

Dissertation Defense:
Improved Trial Wave Functions for Quantum
Monte Carlo Calculations of Nuclear Systems and
Their Applications

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Outline

1 Motivation

2 Research

- QMC Methods
- Trial Wave Function
- Alpha Formation in NS

3 Conclusion

- Conclusion
- Future Work

Outline

- 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 χ EFT potentials as well.
 - Performance scaling, both for x86 computers as well as linear vs. quadratic correlations.
- Other (future) correlations
 - Exponential correlations
 - Eigenvector discontinuity problem and square root matrix fix
 - Preliminary results

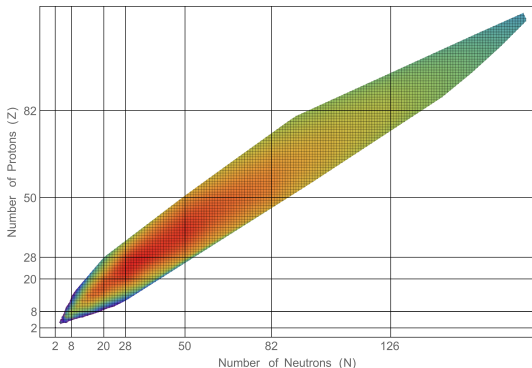
Outline

- Application to α -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

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

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



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.

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

Diffusion Monte Carlo

- The propagated wave function can be written

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

- 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 $\Delta\tau = \tau/N$.

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

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

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.

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

- 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 $\text{int}(w(\mathbf{R}') + \xi)$, where ξ is a uniform random number from $[0, 1]$.

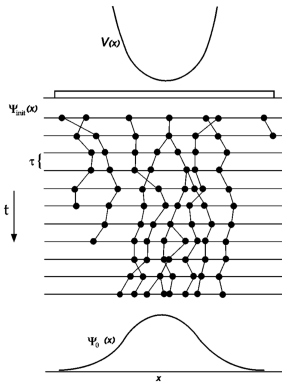


Figure: Reprinted from W.M.C. Foulkes et al. *Rev. Mod. Phys.*, 73:33-83, 2001.

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.

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

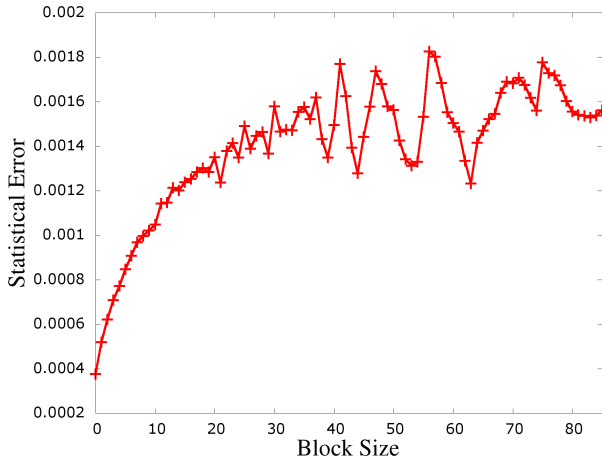
$$\langle \mathcal{O} \rangle_{\text{mixed}} = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle}, \quad \langle \mathcal{O} \rangle_{\text{VMC}} = \frac{\langle \Psi_T | \mathcal{O} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

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

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

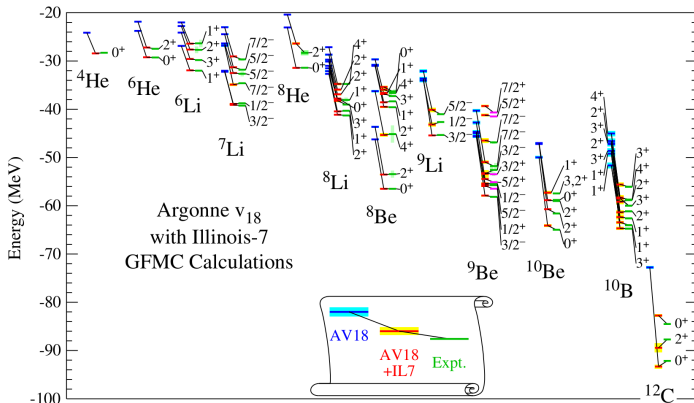
Estimating Error

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.

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

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

- For v_6 , a truncation of the phenomenological Argonne v_{18} potential, the operators are $\sigma_i \cdot \sigma_j$, $\tau_i \cdot \tau_j$, $\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j$, S_{ij} and $S_{ij} \tau_i \cdot \tau_j$, where $S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$

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.

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

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 $i = j$.

$$V_{SD} = \frac{1}{2} \sum_{i\alpha j\beta} \sigma_{i\alpha} A_{i\alpha j\beta}^{\sigma} \sigma_{j\beta} + \frac{1}{2} \sum_{i\alpha j\beta} \sigma_{i\alpha} A_{i\alpha j\beta}^{\sigma\tau} \sigma_{j\beta} \tau_i \cdot \tau_j + \frac{1}{2} \sum_{ij} A_{ij}^{\tau} \tau_i \cdot \tau_j$$

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

$$\sum_{j\beta} A_{i\alpha j\beta}^{\sigma} \psi_{nj\beta}^{\sigma} = \lambda_n^{\sigma} \psi_{ni\alpha}^{\sigma}$$

$$\sum_{j\beta} A_{i\alpha j\beta}^{\sigma\tau} \psi_{nj\beta}^{\sigma\tau} = \lambda_n^{\sigma\tau} \psi_{ni\alpha}^{\sigma\tau}$$

$$\sum_j A_{ij}^{\tau} \psi_{n,j}^{\tau} = \lambda_n^{\tau} \psi_{ni}^{\tau}$$

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

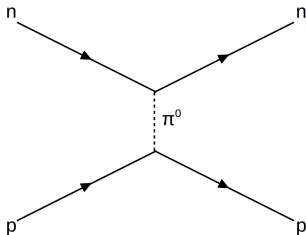
- Since we have squared single particle operators in the propagator we can now rewrite the propagator in terms of the Hubbard-Stratanovich transformation.

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

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

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

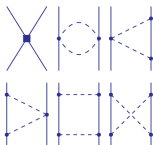
Hamiltonian



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



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



Based on meson exchange

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

Based on χ 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)

Hamiltonian - 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 χ EFT NN and 3N potentials up to N2LO.
- First 6 operators of the AV18 potential

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

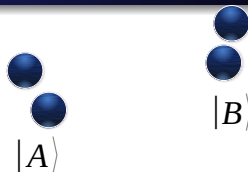
$$\mathcal{O}_{ij}^p = 1, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, S_{ij}, S_{ij} \tau_i \cdot \tau_j$$

$$S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$$

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, $\sigma_i \cdot \sigma_j$, $\tau_i \cdot \tau_j$, $\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j$, S_{ij} and $S_{ij} \tau_i \cdot \tau_j$, where $S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$.

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

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

- 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.

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

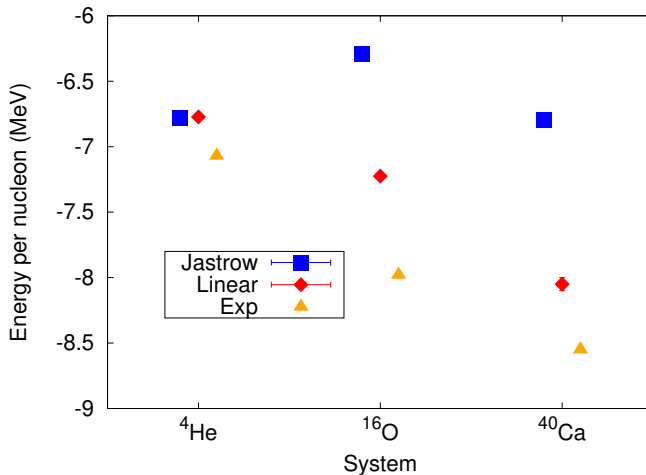
S. Gandolfi et al. *Phys. Rev. Lett.*, **99**, 022507, 2007.

- 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

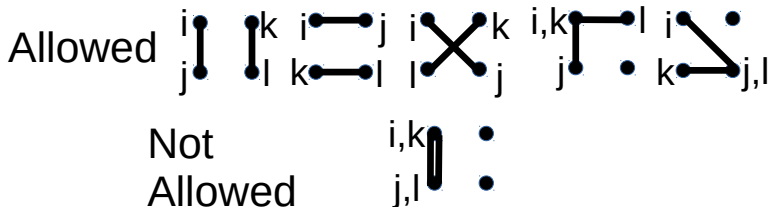


Data taken from each paper respectively.

Symmetrized Product Wave Function

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

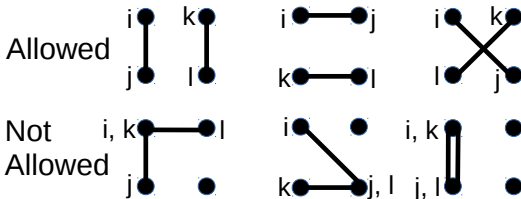
$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij}) \right] \left[1 + \sum_{i<j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p + \frac{1}{2} \sum_{i<j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \sum_{\substack{k<l \\ ij \neq kl}} \sum_q f_q(r_{kl}) \mathcal{O}_{kl}^q \right] |\phi\rangle$$



Independent Pair Quadratic Correlations

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

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



Results - AFDMC

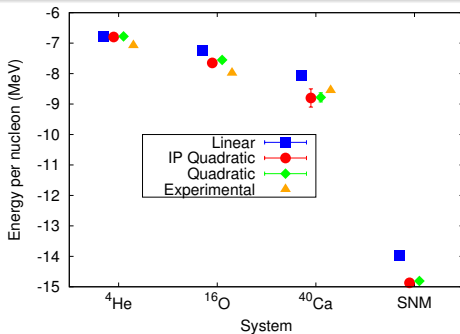
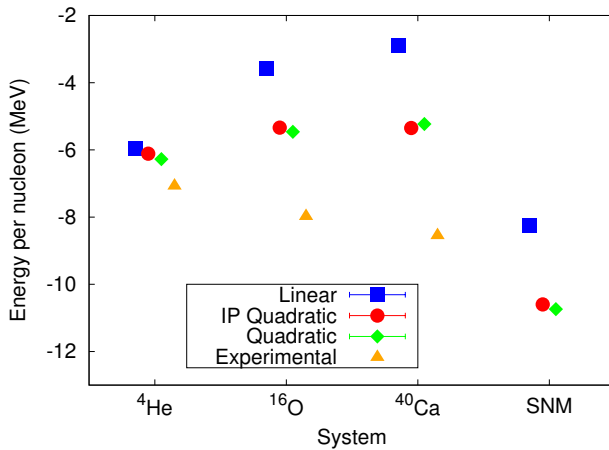


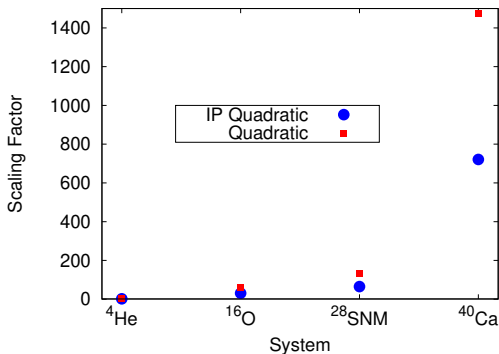
Table 1 : Energy (*per nucleon) in MeV

System	Linear	IP Quadratic	Quadratic	Experimental
^4He	-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)	

Results - VMC



Quadratic Correlation Cost



	^4He	^{16}O	^{28}Si	^{40}Ca
IP Quadratic	1.73	30.7	64.8	720.9
Quadratic	2.00	58.8	133.6	1473.9

Results - χ EFT up to N2LO - Preliminary

Calculation	Correlations	${}^4\text{He}$	${}^{16}\text{O}$	SNM
VMC	Linear	-5.86(1)	-1.08(1)	1.56(5)
VMC	IP Quadratic	—	-4.03(4)	—
VMC	Quadratic	-6.72(1)	-3.95(4)	—
AFDMC	Linear	-6.89(2)	-5.74(4)	-9.5(1)
AFDMC	IP Quadratic	—	-7.3(2)	-12.5(1)
AFDMC	Quadratic	-6.91(2)	-6.9(2)	-12.6(1)

Exponential Correlations

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

Placeholder

blah

Placeholder

blah

Extra Slides

Extra Slides

Slide comparing the AV6' results with N2LO results. Remember that N2LO has the spin-orbit, which decreases binding.