Dissertation Defense:

# Improved Trial Wave Functions for Quantum Monte Carlo Calculations of Nuclear Systems and Their Applications

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# Outline

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- Background
  - What is the problem we are trying to solve?
  - Where are we applicable?
  - Other methods
    - HF - basis for other methods like AFDMC
    - Basis set methods such as ...
    - No-core shell model
    - Coupled cluster
    - self-consistent Green's function
- Methods to solve the nuclear problem and why we use QMC
  - VMC
  - DMC
  - GFMC
    - Excitations up to $^{12}$C
  - AFDMC

# Outline

- Trial wave function and why it's so important
  - Slater Dets (and Pfaffians)
  - Jastrow and linear correlations
    - Results from previous papers showing the improvement
  - Quadratic correlations
    - Results - show with jas $\rightarrow$ lin comparison as well
    - Show the preliminary results we have with $\chi$EFT potentials as well.
    - Performance scaling, both for xsede computers as well as linear vs. quadratic correlations.
- Other (future) correlations
  - Exponential correlations
  - Eigenvector discontinuity problem and square root matrix fix
  - Preliminary results

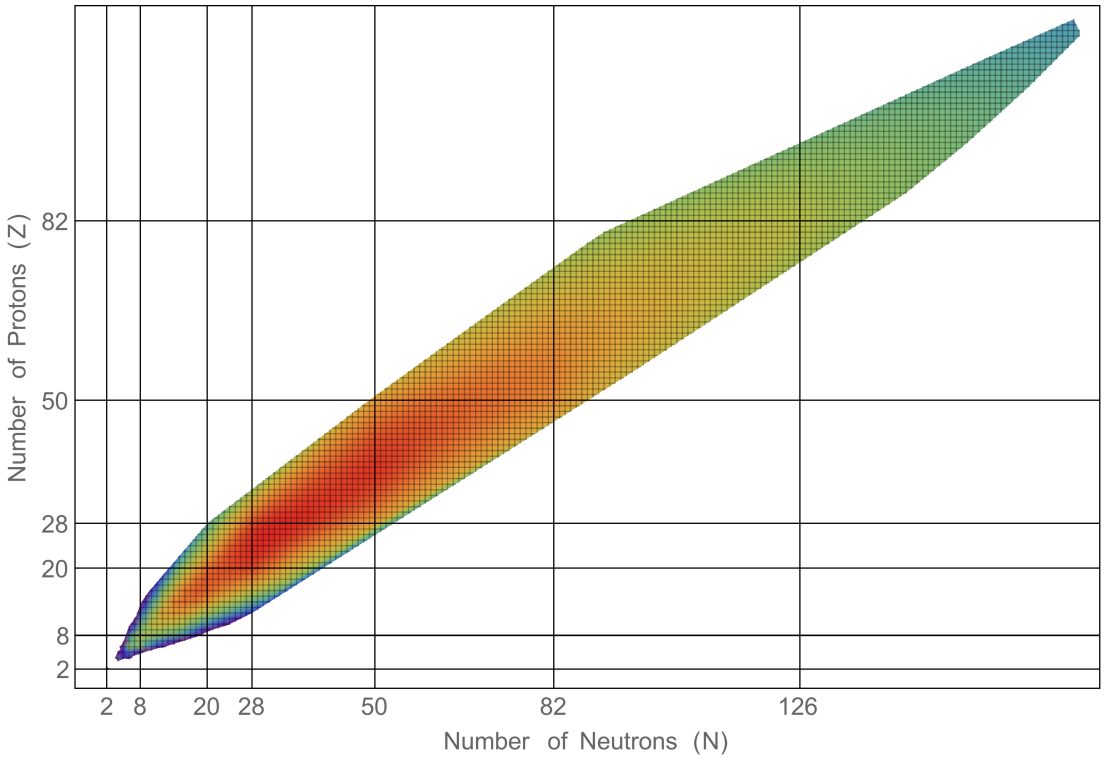
# Outline

- Application to $\alpha$-clustering
  - NS intro and why clustering is an interesting problem
    - Clustering is often put in by hand, but we can do it *ab initio*.
  - Stefano's original results
  - Results with quadratic correlations
- Conclusion
- Extra Slides
  - Add possible extra slides here when you think of them

# Nuclear Many Body Problem

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \Psi^*(\boldsymbol{R}) H \Psi(\boldsymbol{R}) d\boldsymbol{R}$$

$$H = \sum_{i=1}^{A} \frac{\boldsymbol{p}^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \dots$$



# Nuclear Many Body Methods

- There are a number of ways to solve this problem.
  - Hartree-Fock
  - Basis-set methods
    - No-core shell model
    - Coupled-cluster
    - Self consistent Green's function method
  - Quantum Monte Carlo
    - VMC
    - GFMC
    - AFDMC

# Variational Monte Carlo

- VMC starts with a trial wave function which includes variable parameters.
- The variational principle guarantees

$$E_V = \frac{\int \psi_T^*(\mathbf{R}) H \psi_T(\mathbf{R}) d\mathbf{R}}{\int \psi_T^*(\mathbf{R}) \psi_T(\mathbf{R}) d\mathbf{R}} \geq E_0$$

- We want this to look like this

$$E_V = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R} \approx \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{R}_n)$$

# Variational Monte Carlo

$$E_V = \int P(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R}$$

- We can do that if we multiply by $\Psi_T(\mathbf{R})\Psi_T^{-1}(\mathbf{R})$.

$$P(\mathbf{R}) = \frac{|\Psi_T(\mathbf{R})|^2}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}, \quad E_L(\mathbf{R}) = \frac{\Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R})}{\Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})}$$

- Now using Monte Carlo integration we can write

$$E_V \approx \frac{1}{N} \sum_{n=1}^{N} E_L(\mathbf{R_n}),$$

where the $\mathbf{R}_n$ are samples from $P(\mathbf{R})$.

# Variational Monte Carlo

- The statistical error in the energy is then given in the typical way

$$\sigma_{E_V} = \sqrt{\frac{\langle E_L^2 \rangle - \langle E_L \rangle^2}{N}} \approx \sqrt{\frac{\left(\frac{1}{N}\sum_{n=1}^{N} E_L^2(\mathbf{R}_n)\right) - \left(\frac{1}{N}\sum_{n=1}^{N} E_L(\mathbf{R}_n)\right)^2}{N-1}}$$

- We can then vary the parameters in the trial wave function and calculate this until we minimize the energy or statistical error, since $E_V \geq E_0$.

# Diffusion Monte Carlo

- Diffusion Monte Carlo uses a Green's function to diffuse in imaginary time to estimate the ground state energy and wave function based on a trial wave function.

$$H\Psi = i\hbar\frac{d\Psi}{dt} \xrightarrow{\tau = it/\hbar} H\Psi = -\frac{d\Psi}{d\tau}$$

Using separation of variables we can write

$$\Psi(\mathbf{R},\tau) = \sum_{n=0}^{\infty} c_n \phi_n(\mathbf{R}) e^{-\tau(E_n - E_0)}$$

- The long imaginary time limit of this goes to the ground state.

$$\lim_{\tau\to\infty} \Psi(\mathbf{R},\tau) = c_0\phi_0(\mathbf{R})$$

# Diffusion Monte Carlo

- The propagated wave function can be written

$$\left\langle \mathbf{R}' \middle| \Psi_T(\tau) \right\rangle = \int d\mathbf{R} \left\langle \mathbf{R}' \middle| e^{-(H-E_0)\tau} \middle| \mathbf{R} \right\rangle \left\langle \mathbf{R} \middle| \Psi_T(0) \right\rangle$$

- Now we use $e^{-H\tau} = e^{-V\tau/2} e^{-T\tau} e^{-V\tau/2} + \mathcal{O}(\tau^3)$ and break up the propagator into small time steps $\Delta\tau = \tau/N$.

$$\left\langle \mathbf{R}_N \middle| \Psi_T(\tau) \right\rangle = \int d\mathbf{R}_1 \ldots d\mathbf{R}_N \left[ \prod_{i=1}^{N} G(\mathbf{R}_i, \mathbf{R}_{i-1}, \Delta\tau) \right] \left\langle \mathbf{R}_0 \middle| \Psi_T(0) \right\rangle$$

$$G(\mathbf{R}', \mathbf{R}, \Delta\tau) = \left\langle \mathbf{R}' \middle| e^{-(H-E_0)\Delta\tau} \middle| \mathbf{R} \right\rangle$$

# Diffusion Monte Carlo

- In the small $\Delta\tau$ limit this propagator can be split up with the kinetic term being used to diffuse the walkers along a random path.

$$\left\langle \mathbf{R}' \right| e^{-T\Delta\tau} \left| \mathbf{R} \right\rangle = \left( \frac{m}{2\pi\hbar^2\Delta\tau} \right)^{3A/2} e^{-m(\mathbf{R}'-\mathbf{R})^2/2\hbar^2\Delta\tau}$$

- The potential term can then be used as a weight in a branching algorithm.

$$w(\mathbf{R}') = e^{-(V(\mathbf{R}')+V(\mathbf{R})-2E_0)\Delta\tau/2}$$

- Importance sampling improves the variance of the sampling and can be included with

$$G(\mathbf{R}', \mathbf{R}, \Delta\tau) \rightarrow G(\mathbf{R}', \mathbf{R}, \Delta\tau) \frac{\langle \mathbf{R} | \Psi_I \rangle}{\langle \mathbf{R}' | \Psi_I \rangle}$$

# Diffusion Monte Carlo

Branching: Each walker can be deleted or multiply. The number of walkers that continues is equal to $\mathrm{int}\,(w(\mathbf{R}') + \xi)$, where $\xi$ is a uniform random number from $[0, 1]$.

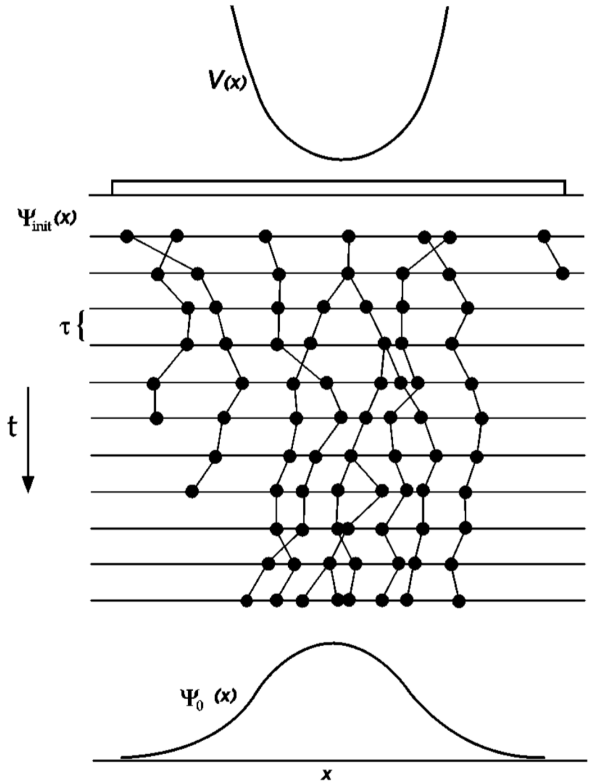



Figure: Reprinted from W.M.C. Foulkes et al. *Rev. Mod. Phys.*, 73:33-83, 2001.

# Estimating Expectation Values

We want to solve something like this

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}.$$

In practice a linear extrapolation is used because $\mathcal{O}\Psi(\tau)$ is hard.

$$\langle \mathcal{O} \rangle \approx 2 \langle \mathcal{O} \rangle_{\text{mixed}} - \langle \mathcal{O} \rangle_{\text{VMC}}$$

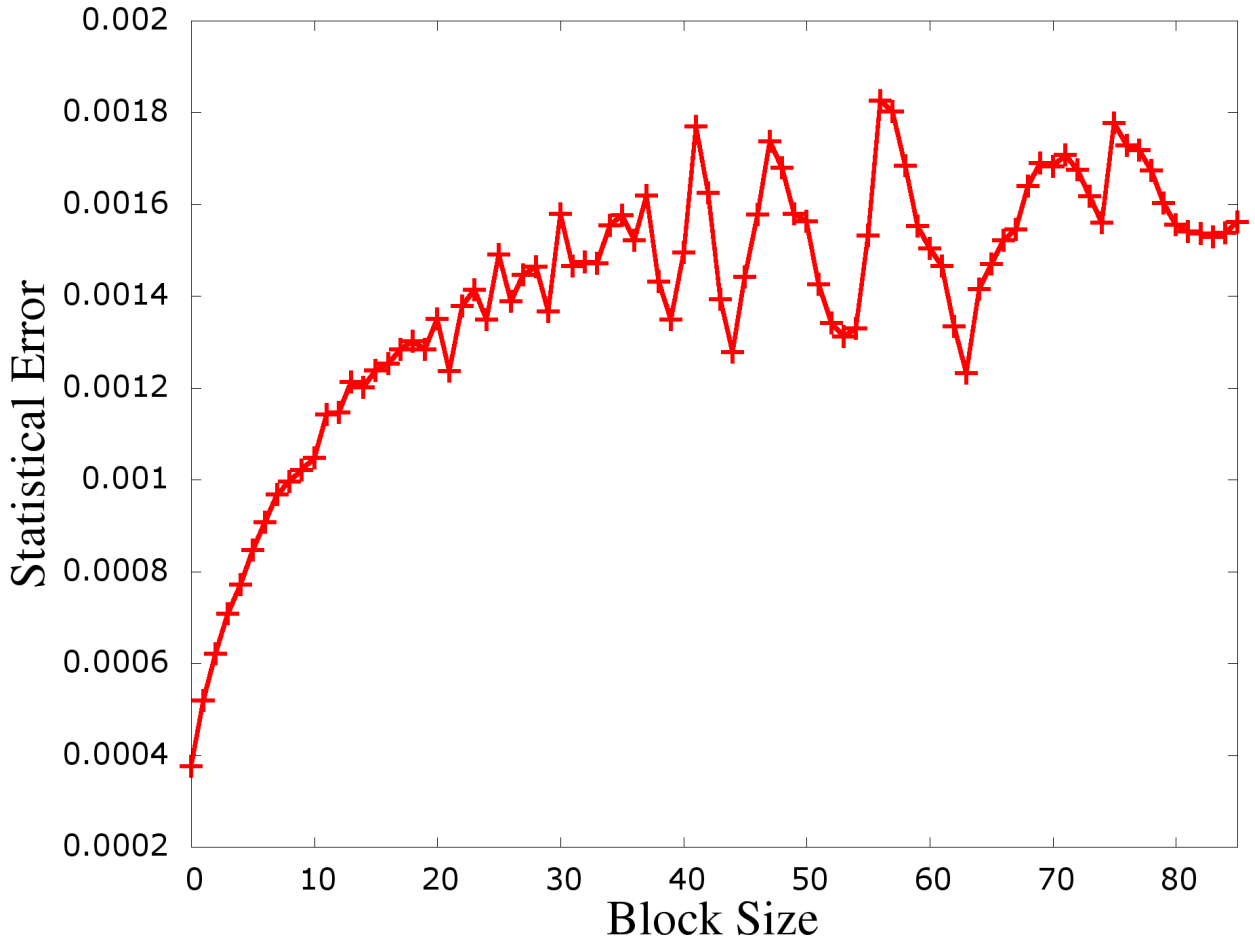
$$\langle \mathcal{O} \rangle_{\text{mixed}} = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle}, \qquad \langle \mathcal{O} \rangle_{\text{VMC}} = \frac{\langle \Psi_T | \mathcal{O} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

In the large $\tau$ limit when $[\mathcal{O}, H]$=0

$$\lim_{\tau \to \infty} \langle \mathcal{O} \rangle_{\text{mixed}} = \langle \mathcal{O} \rangle$$

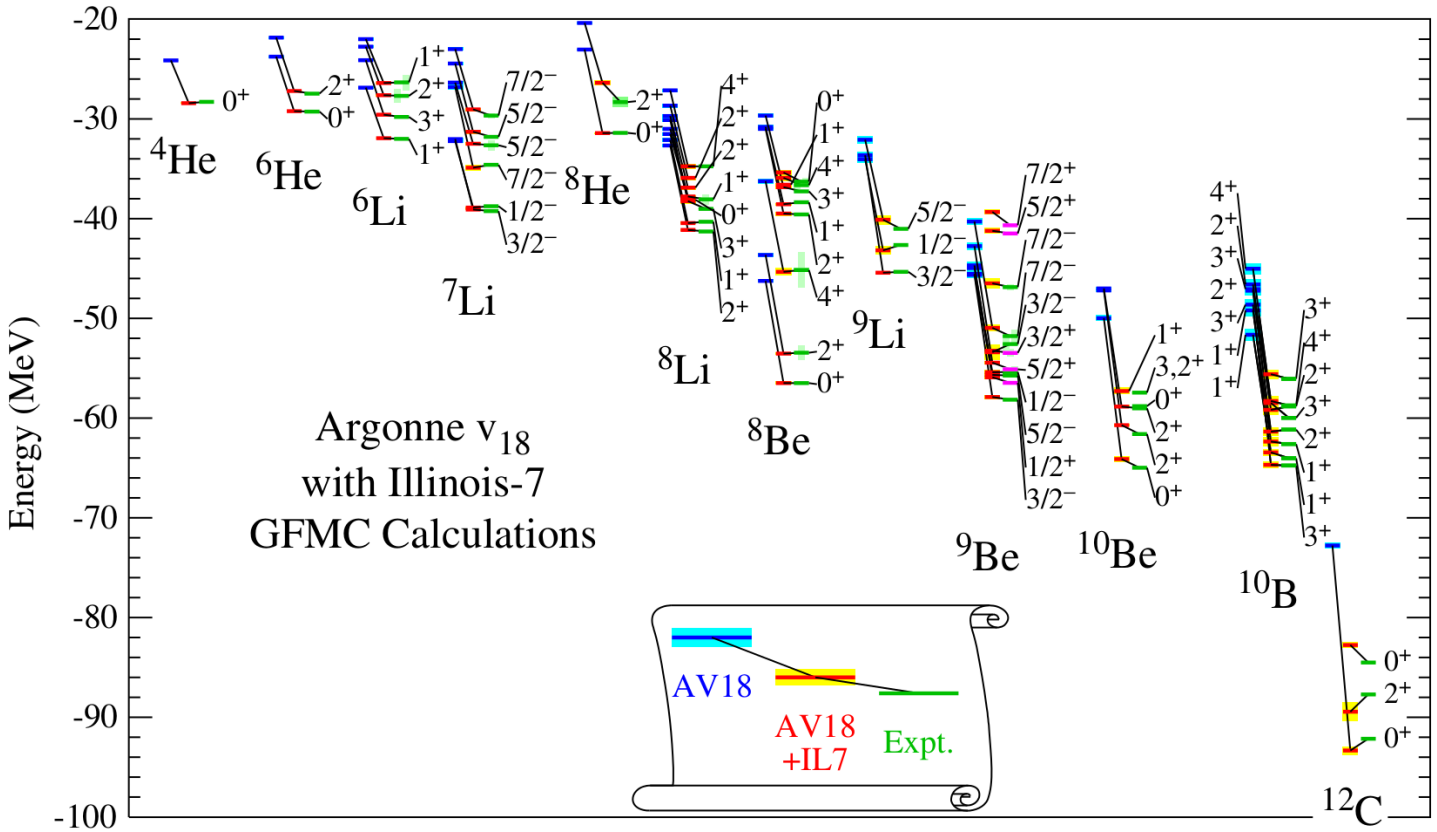
# Estimating Error

Our energy estimates are correlated and so we estimate error using block averaging



# Green's Function Monte Carlo

- GFMC follows DMC exactly for the spatial integrals, but performs the sums of $2^A$ spin and $\frac{A!}{Z!(A-Z)!}$ isospin states, for $A$ nucleons with $Z$ protons explicitly.



# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- AFDMC samples auxiliary fields to rotate the spins/isospins of the walkers.
- The spin/isospin dependent part of the potential is what is used in the spin/isospin dependent part of the propagator.

$$G_{SD}(R'S', RS, \Delta\tau) = \left\langle R'S' \right| e^{-V_{SD}\Delta\tau} \left| RS \right\rangle$$

$$V_{SD} = \sum_{p=2}^{6} \sum_{i<j} v_p(r_{ij}) \mathcal{O}_{ij}^{p}$$

- For $v_6$, a truncation of the phenomenological Argonne $v_{18}$ potential, the operators are $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $S_{ij}$ and $S_{ij}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, where $S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- To avoid explicitly doing the $2^A \frac{A!}{Z!(A-Z)!}$ sums over the spin-isospin states AFDMC writes the spin-isospin dependent propagator in terms of squared single particle operators.
- The spin-isospin dependent operators

$$e^{-V_{SD}\Delta\tau}$$

is sampled by using the Hubbard-Stratanovich transformation.

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

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The potential can be written in terms of matrices that are made of the $v_p(r_{ij})$, are symmetric, and 0 if $i = j$.

$$V_{SD} = \frac{1}{2}\sum_{i\alpha j\beta} \sigma_{i\alpha} A^{\sigma}_{i\alpha j\beta} \sigma_{j\beta} + \frac{1}{2}\sum_{i\alpha j\beta} \sigma_{i\alpha} A^{\sigma\tau}_{i\alpha j\beta} \sigma_{j\beta} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + \frac{1}{2}\sum_{ij} A^{\tau}_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

- We can construct these matrices and then solve for their eigenvalues and eigenvectors.

$$\sum_{j\beta} A^{\sigma}_{i\alpha j\beta} \psi^{\sigma}_{nj\beta} = \lambda^{\sigma}_{n} \psi^{\sigma}_{ni\alpha}$$

$$\sum_{j\beta} A^{\sigma\tau}_{i\alpha j\beta} \psi^{\sigma\tau}_{nj\beta} = \lambda^{\sigma\tau}_{n} \psi^{\sigma\tau}_{ni\alpha}$$

$$\sum_{j} A^{\tau}_{ij} \psi^{\tau}_{n,j} = \lambda^{\tau}_{n} \psi^{\tau}_{ni}$$

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The potential can then be written in terms of the square of new single particle operators.

$$V_{SD} = \frac{1}{2}\sum_{n=1}^{3A}(O_n^{\sigma})^2\,\lambda_n^{\sigma} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A}(O_{n\alpha}^{\sigma\tau})^2\,\lambda_n^{\sigma\tau} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{A}(O_{n\alpha}^{\tau})^2\,\lambda_n^{\tau}$$

$$O_n^{\sigma} = \sum_{j\beta}\sigma_{j\beta}\psi_{nj\beta}^{\sigma}$$

$$O_{n\alpha}^{\sigma\tau} = \sum_{j\beta}\tau_{j\alpha}\sigma_{j\beta}\psi_{nj\beta}^{\sigma\tau}$$

$$O_{n\alpha}^{\tau} = \sum_{j}\tau_{j\alpha}\psi_{nj}^{\tau}$$

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

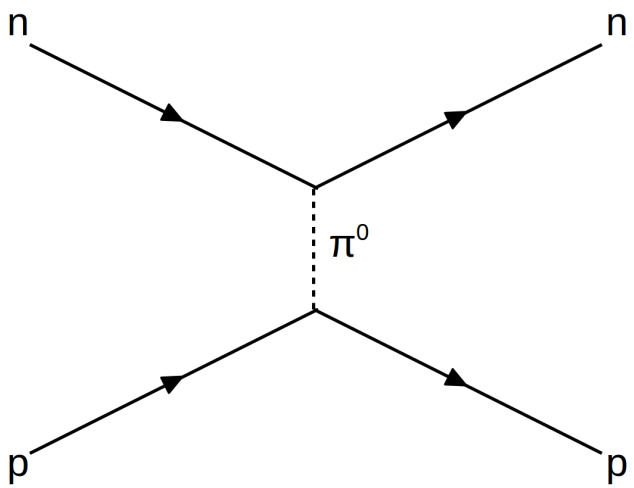
- Since we have squared single particle operators in the propagator we can now rewrite the propagator in terms of the Hubbard-Stratanovich transformation.

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

- Since we have 15A operators ($3A$ for $O_n^\sigma$, $9A$ for $O_{n\alpha}^{\sigma\tau}$, and $3A$ for $O_{n\alpha}^{\tau}$), the spin-isospin dependent part of the propagator becomes

$$G_{SD}(R'S', RS, \Delta\tau) = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n \Delta\tau} x_n O_n}.$$

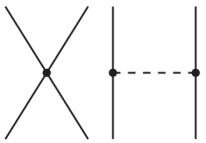
# Hamiltonian



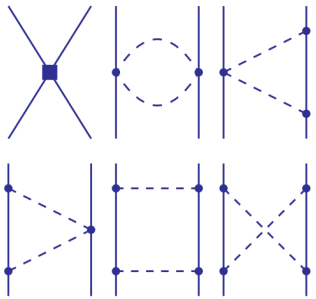

Based on meson exchange

- Argonne $v_{18}$ (NN)
- CD-Bonn (NN)
- Urbana UIX (NNN)
- Illinois (NNN)

**LO**
$(Q/\Lambda_\chi)^0$



**NLO**
$(Q/\Lambda_\chi)^2$



Based on $\chi$EFT expansion in momentum (up to N2LO)

Figure from R. Machleidt and D.R. Entem, *Chiral effective field theory and nuclear forces*, Phys. Rep. **503**, 1 (2011)

# Hamilatonian - Argonne $v6'$ (AV6′)

- For this work I have used the NN AV6′ potential with no 3N interaction, though I will be showing some preliminary results with the $\chi$EFT NN and 3N potentials up to N2LO.
- First 6 operators of the AV18 potential

$$v_{ij} = \sum_{p=1}^{6} v_p(\mathbf{r}_{ij}) \mathcal{O}_{ij}^p$$

$$\mathcal{O}_{ij}^p = 1,\ \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j,\ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j,\ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j,\ S_{ij},\ S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

$$S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

# Slater Determinant

- Properties:
  - Antisymmetric
  - Cluster Decomposable
    $|A+B\rangle = |A\rangle\,|B\rangle$


- The simplest wave function for a many-fermion system obeying these properties is a Slater determinant where $\phi_i(\mathbf{r}_i, s_i)$ are single particle nucleon states.

$$\psi_T = \langle RS|\phi\rangle = \mathcal{A}\prod_{i=1}^{A}\phi_i(\mathbf{r}_i, s_i) = \frac{1}{A!}\det\,\phi_i(\mathbf{r}_i, s_i)$$

- Short range correlations need to be put in by hand via Jastrow-like correlations.

$$|\psi_T\rangle = \prod_{i<j} f(r_{ij})\,|\phi\rangle\,.$$

# Spin Dependent Correlations

- Two spin dependent wave functions that obey these two properties are the exponentially correlated and symmetrized product wave functions, where $\mathcal{O}_{ij}^{p}$ are the AV6 operators, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $S_{ij}$ and $S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, where $S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$.

$$|\psi_T\rangle = \left[ \prod_{i<j} f_c(r_{ij}) \right] e^{\sum_{i<j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^{p}} |\phi\rangle$$

$$|\psi_T\rangle = \left[ \prod_{i<j} f_c(r_{ij}) \right] \mathcal{S} \prod_{i<j} \left( 1 + \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^{p} \right) |\phi\rangle$$

- These two wave functions are the same up to second order except for commutator terms.

# Expand to Linear Correlations

- Because of the cost for larger systems in 2007 they only included Jastrow correlations.

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] |\phi\rangle$$

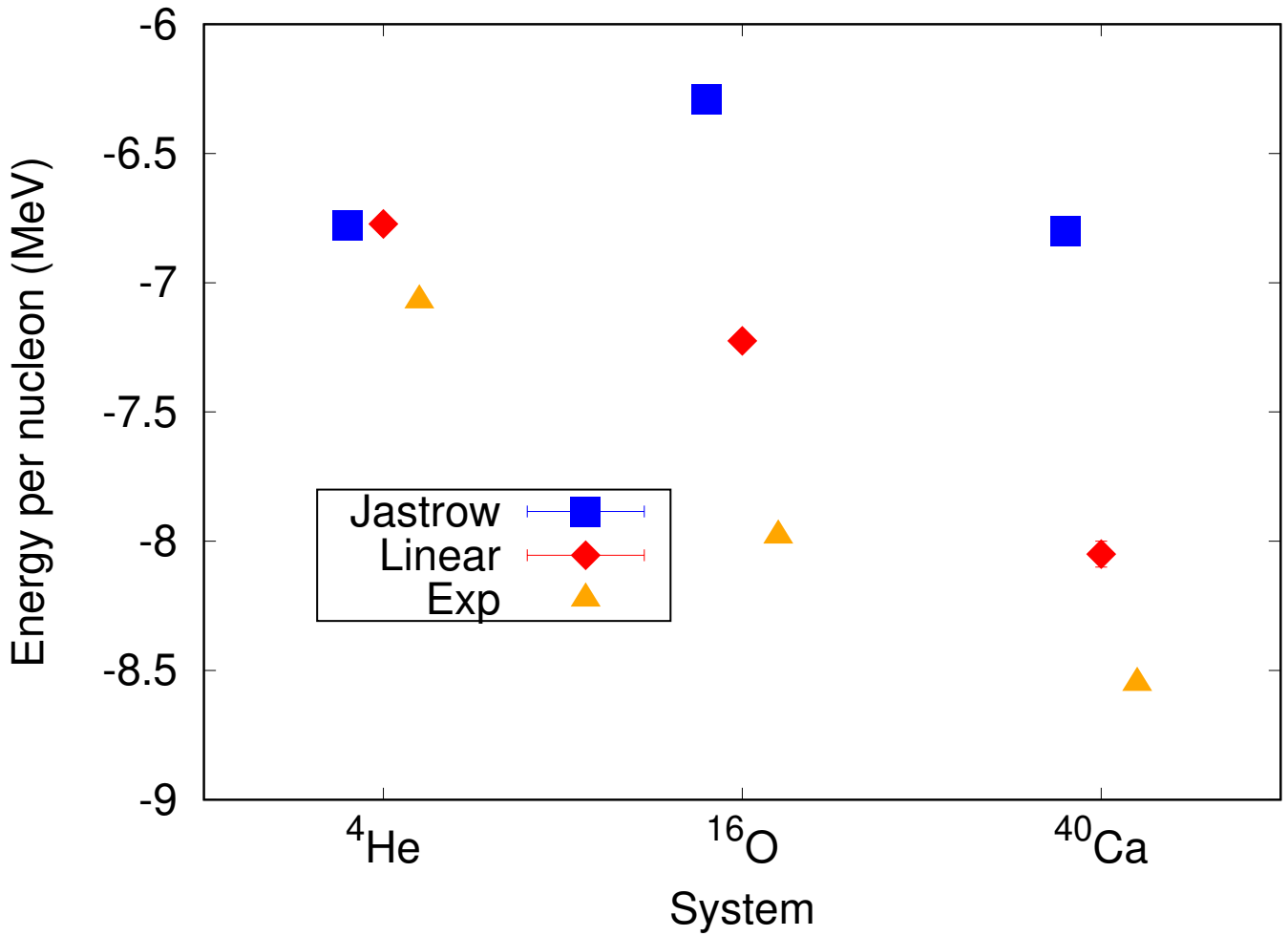
S. Gandolfi et al. *Phys. Rev. Lett.*, **99**, 022507, 2007.

- By 2014 they added spin-isospin correlations to improve overlap with tensor. This is a truncated expansion of either full wave function from before.

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] \left(1 + \sum_{i<j} \sum_{p} f_p(r_{ij}) \mathcal{O}_{ij}^{p}\right) |\phi\rangle$$

S. Gandolfi et al. *Phys. Rev. C.*, **90**, 061306(R), 2014.

# Compare Jastrow to Jastrow+Linear



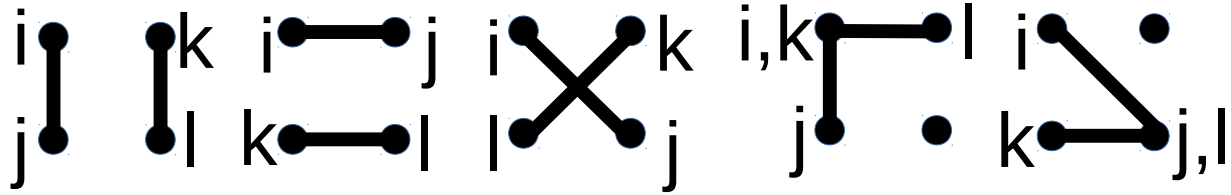

Data taken from each paper respectively.

# Symmetrized Product Wave Function

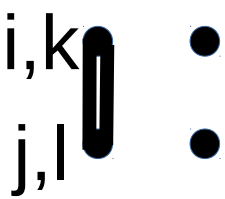
- The logical next step was to keep more terms in the expansion.

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_{p} f_p(r_{ij})\mathcal{O}^p_{ij} + \frac{1}{2}\sum_{i<j}\sum_{p} f_p(r_{ij})\mathcal{O}^p_{ij} \sum_{\substack{k<l \\ ij\neq kl}}\sum_{q} f_q(r_{kl})\mathcal{O}^q_{kl}\right]|\phi\rangle$$

Allowed



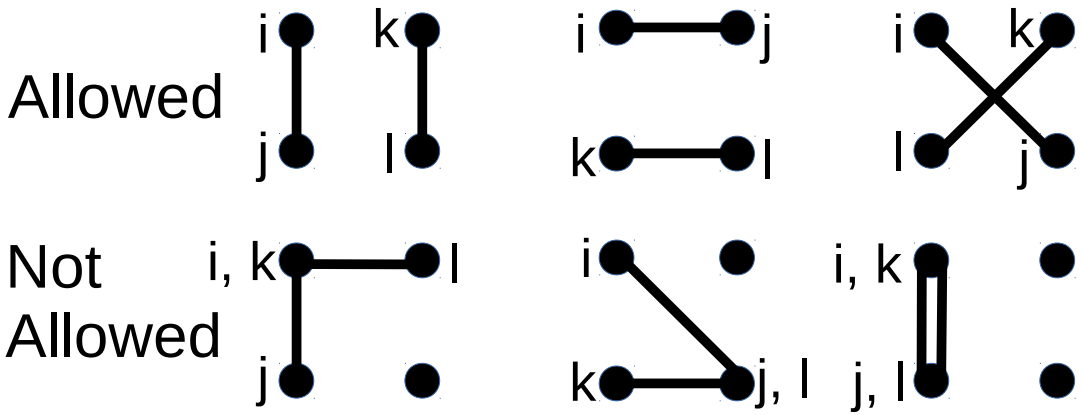

Not Allowed



# Independent Pair Quadratic Correlations

- Or it can be expanded to get independent pair quadratic terms

$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right]\left[1 + \sum_{i<j}\sum_{p} f_p(r_{ij})\mathcal{O}^p_{ij} + \sum_{i<j}\sum_{p} f_p(r_{ij})\mathcal{O}^p_{ij} \sum_{k<l,\mathrm{ip}}\sum_{q} f_q(r_{kl})\mathcal{O}^q_{kl}\right]|\phi\rangle$$



# Results - AFDMC

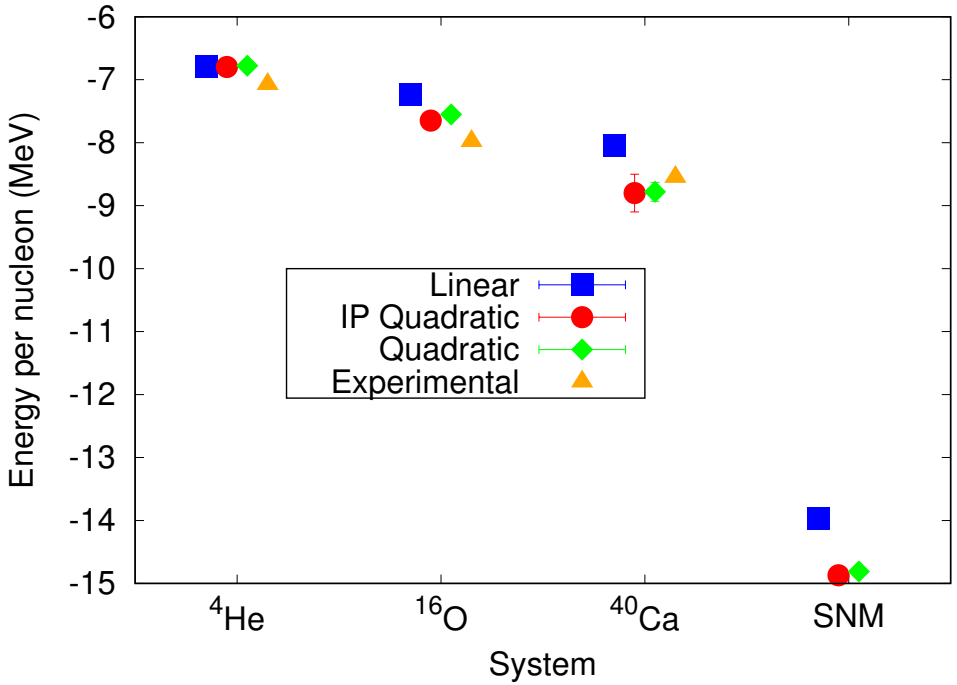
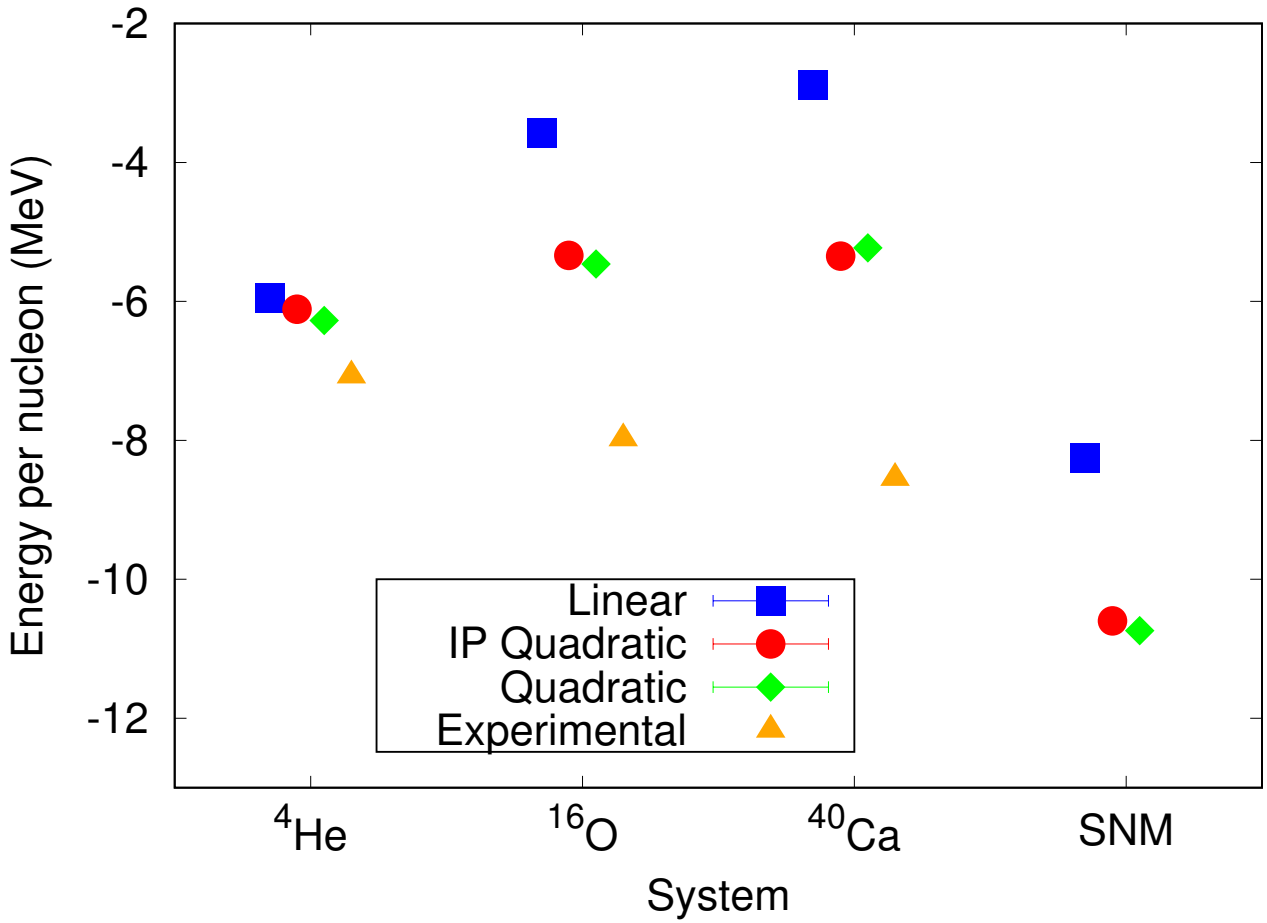



Table 1: Energy (*per nucleon) in MeV

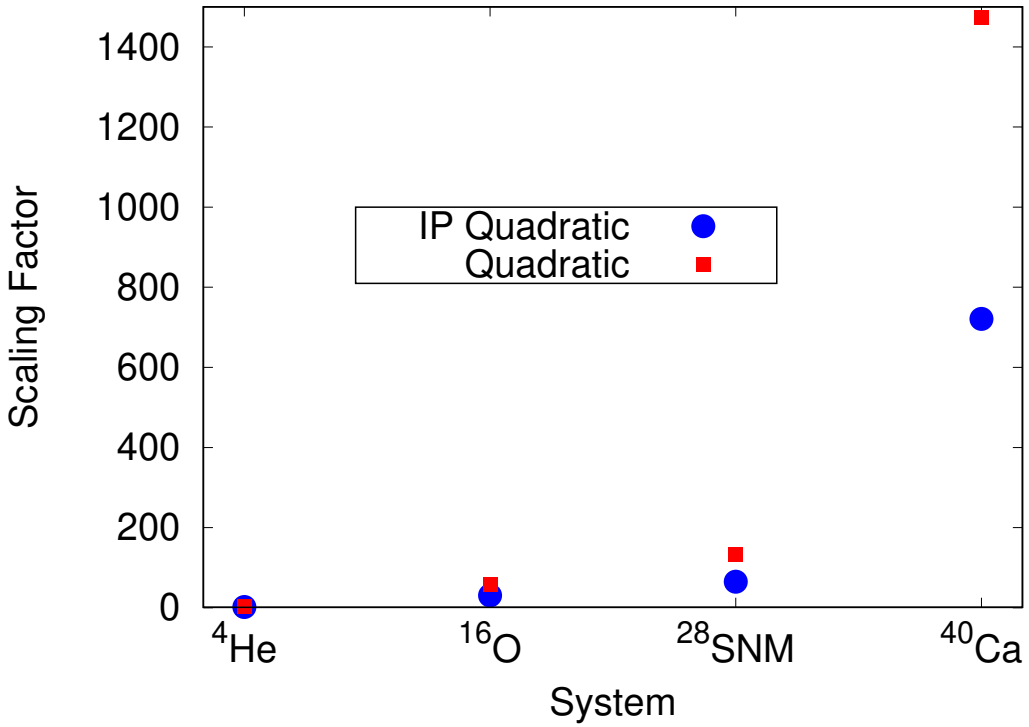
| System | Linear | IP Quadratic | Quadratic | Experimental |
|---|---|---|---|---|
| $^{4}$He | -27.14(4) | -27.19(3) | -27.11(3) | -28.296 |
| $^{16}$O | -115.7(9) | -122.4(1.5) | -120.8(1.3) | -127.62 |
| $^{40}$Ca | -322(3) | -350(10) | -351(6) | -342.1 |
| SNM* | -13.97(3) | -14.87(4) | -14.81(3) | |

D. Lonardoni et al. *Phys. Rev. C.*, **97**, 044318, 2018.

# Results - VMC


-2
-4
-6
-8
-10
-12
Energy per nucleon (MeV)
Linear
IP Quadratic
Quadratic
Experimental
$^4$He
$^{16}$O
$^{40}$Ca
SNM
System

# Quadratic Correlation Cost




| | $^4$He | $^{16}$O | SNM(28) | $^{40}$Ca |
|---|---|---|---|---|
| IP Quadratic | 1.73 | 30.7 | 64.8 | 720.9 |
| Quadratic | 2.00 | 58.8 | 133.6 | 1473.9 |

# Results - $\chi$EFT up to N2LO - Preliminary

ADD RESULTS HERE

# Placeholder

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# Placeholder

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