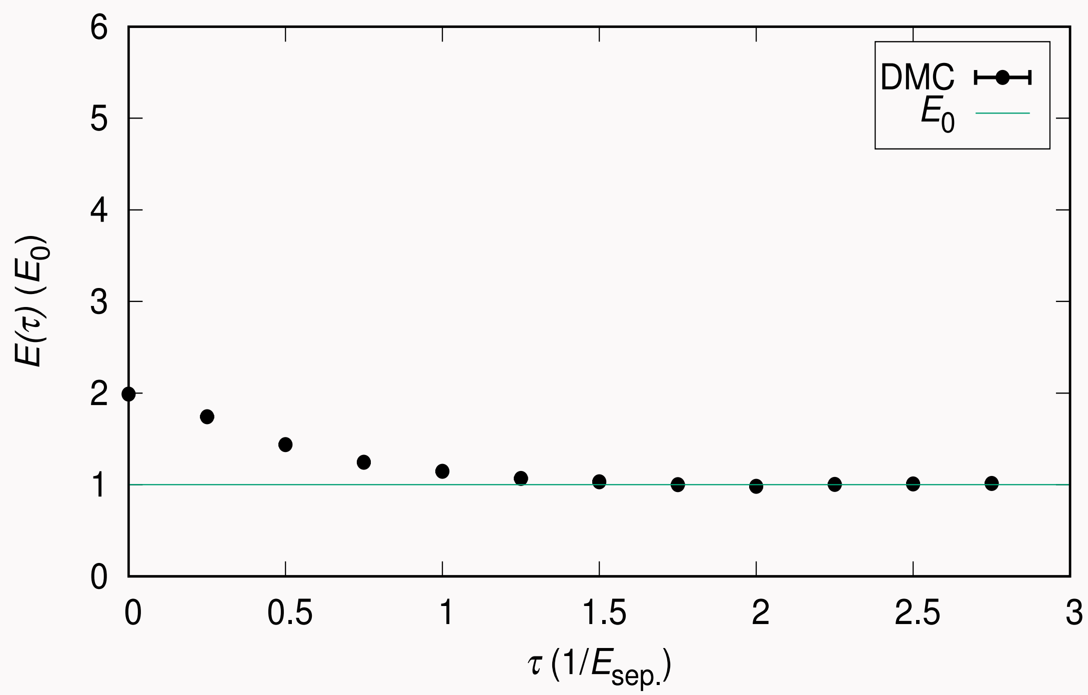


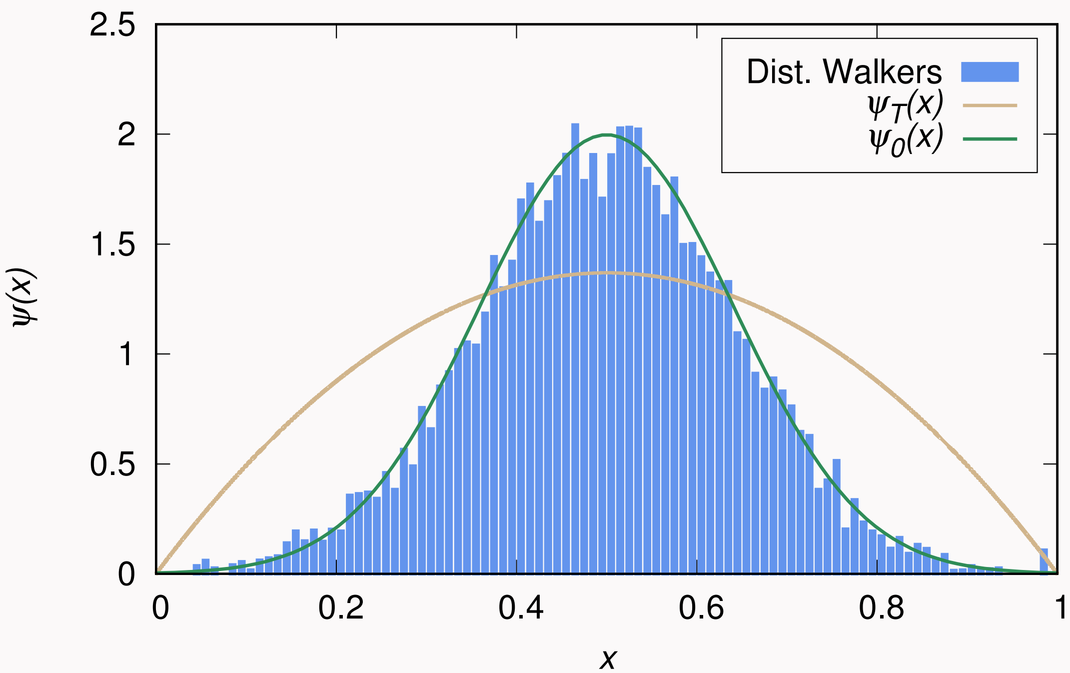
QMC Methods - An Example

Now, imaginary-time evolution:

$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

$$\tau = 2.75\,(1/E_{\text{sep}})$$



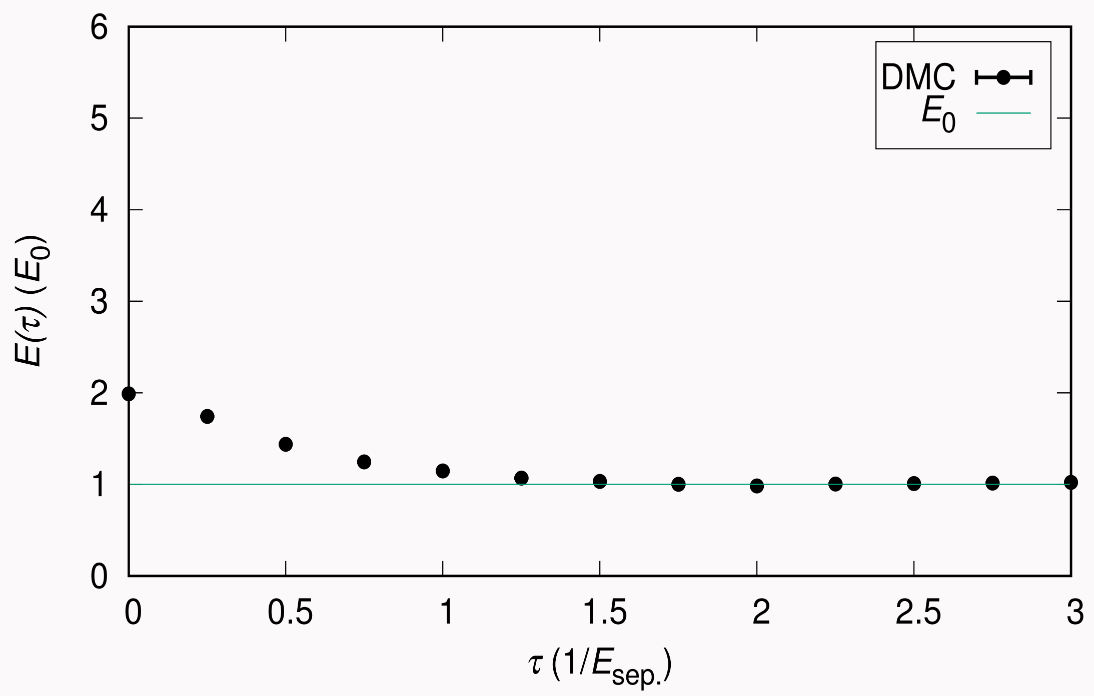


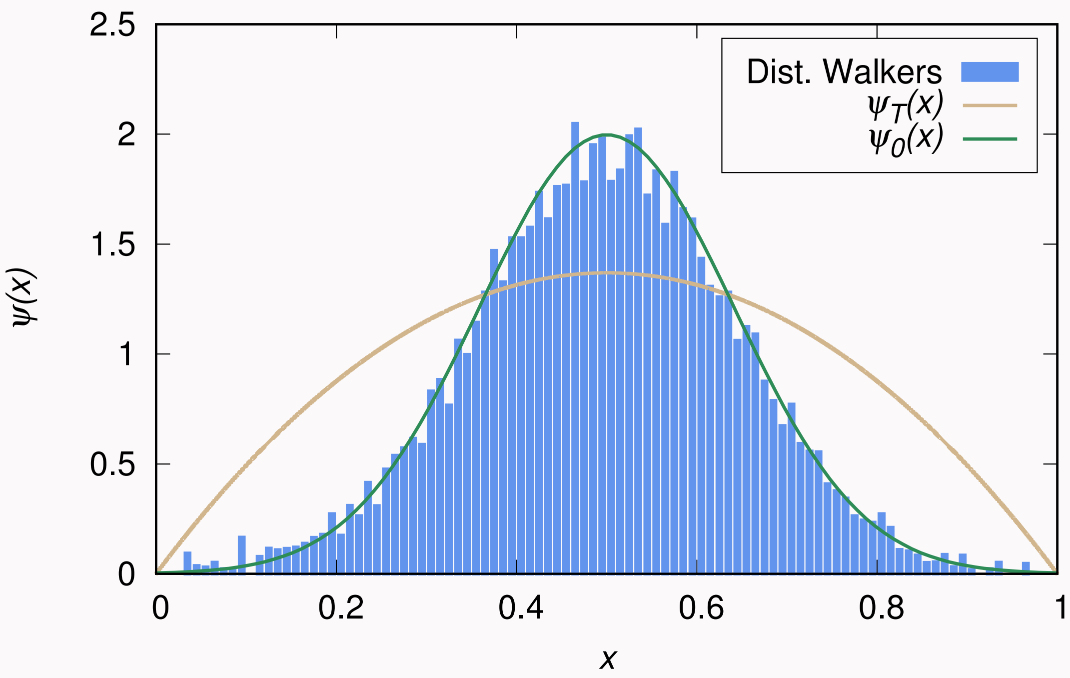
QMC Methods - An Example

Now, imaginary-time evolution:

$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

$$\tau = 3.00(1/E_{\text{sep}})$$



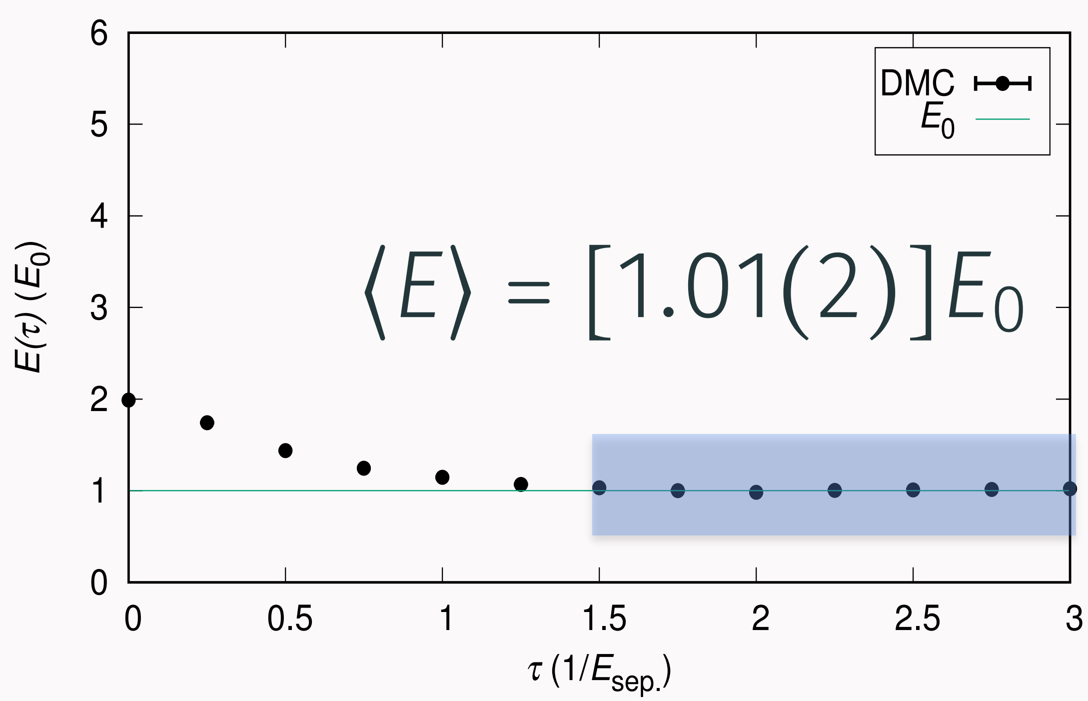


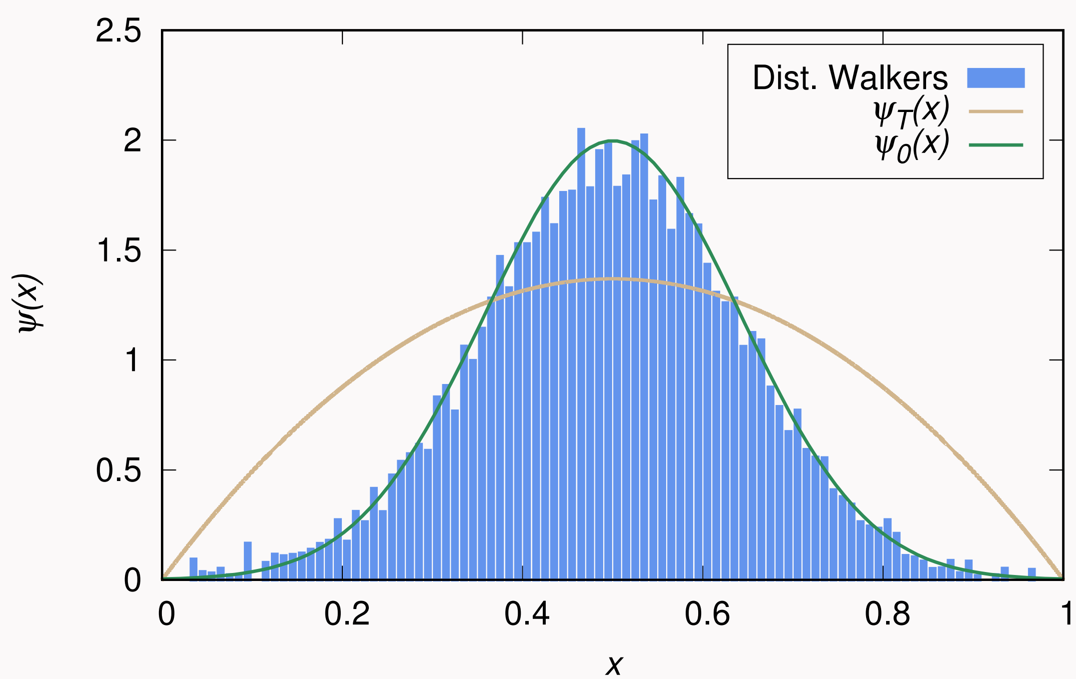
QMC Methods - An Example

Now, imaginary-time evolution:

$$\frac{\langle \psi_T | e^{-(H-E_T)\tau} H | \psi_T \rangle}{\langle \psi_T | e^{-(H-E_T)\tau} | \psi_T \rangle}$$

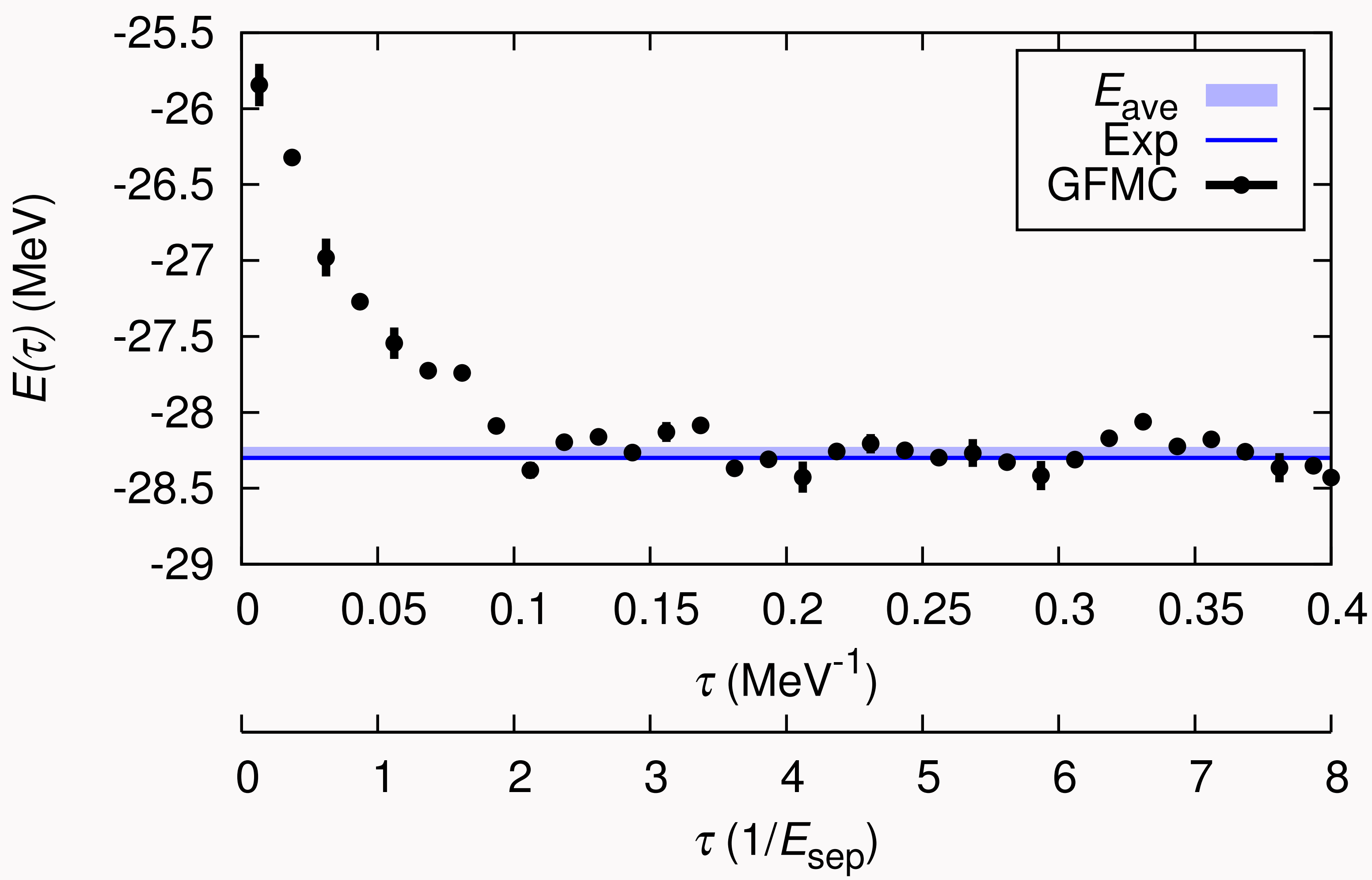
$$\tau = 3.00(1/E_{\mathrm{sep}})$$





QMC Methods - An Example

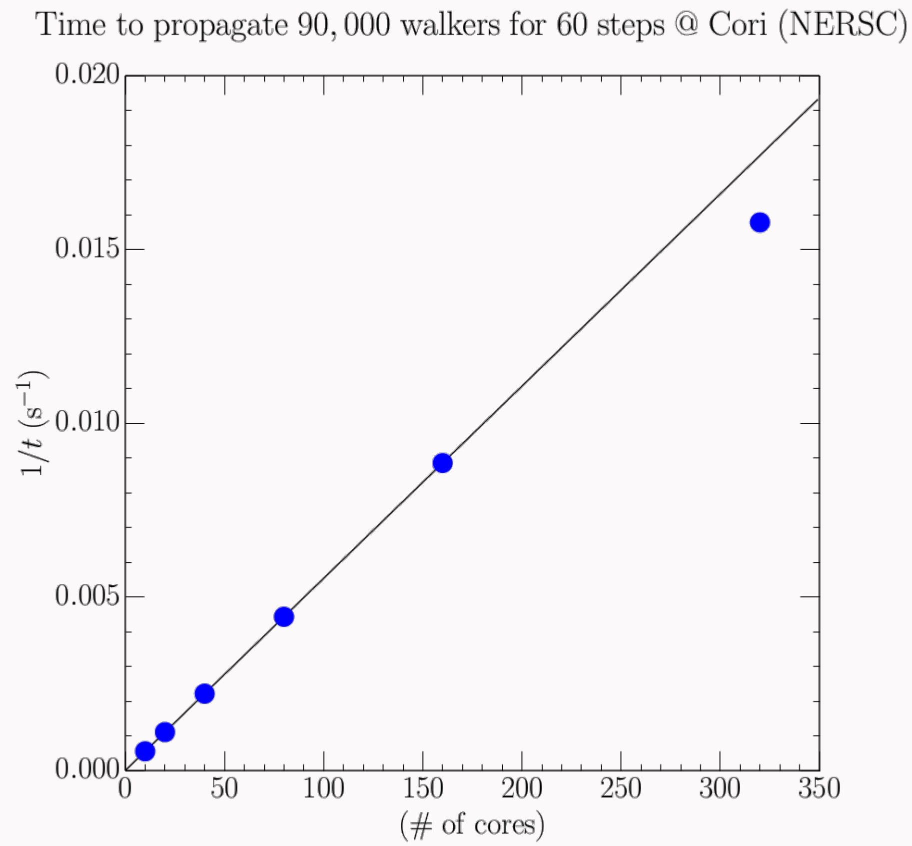
For ^{4}He, $1/E_{sep} = 1/|E_\alpha - E_t| \approx 0.05\ \text{MeV}^{-1}$.

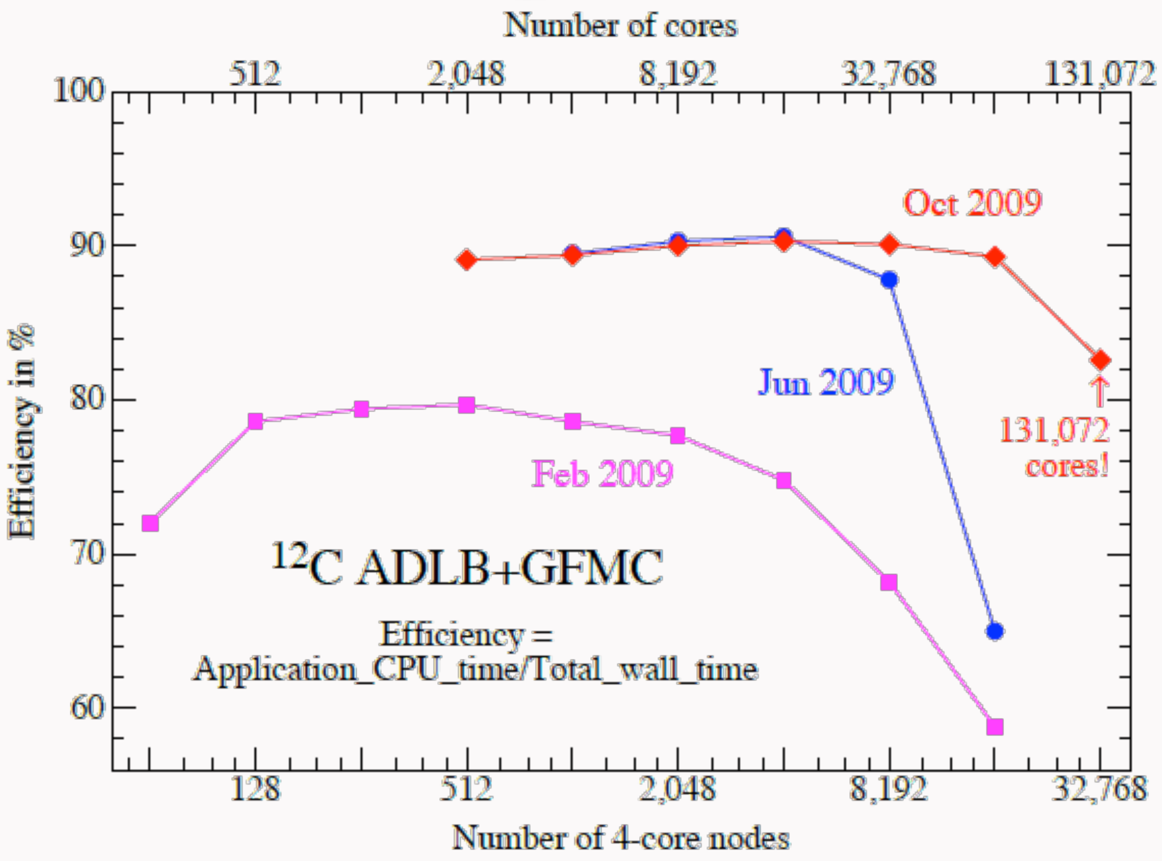


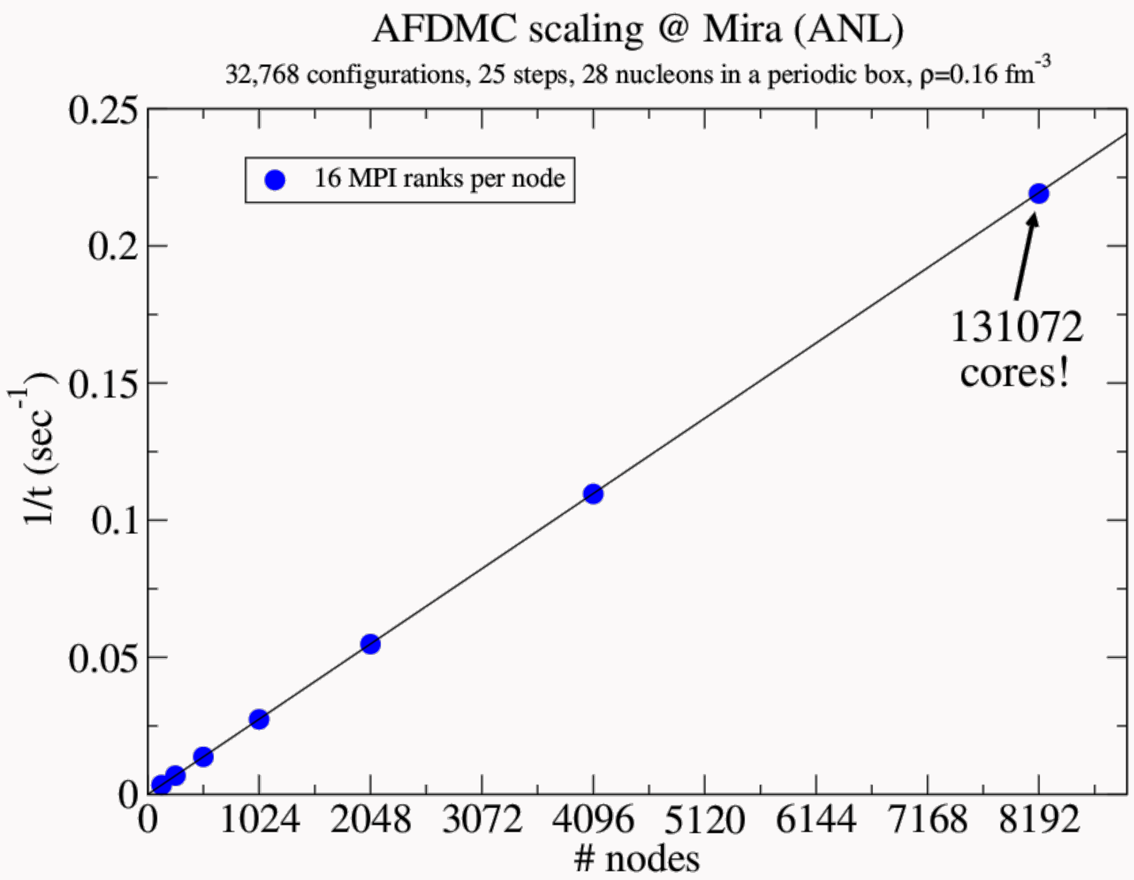
QMC Methods - Compare/Contrast GFMC & AFDMC

Green's function Monte Carlo (GFMC)	Auxiliary-field diffusion Monte Carlo (AFDMC)
· $\lvert\Psi_T\rangle \sim 3A$ coordinates & $2^A\binom{A}{Z}$ complex amplitudes.	· $\lvert\Psi_T\rangle \sim 3A$ coordinates & $4A$ complex amplitudes $(\lvert n\uparrow\rangle, \lvert n\downarrow\rangle, \lvert p\uparrow\rangle, \lvert p\downarrow\rangle)$.
· General treatment of (local) $2N$ and $3N$ forces.	· Some difficulty with $3N$ interactions in propagator. (Work ongoing).
· Robust sign-problem treatment.	· Sign-problem treatment in active development.

QMC Methods - Some Computing Details







The Hamiltonian

Of course, the Hamiltonian is much more complicated in nuclear physics.

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk} + \cdots$$

Where should it come from?

Chiral Effective Field Theory (EFT)

Chiral EFT

Chiral EFT in two lines:

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{2g^2}\mathrm{Tr}(G_{\mu\nu}G^{\mu\nu}) + \bar{q}i\gamma^\nu D_\nu q - \cancel{\bar{q}\mathcal{M}q} \rightarrow \text{Chiral symmetry}$$

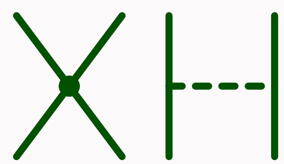
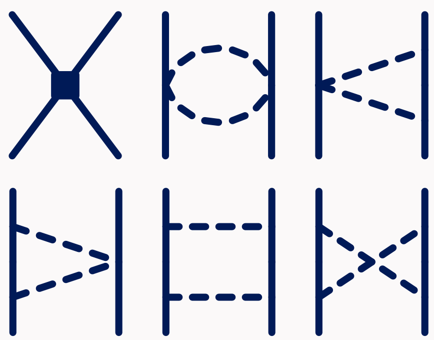
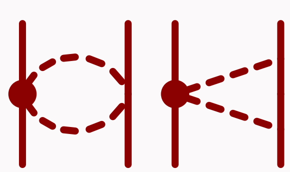
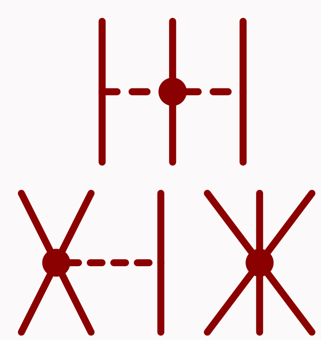
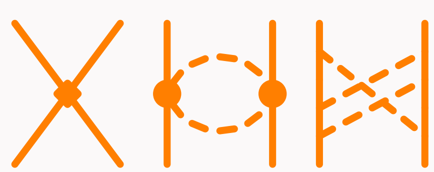
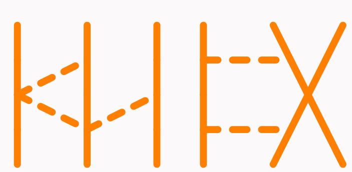
$$\mathcal{L}_{\mathrm{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \cdots$$

More Details:

E. Epelbaum et al, RMP **81**, 1773 (2009);

R. Machleidt et al, Phys. Rep. **503**, (2011).

Chiral EFT

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		–
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		–
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$	
N^{3}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$

- Chiral EFT: Expand in powers of Q/Λ_b.
  $Q \sim m_\pi \sim 100$ MeV
  $\Lambda_b \sim 800$ MeV
- Long-range physics: π exchanges.
- Short-range physics: Contacts × LECs.
- Many-body forces & currents enter systematically.

Chiral EFT

Local construction possible[1] up to N^2LO.

Definitions.

$$\mathbf{q} = \mathbf{p} - \mathbf{p}', \quad \mathbf{k} = \mathbf{p} + \mathbf{p}'$$

Regulator:

$$f(p, p') = e^{-(p/\Lambda)^n} e^{-(p'/\Lambda)^n}$$

Contacts:

$\propto$ $\mathbf{q}$ and $\mathbf{k}$

[1] A. Gezerlis et al, PRL **111** 032501 (2013); JEL et al, PRL **113** 192501 (2014); A. Gezerlis et al, PRC **90** 054323 (2014)

Chiral EFT

Local construction possible[1] up to N^2LO.

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Regulator:

$$f(p, p') = e^{-(p/\Lambda)^n} e^{-(p'/\Lambda)^n}$$

$$\rightarrow f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4} \; : \; R_0 = 1.0, 1.1, 1.2 \text{ fm}.$$

Contacts:

$\propto \mathbf{q}$ and $\mathbf{k}$

$\rightarrow$ Choose contacts $\propto \mathbf{q}$ (As much as possible!)

[1]A. Gezerlis et al, PRL **111** 032501 (2013); JEL et al, PRL **113** 192501 (2014); A. Gezerlis et al, PRC **90** 054323 (2014)

Chiral EFT

Local construction possible[1] up to N^{2}LO.

Definitions.

$$\mathbf{q} = \mathbf{p} - \mathbf{p}', \ \mathbf{k} = \mathbf{p} + \mathbf{p}'$$

Regulator:

~~$f(p, p') = e^{-(p/\Lambda)^n} e^{-(p'/\Lambda)^n}$~~

$$\rightarrow f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4} \ : \ R_0 = 1.0, 1.1, 1.2 \text{ fm}.$$?

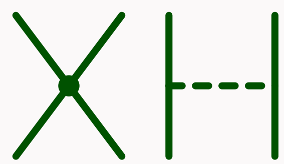
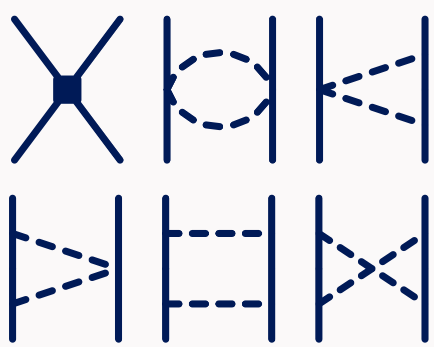
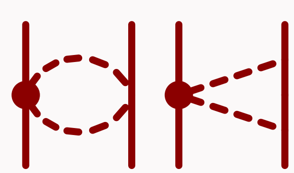
Contacts:

~~$\propto \mathbf{q}$ and $\mathbf{k}$~~

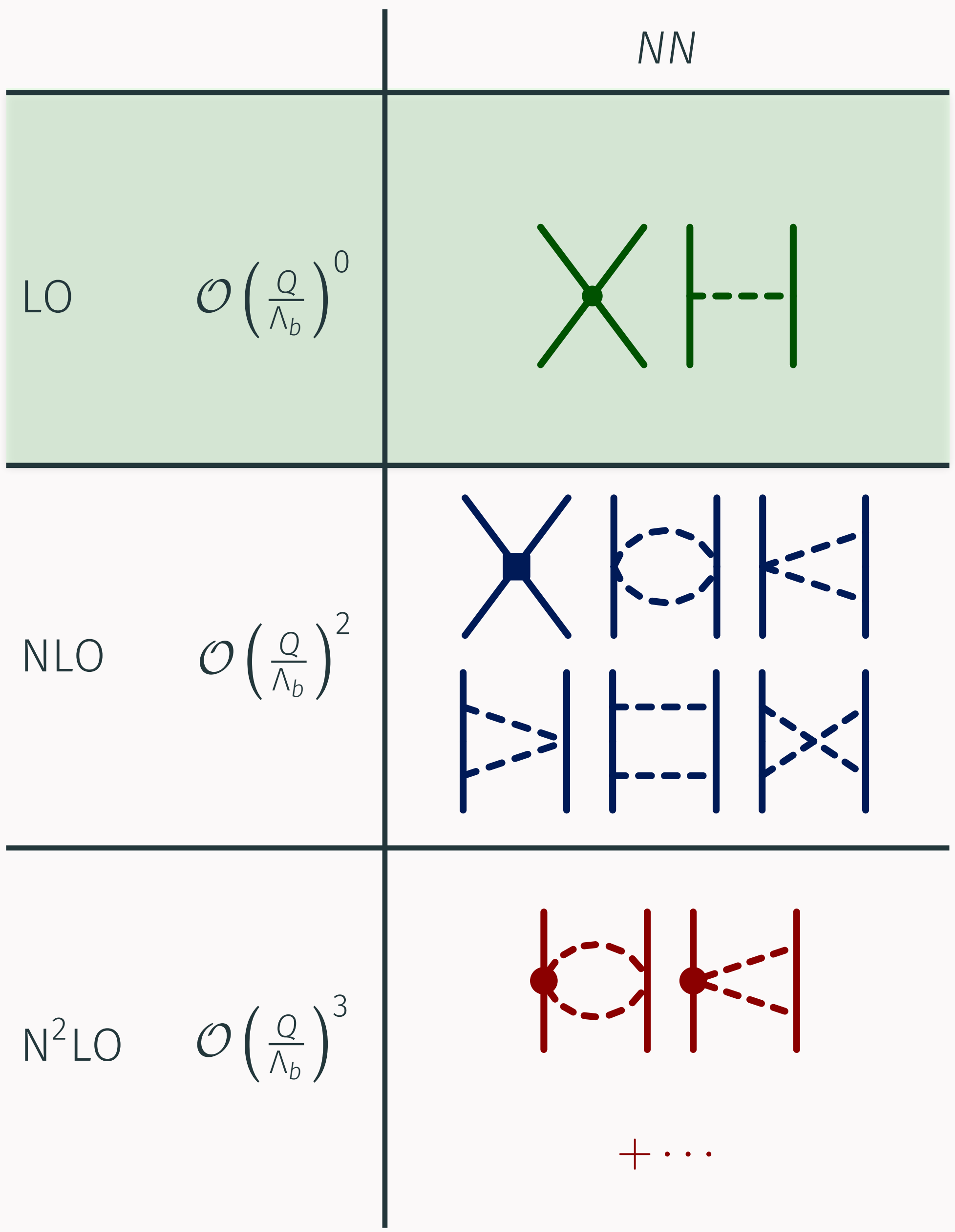
$\rightarrow$ Choose contacts $\propto \mathbf{q}$ (As much as possible!) ?

[1] A. Gezerlis et al, PRL **111** 032501 (2013); JEL et al, PRL **113** 192501 (2014); A. Gezerlis et al, PRC **90** 054323 (2014)

Chiral EFT

		NN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$	
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$	
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$

Chiral EFT



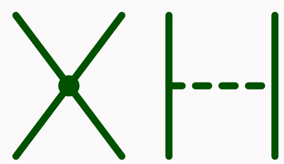
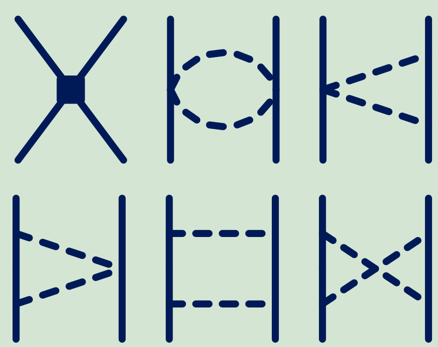
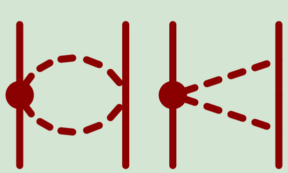
$$V_{\text{cont}}^{(0)} = \alpha_1 + \alpha_2(\sigma_1 \cdot \sigma_2) + \alpha_3(\tau_1 \cdot \tau_2) + \alpha_4(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$$

Pauli Exclusion Principle

$\rightarrow$ Only two independent contacts!

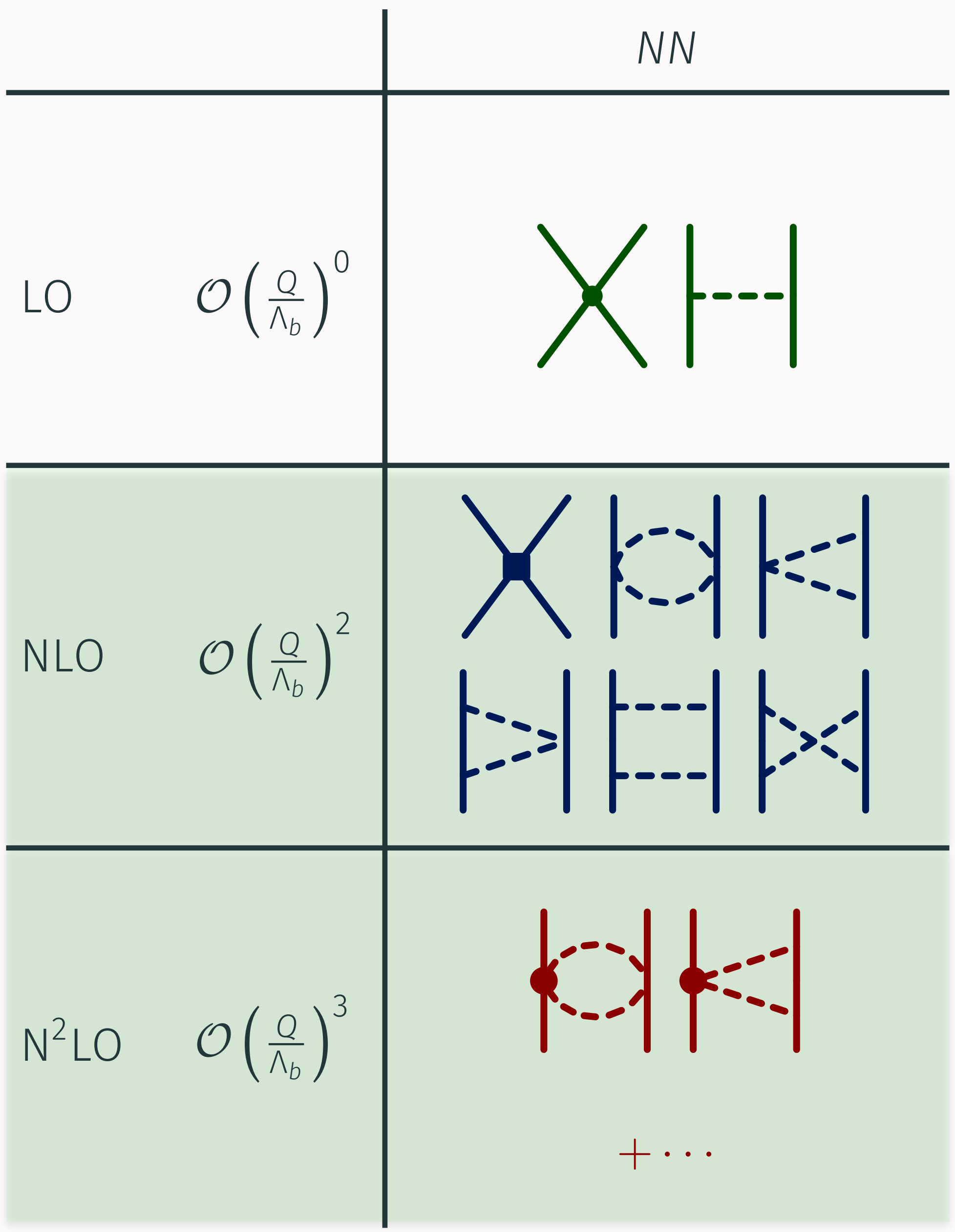
$$V_{\text{cont}}^{(0)} = C_S + C_T(\sigma_1 \cdot \sigma_2)$$

Chiral EFT

		NN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$	
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$	
N^{2}LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	 $+\cdots$

$$
\begin{aligned}
V^{(2)}_{\text{cont}} &= \gamma_1 q^2 + \gamma_2 q^2 (\sigma_1 \cdot \sigma_2) \\
&+ \gamma_3 q^2 (\tau_1 \cdot \tau_2) + \gamma_4 q^2 (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \\
&+ \gamma_5 k^2 + \gamma_6 k^2 (\sigma_1 \cdot \sigma_2) + \gamma_7 k^2 (\tau_1 \cdot \tau_2) \\
&+ \gamma_8 k^2 (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \\
&+ (\sigma_1 + \sigma_2)(\mathbf{q} \times \mathbf{k})(\gamma_9 + \gamma_{10}(\tau_1 \cdot \tau_2)) \\
&+ (\sigma_1 \cdot \mathbf{q})(\sigma_2 \cdot \mathbf{q})(\gamma_{11} + \gamma_{12}(\tau_1 \cdot \tau_2)) \\
&+ (\sigma_1 \cdot \mathbf{k})(\sigma_2 \cdot \mathbf{k})(\gamma_{13} + \gamma_{14}(\tau_1 \cdot \tau_2))
\end{aligned}
$$

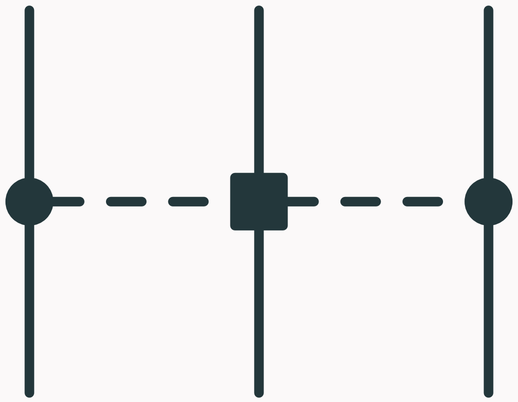
Chiral EFT



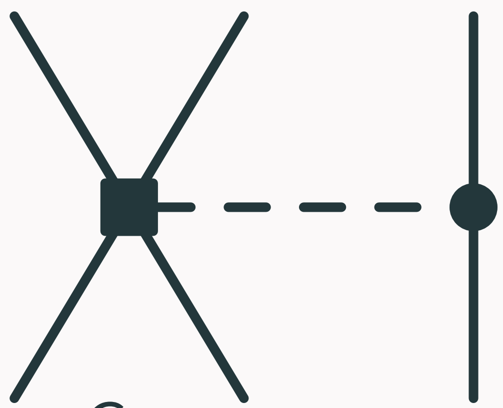
$$
\begin{aligned}
V^{(2)}_{\text{cont}} = {} & \gamma_1 q^2 + \gamma_2 q^2 (\sigma_1 \cdot \sigma_2) \\
& + \gamma_3 q^2 (\tau_1 \cdot \tau_2) + \gamma_4 q^2 (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \\
& + \gamma_5 k^2 + \gamma_6 k^2 (\sigma_1 \cdot \sigma_2) + \gamma_7 k^2 (\tau_1 \cdot \tau_2) \\
& + \gamma_8 k^2 (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \\
& + (\sigma_1 + \sigma_2)(\mathbf{q} \times \mathbf{k})(\gamma_9 + \gamma_{10}(\tau_1 \cdot \tau_2)) \\
& + (\sigma_1 \cdot \mathbf{q})(\sigma_2 \cdot \mathbf{q})(\gamma_{11} + \gamma_{12}(\tau_1 \cdot \tau_2)) \\
& + (\sigma_1 \cdot \mathbf{k})(\sigma_2 \cdot \mathbf{k})(\gamma_{13} + \gamma_{14}(\tau_1 \cdot \tau_2))
\end{aligned}
$$

Three-Nucleon Interaction

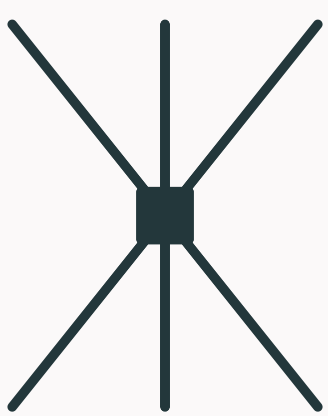
Three-Nucleon Interaction



c_1, c_3, c_4

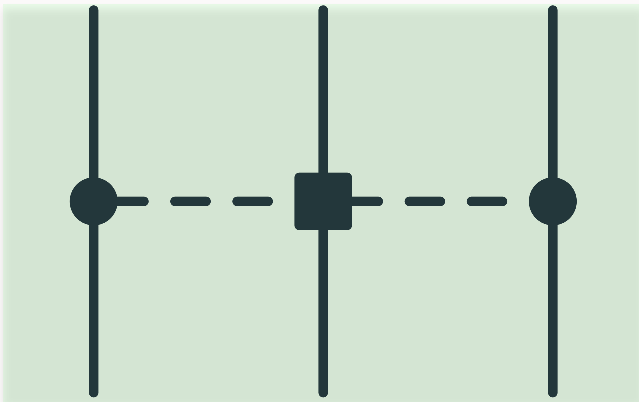


c_D

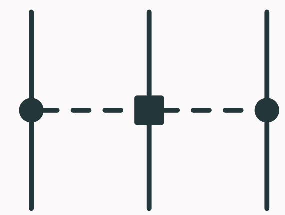


c_E

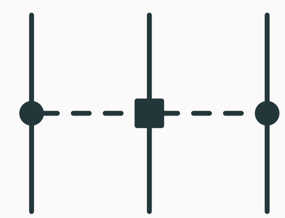
Three-Nucleon Interaction



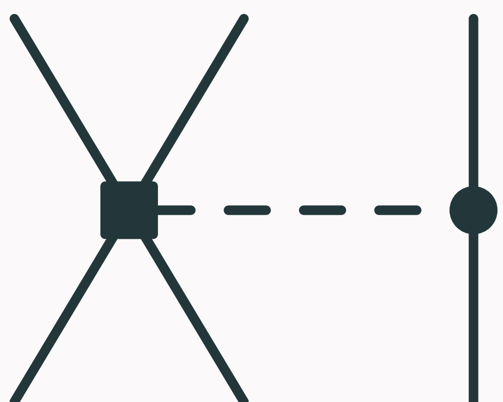
c_1, c_3, c_4

$\mathcal{F}\Big\{$  $\Big\} \rightarrow \sim$ Tucson-Melbourne a' Term

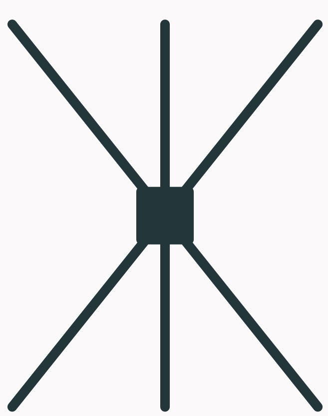
c_1

$\mathcal{F}\Big\{$  $\Big\} \rightarrow \sim$ Fujita-Miyazawa

c_3, c_4

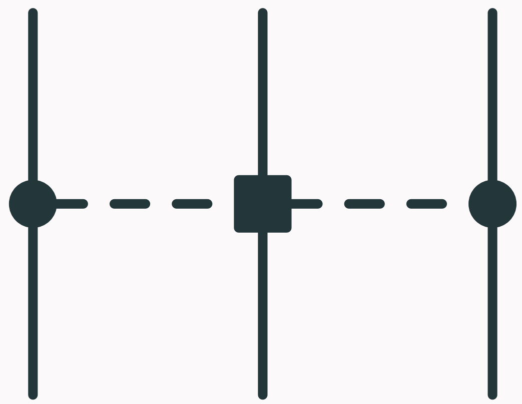


c_D

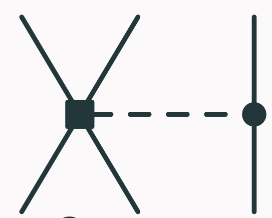


c_E

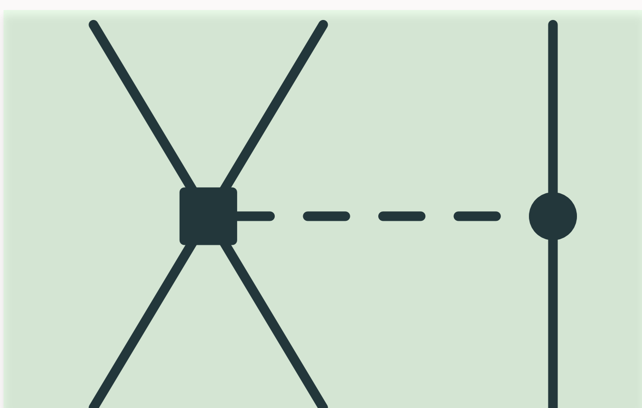
Three-Nucleon Interaction



$c_1,\ c_3,\ c_4$

$$\mathcal{F}\left\{ \right.$$  $$\left. \right\} \rightarrow 1\pi\text{-Exchange} + \text{Contact}$$

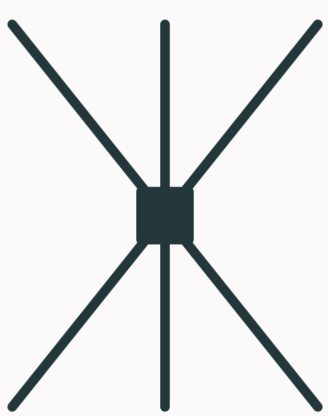
c_D



c_D

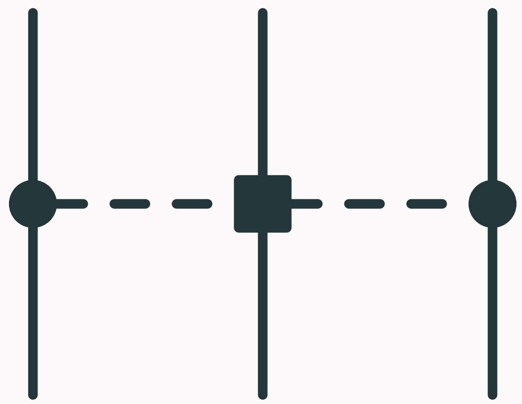
$$V_{D1} \propto \sum_{i<j<k} \sum_{\text{cyc.}} (\tau_i \cdot \tau_k) \times \left[X_{ik}(\mathbf{r}_{kj})\Delta_{ij} + X_{ik}(\mathbf{r}_{ij})\Delta_{kj} - \frac{2^3\pi}{m_\pi^3}(\sigma_i \cdot \sigma_k)\Delta_{ij}\Delta_{kj} \right]$$

$$V_{D2} \propto \sum_{i<j<k} \sum_{\text{cyc.}} (\tau_i \cdot \tau_k) \times \left[X_{ik} - \frac{2^2\pi}{m_\pi^3}(\sigma_i \cdot \sigma_k)\Delta_{ik} \right] (\Delta_{ij} + \Delta_{kj})$$

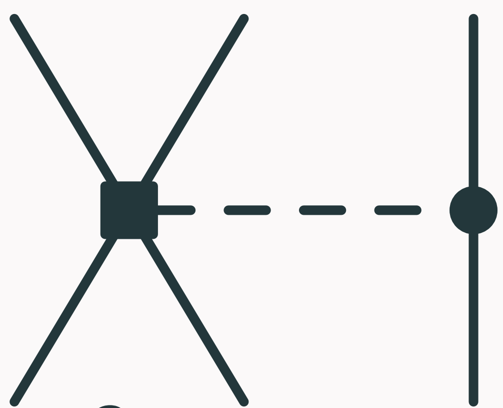


c_E

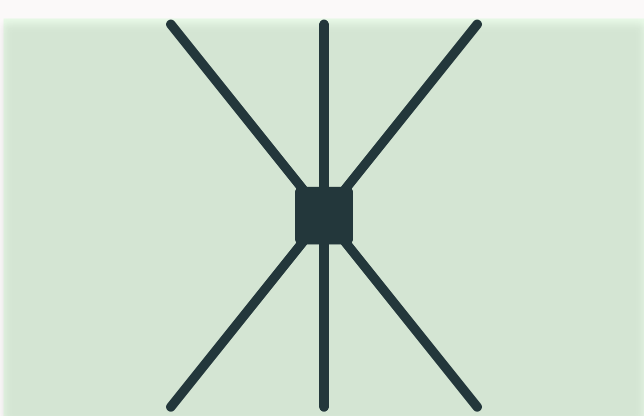
Three-Nucleon Interaction



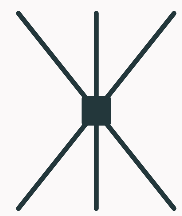
$c_1,\ c_3,\ c_4$



c_D



c_E

$\mathcal{F}\{$  $\} \rightarrow$ Contact

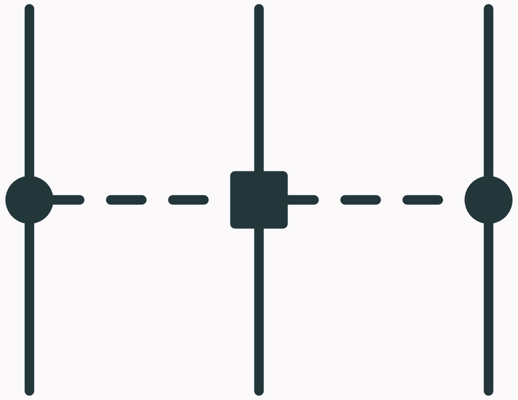
c_E

$$V_E \propto \sum_{i<j<k} \sum_{\text{cyc.}} O_{ijk} \Delta_{ij} \Delta_{kj}$$

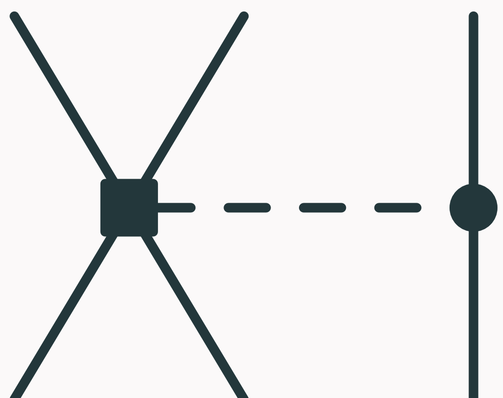
Fierz rearrangement freedom

$$O_{ijk} = \{\mathbb{1}, \sigma_i \cdot \sigma_j, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_k, [(\sigma_i \times \sigma_j) \cdot \sigma_k][(\tau_i \times \tau_j) \cdot \tau_k]\}$$

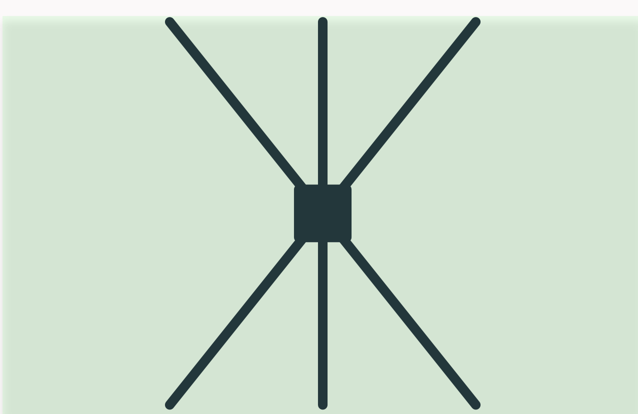
Three-Nucleon Interaction



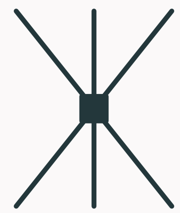
$c_1,\ c_3,\ c_4$



c_D



c_E

$\mathcal{F}\Big\{$  $\Big\}$ → Contact

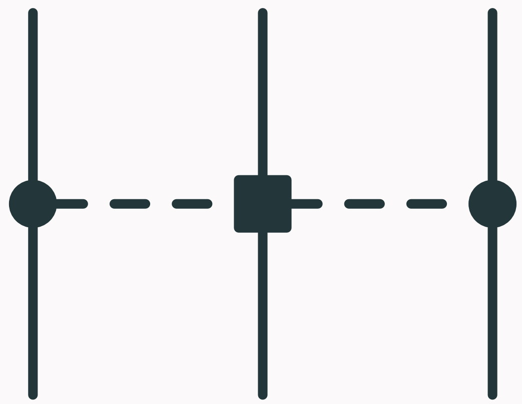
c_E

$$V_E \propto \sum_{i<j<k} \sum_{\text{cyc.}} O_{ijk} \Delta_{ij} \Delta_{kj},\ \Delta_{ij} \propto e^{-(r_{ij}/R_0)^4}$$

~~Fierz rearrangement freedom~~

$$O_{ijk} = \{\mathbb{1}, \sigma_i \cdot \sigma_j, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j,$$
$$\sigma_i \cdot \sigma_j \tau_i \cdot \tau_k, [(\sigma_i \times \sigma_j) \cdot \sigma_k][(\tau_i \times \tau_j) \cdot \tau_k]\}$$

Three-Nucleon Interaction



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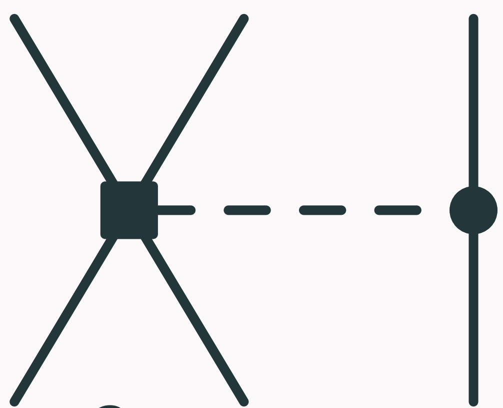
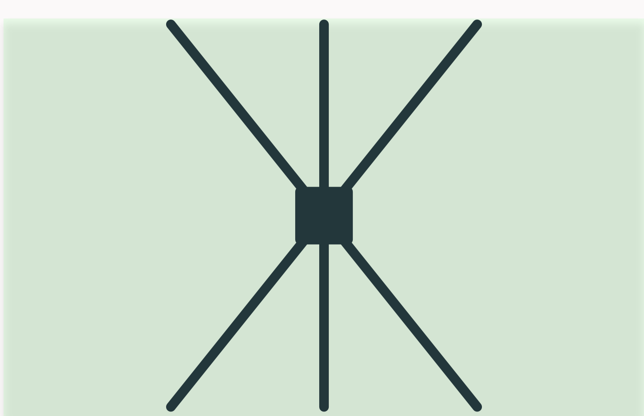
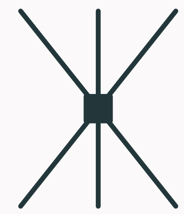


c_D



c_E

$\mathcal{F}\Big\{$  $\Big\} \to$ Contact

c_E

$$V_{E\tau} \propto \sum_{i<j<k} \sum_{\text{cyc}} \tau_i \cdot \tau_k \Delta_{ij} \Delta_{kj}$$

$$V_{E\mathbb{1}} \propto \sum_{i<j<k} \sum_{\text{cyc}} \Delta_{ij} \Delta_{kj}$$

$$V_{E\mathcal{P}} \propto \sum_{i<j<k} \sum_{\text{cyc}} \mathcal{P} \Delta_{ij} \Delta_{kj},$$

$$\mathcal{P} = \frac{1}{36}\Big(3 - \sum_{i<j} \sigma_i \cdot \sigma_j\Big)\Big(3 - \sum_{k<\ell} \tau_k \cdot \tau_\ell\Big)$$

Fits

Choosing Observables

What to fit c_D and c_E to?

- Uncorrelated observables.
- Probe properties of light nuclei: ^{4}He E_B.
- Probe $T = 3/2$ physics: n-α scattering phase shifts.

n-α Scattering - Details

For low-energy scattering and one open channel of total angular momentum J,

$$\Psi \propto \{\Phi_{c_1}\Phi_{c_2}Y_L\}_J[\cos\delta_{JL}j_L(kr_c) - \sin\delta_{JL}n_L(kr_c)],$$

Impose[2]

$$\hat{n}\cdot\nabla_{r_c}\Psi = \gamma\Psi \text{ at } r_c = R.$$

$$\Rightarrow \tan\delta_{JL} = \frac{\gamma j_L(kR) - kj_L'(kR)}{\gamma n_L(kR) - kn_L'(kR)}$$

[2] K. M. Nollet et al, PRL **99** 022502 (2007)

n-α Scattering - Details

Reject samples with $r_c > R$, but

$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}_c|<R} d\mathbf{R}_{c_1} d\mathbf{R}_{c_2} d\mathbf{r}_c G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R}) + \int_{|\mathbf{r}_c|>R} d\mathbf{R}_{c_1} d\mathbf{R}_{c_2} d\mathbf{r}_c G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R})$$

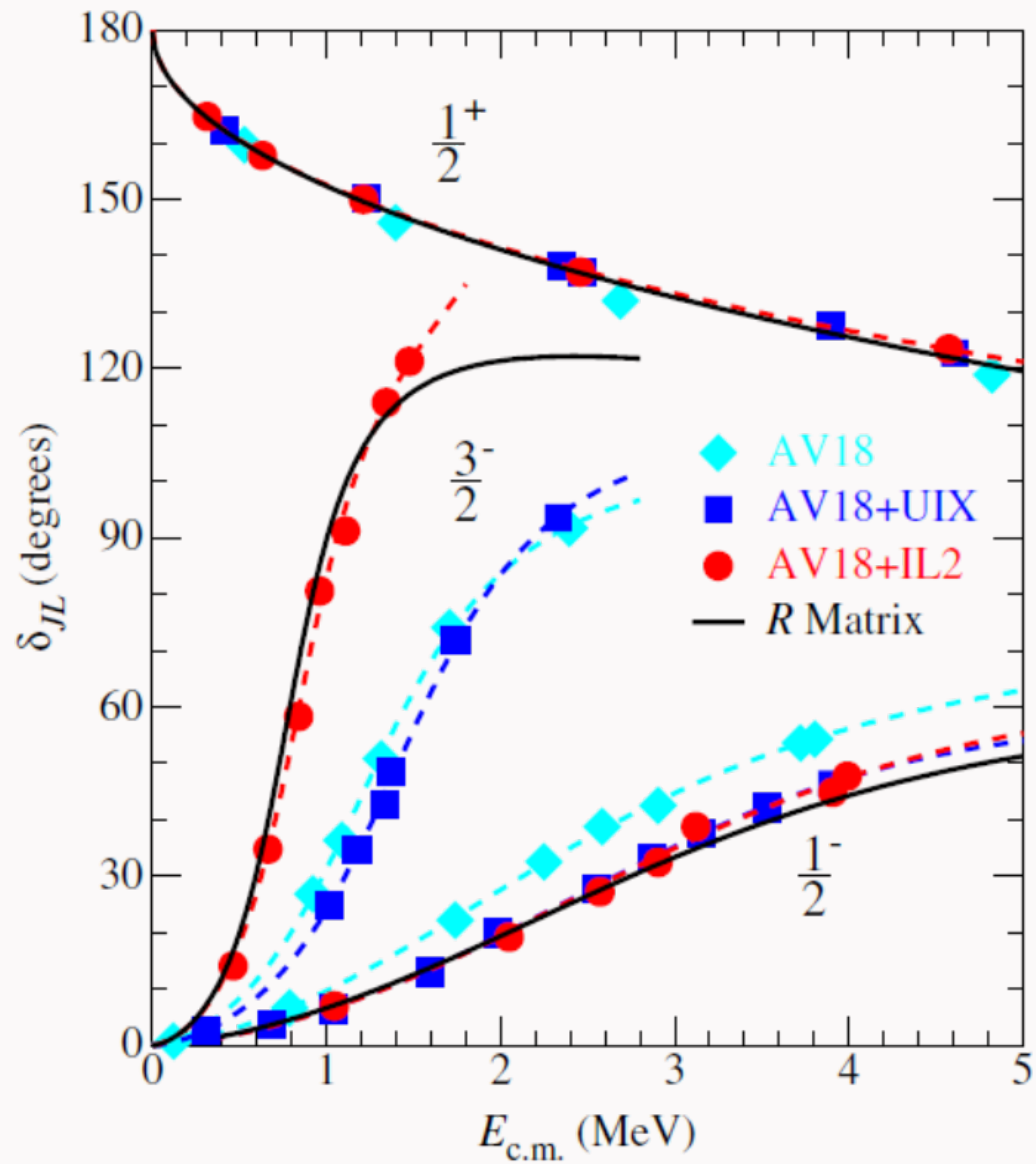
maps to

$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}_c|<R} d\mathbf{R}_{c_1} d\mathbf{R}_{c_2} d\mathbf{r}_c G(\mathbf{R}', \mathbf{R}; \Delta\tau) \times \left[\Psi_n(\mathbf{R}) + \frac{G(\mathbf{R}', \mathbf{R}_e; \Delta\tau)}{G(\mathbf{R}', \mathbf{R}; \Delta\tau)} \left(\frac{r_e}{r_c}\right)^3 \Psi_n(\mathbf{R}_e)\right]$$

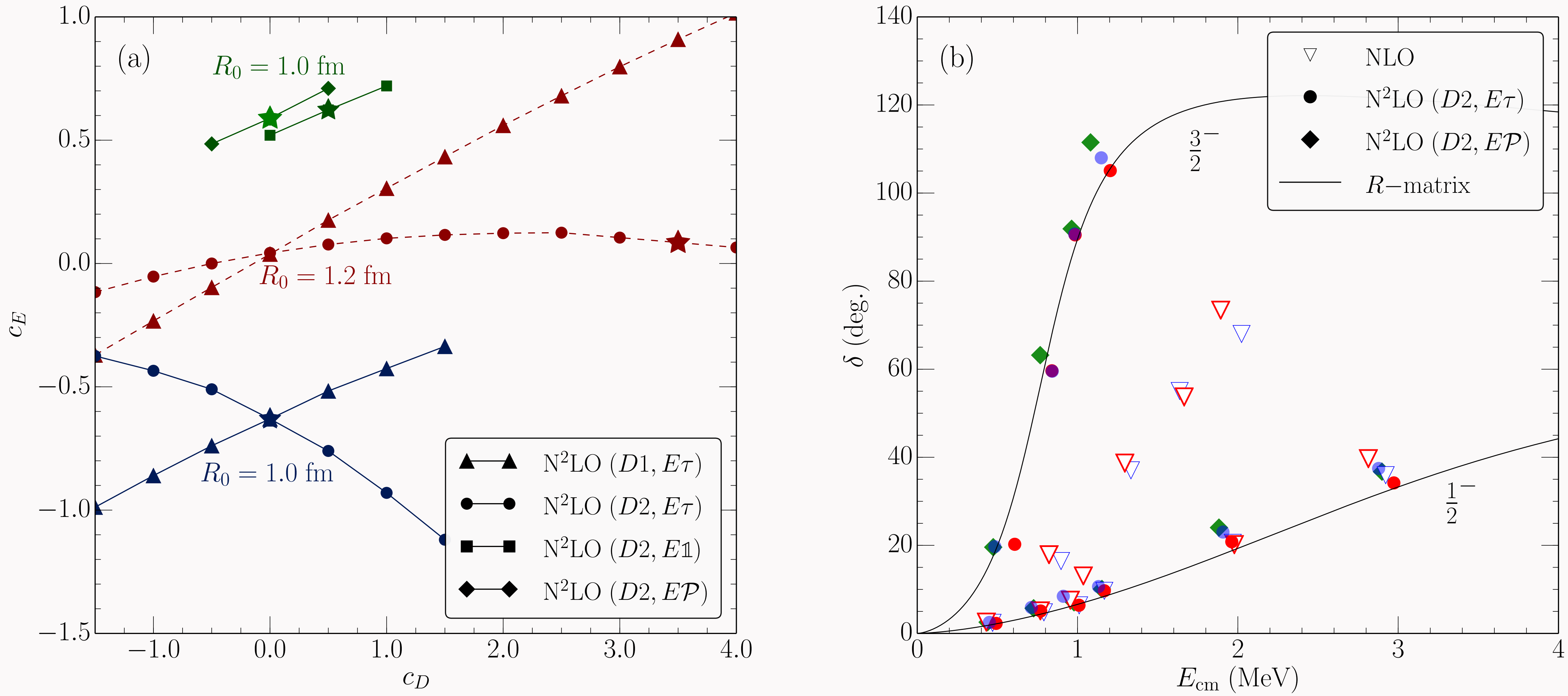
That is, the wave function at the (n+1)th point gets a contribution from the previous point $\mathbf{R}$ and an "image" point $\mathbf{R}_e$.

n-α Scattering - Details

- Results showed need for greater spin-orbit splitting than was provided for by the Urbana IX (UIX) 3*N* interaction.
- Interpretation was *T*=3/2 component in Illinois 3*N* interaction was necessary. (?)



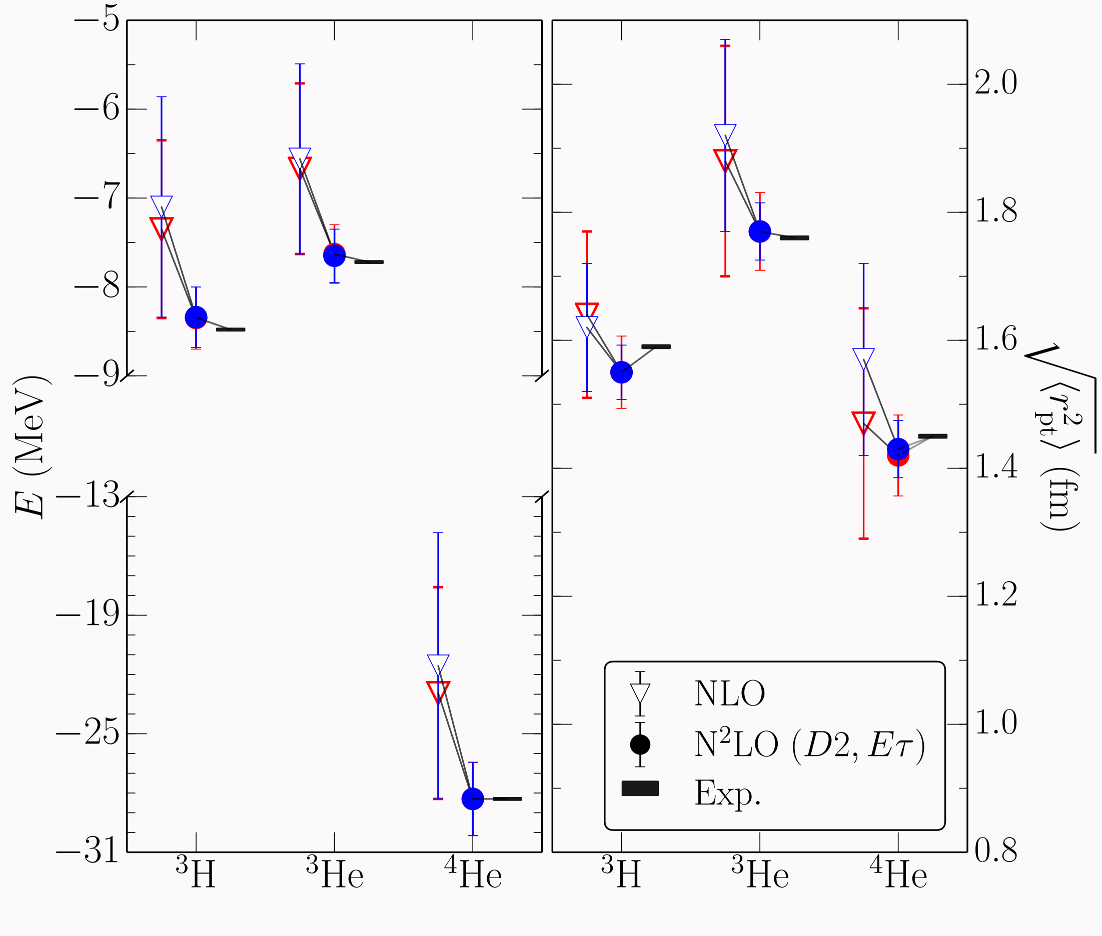
Fits

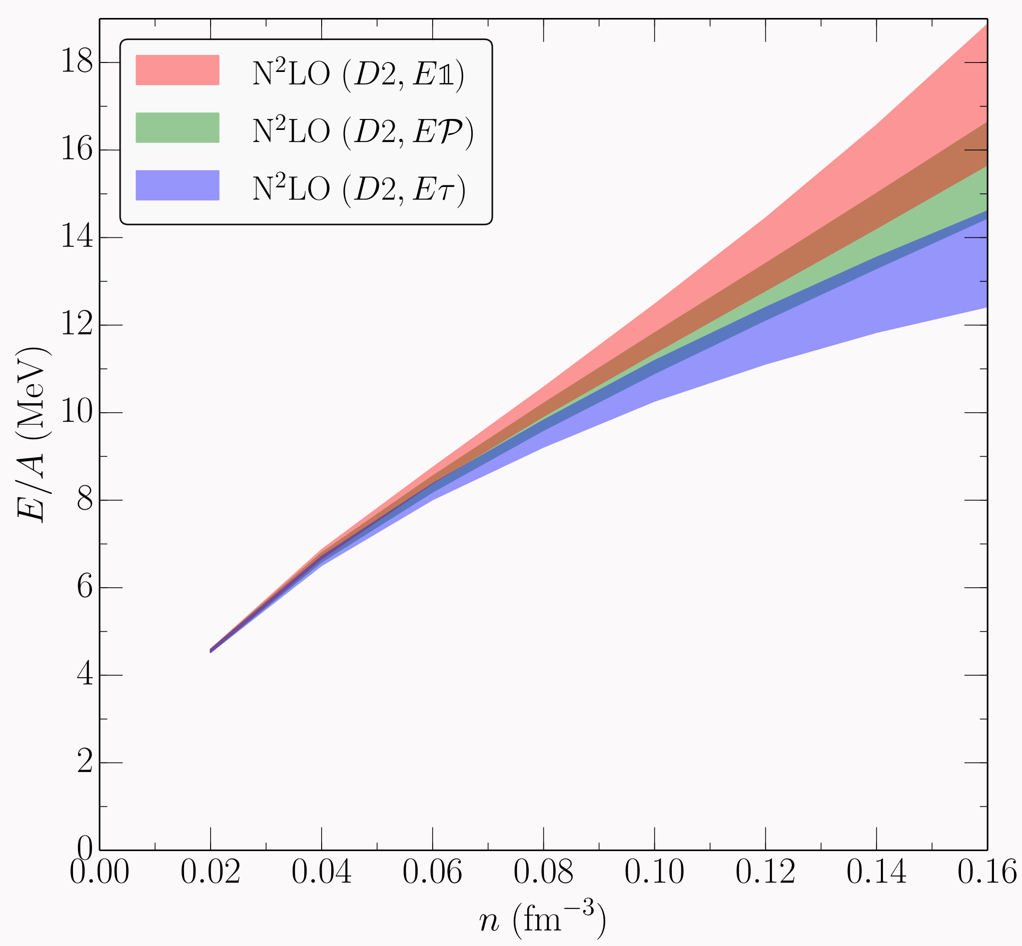


JEL et al, PRL **116**, 062501 (2016)

Results

A simultaneous description of properties of light nuclei, n-α scattering and neutron matter is possible. Uncertainty analysis as in E. Epelbaum et al, EPJ **A51**, 53 (2015).





JEL et al, PRL **116**, 062501 (2016)

A Recent Application

Motivation - Nuclei In Finite Volume

- Lattice QCD is the only *ab initio* method available to solve QCD directly at low energies.
- Computational costs mean in our lifetimes, Lattice QCD will not likely simulate, e.g., ^{12}C.
- Need some connection between Lattice QCD and *ab initio* low-energy nuclear theory;
  e.g. obtaining LECs in chiral EFT from Lattice simulations.

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  e.g. obtaining LECs in chiral EFT from Lattice simulations. Now add filler text! Yeah. I like this
  Use Lattice ideas to extract resonant properties from finite volume calculations.

Motivation - Lüscher Formula

- Take a simple scattering problem $np \to d\gamma$.
  Near threshold radiative capture in the $^1S_0$ channel.

- Might expect $L \gg |a^{^1S_0}|, |a^{^3S_1}|$, with, e.g.
  $a^{^1S_0} = -23.71$ fm.

- Not so! Lüscher $\to p\cot\delta_0(p) = \frac{1}{\pi L} S\left[\left(\frac{Lp}{2\pi}\right)^2\right]$,

$$S(\eta) \equiv \lim_{\Lambda_j \to \infty} \left(\sum_{\mathbf{j}}^{\Lambda_j} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda_j \right).$$

More On The Lüscher Formula

For low-energy S-wave scattering, can use the effective-range expansion:

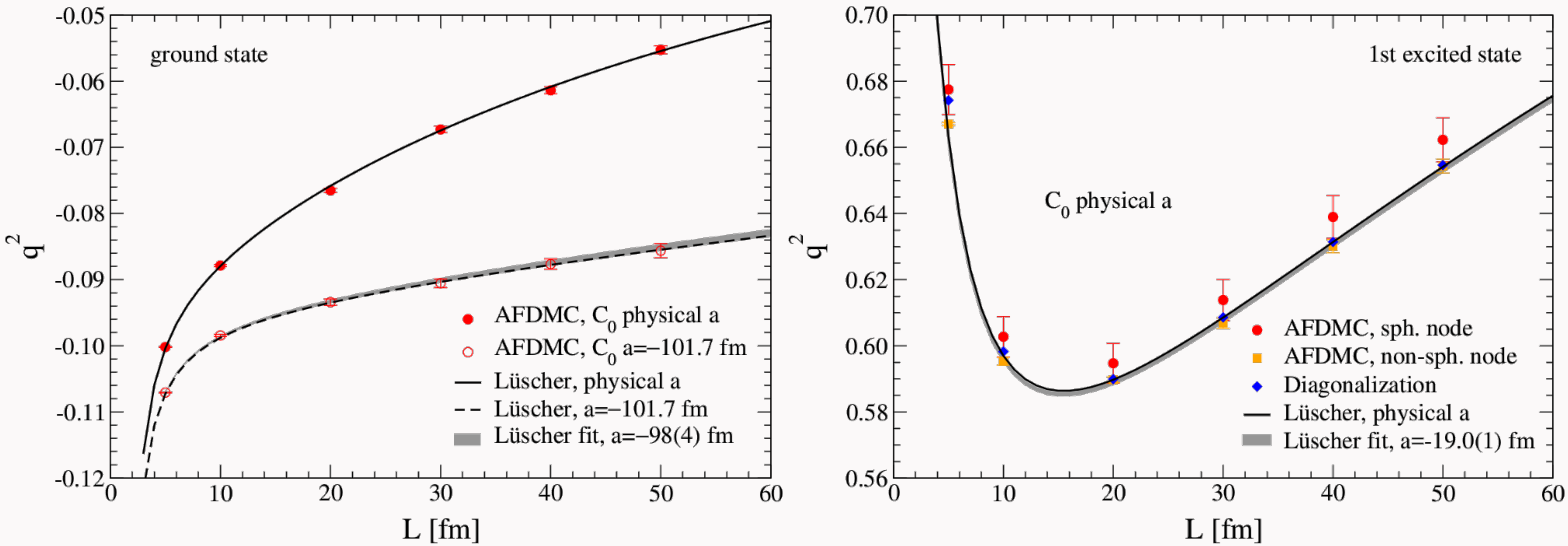
$$-\frac{1}{a^{(^1S_0)}} + \frac{1}{2} r_0^{(^1S_0)} p^2 = \frac{1}{\pi L} S\left[\left(\frac{Lp}{2\pi}\right)^2\right].$$

Consider first two neutrons only and a contact interaction (smeared out)

$$V(r) = C_0 \exp\left[-\left(\frac{r}{R_0}\right)^4\right].$$

Introduce $q = pL/2\pi$.

Results - Contact



First AFDMC calculations of excited states.

P. Klos et al, arXiv:1604.01387 [nucl-th]

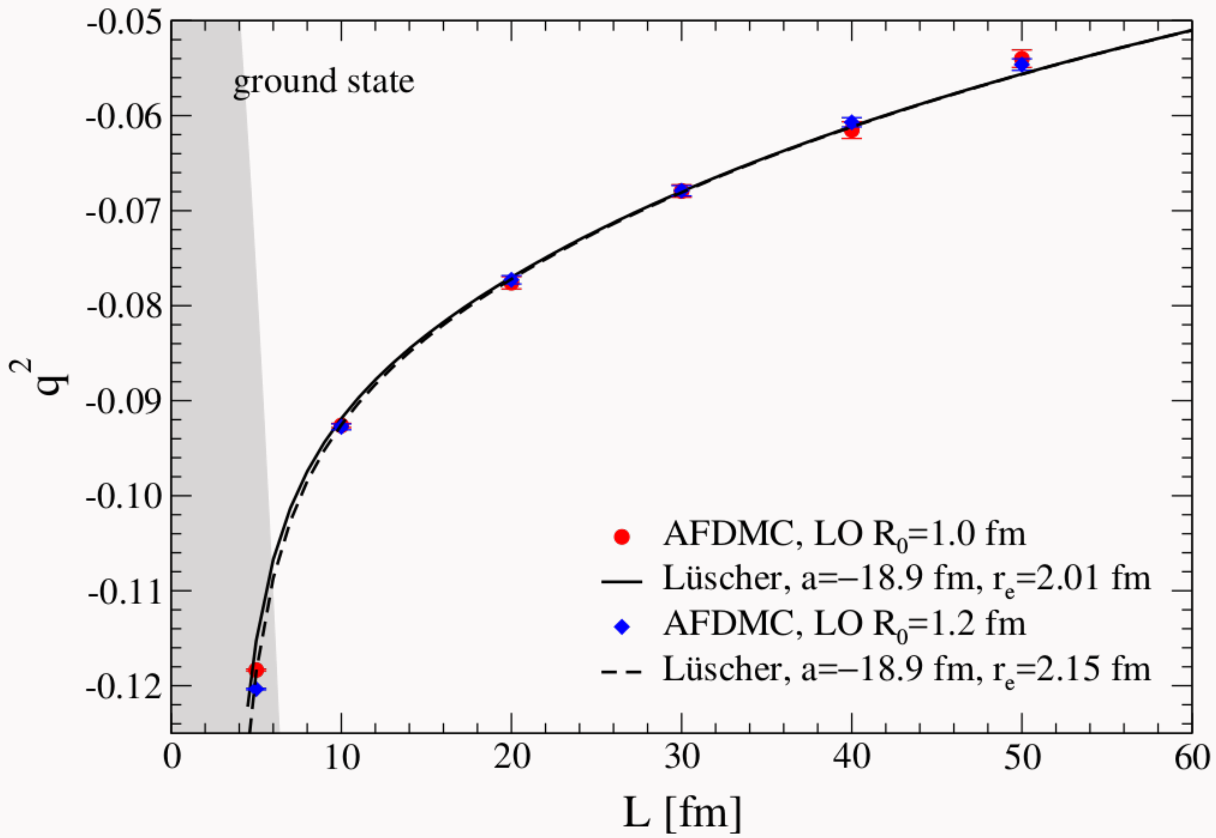
$2n$ In Finite Volume With Chiral Interactions

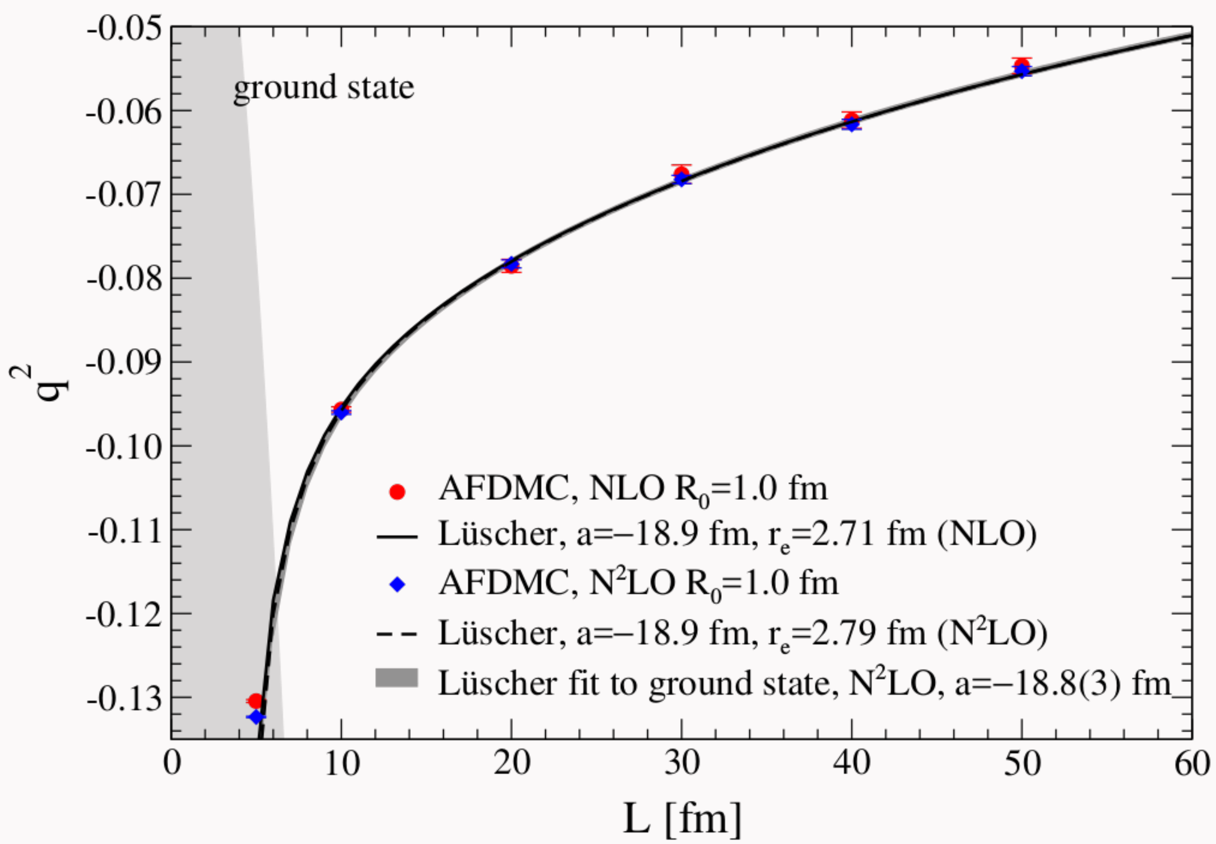
Now consider chiral EFT interactions.

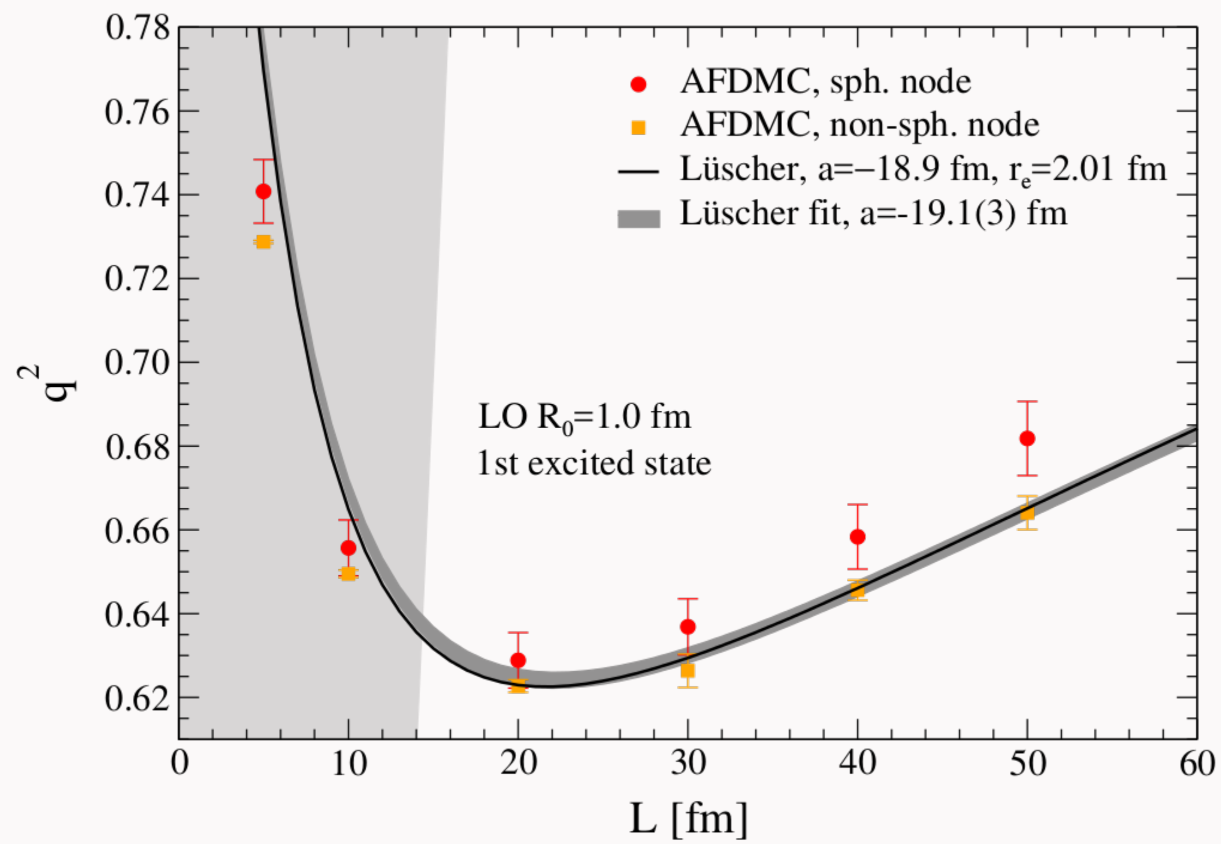
Standard Lüscher formula assumes $\not\pi$ EFT.

$$p \lesssim m_\pi/2$$

Results - Chiral EFT







P. Klos et al, arXiv:1604.01387 [nucl-th]

Summary

- QMC + Chiral EFT is possible and yields new insights.
- More studies of regulator choices and effects are necessary.
- Chiral two- and three-nucleon interactions at N^2LO have sufficient freedom to give a good description of light nuclei, n-α scattering, and neutron matter.
- Calculations of nuclei in finite volume will eventually allow for comparison to Lattice QCD calculations.

Outlook

- Larger A (how does the spin-orbit splitting in light nuclear levels look?) & studies of electroweak properties of nuclei (currents are in development at TU Darmstadt with P. Klos).
- Further investigations of nuclei/neutrons in finite volume.
- Extend n-α calculations to other scattering cases.
- Extend our recent work on the EMC effect and EFT. (See arXiv:1607.03065 [hep-ph]).
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Thank you for your attention!