

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

- Future Work
- Conclusion

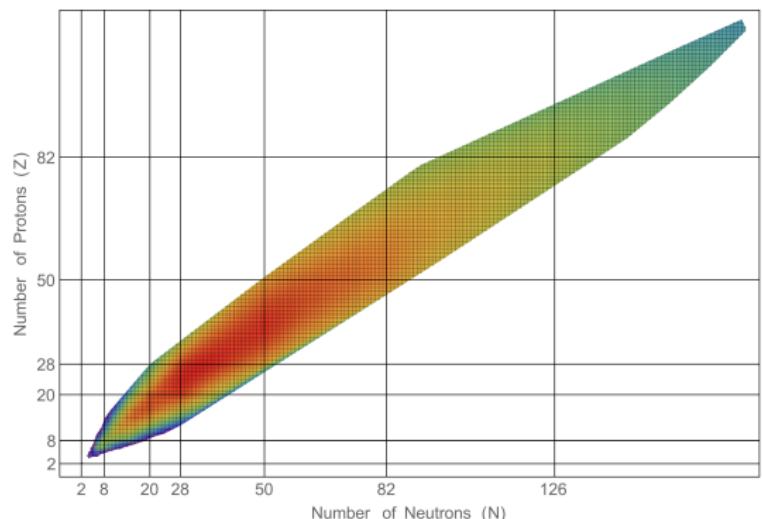
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└ Outline

Nuclear Many Body Problem

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

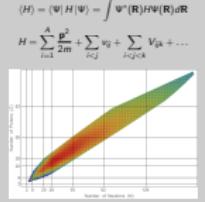
$$H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m} + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$



└ Motivation

└ Nuclear Many Body Problem

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- Many-body quantum problem with n and p dof.
- GROUND STATE properties.
- Up to ^{40}Ca and $\sim A=100$ for nuclear matter.
- Show on the chart up to where our method is applicable.

Nuclear Many Body Methods

└ Motivation

└ Nuclear Many Body Methods

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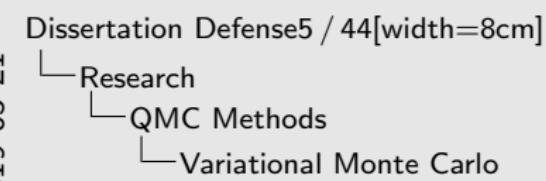
- There are a number of ways to solve this problem.
 - Hartree-Fock
 - Basis-set methods
 - No-core shell model
 - Coupled-cluster
 - Self consistent Green's function method
 - Quantum Monte Carlo
 - VMC
 - GFMC
 - AFDMC

- HF and basis set methods can only use “soft” potentials, but can do non-local potentials.
- QMC complements those because it can do “hard” potentials, but can’t do non-local potentials.

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Variational Monte Carlo

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- VMC starts with a trial wave function which includes variable parameters.
- Variational energy is an upper bound to the ground state energy.

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

- Integral is solved with MC integration.

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

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Variational Monte Carlo

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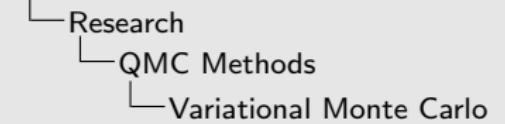
- Multiply and divide the numerator by $\Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})$.

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

- 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 $P(\mathbf{R})$.



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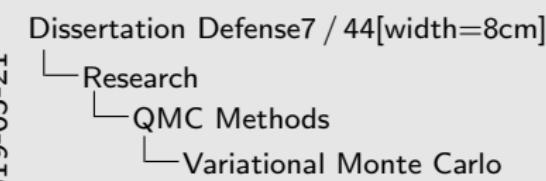
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Variational Monte Carlo

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- 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 $E_V \geq E_0$.

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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.

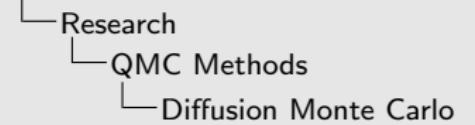
$$H\Psi = i\hbar \frac{d\Psi}{dt} \xrightarrow{\tau=it/\hbar} H\Psi = -\frac{d\Psi}{d\tau}$$

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.

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



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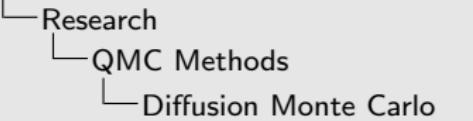
- The propagated wave function can be written

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

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

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

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- In practice: Green's function (propagator).
- Can't do full time propagation.
- Can do short time propagation.
- Stress the importance of having an accurate and “cheap” wave function.

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.

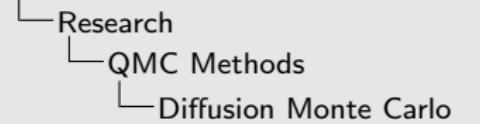
$$\langle \mathbf{R}' | e^{-T\Delta\tau} | \mathbf{R} \rangle = \left(\frac{m}{2\pi\hbar^2\Delta\tau} \right)^{3A/2} e^{-m(\mathbf{R}'-\mathbf{R})^2/2\hbar^2\Delta\tau}$$

- 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

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



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Diffusion Monte Carlo - Branching

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 $[0, 1]$.

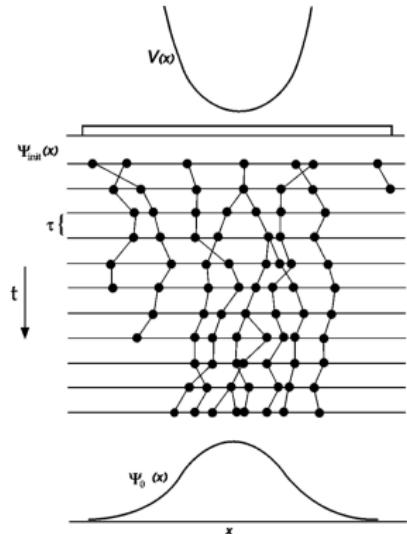


Figure: Reprinted from W.M.C. Foulkes et al.
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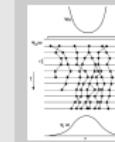


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Estimating Expectation Values

We want to solve something like this

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

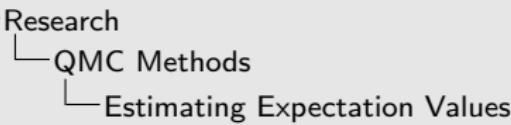
In practice a linear extrapolation is used because $\mathcal{O}\Psi(\tau)$ is hard.

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

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

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

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



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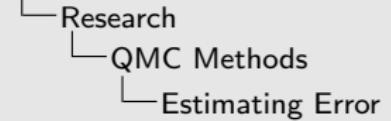
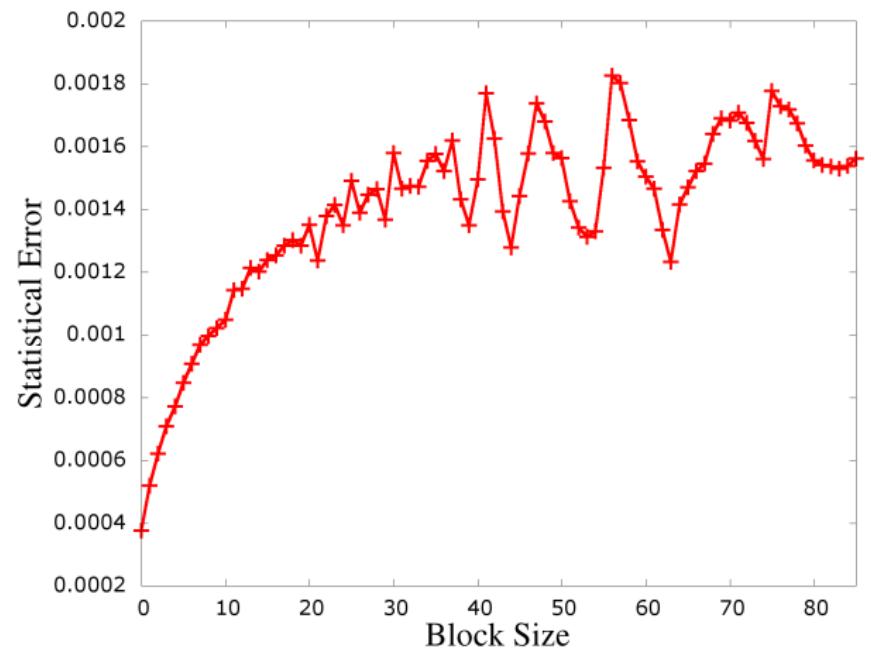
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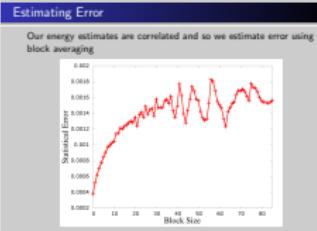
- It's difficult to operate through the propagator.
- Accurate to $\mathcal{O}[(\psi(\tau) - \psi_T)^2]$
- This could be done with **forward walking** but it typically isn't necessary.

Estimating Error

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



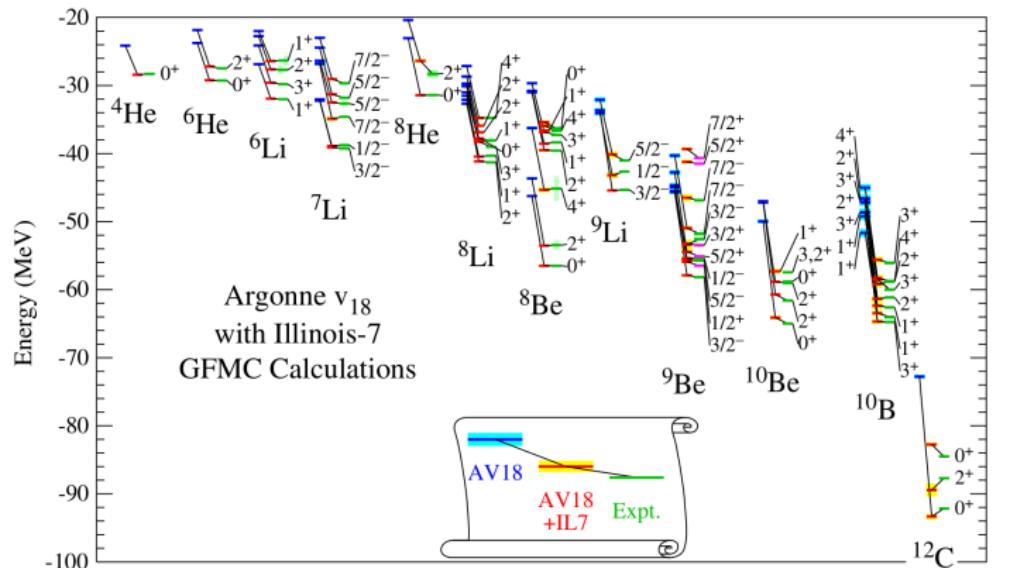
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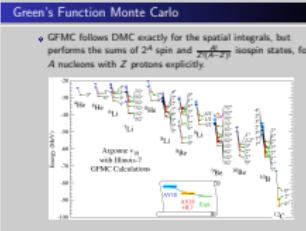
- We don't usually (though you could) talk about the uncertainty in the statistical errors. It's the wiggles at the plateau. We just report 1 digit.

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.



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- The excited states come by changing the J^π and T of the wave function.

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- Mimicking the diffusion in DMC, 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 $S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$

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Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The spin-isospin dependent operators

$$\begin{aligned} G_{SD}(R'S', RS, \Delta\tau) &= \langle R'S' | e^{-V_{SD}\Delta\tau} | RS \rangle \\ &= \langle R'S' | e^{-\sum_{p=2}^6 \sum_{i < j} v_p(r_{ij}) \mathcal{O}_{ij}^p \Delta\tau} | RS \rangle \end{aligned}$$

is sampled by using the Hubbard-Stratanovich transformation.

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



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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 $i = j$.

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

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

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

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

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Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

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

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

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Research

QMC Methods

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

• 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

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

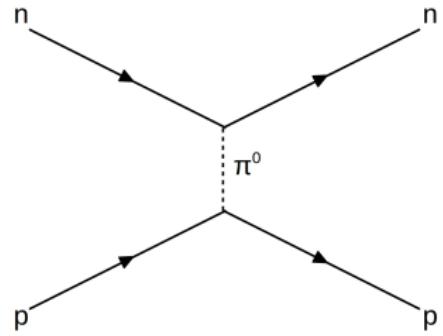
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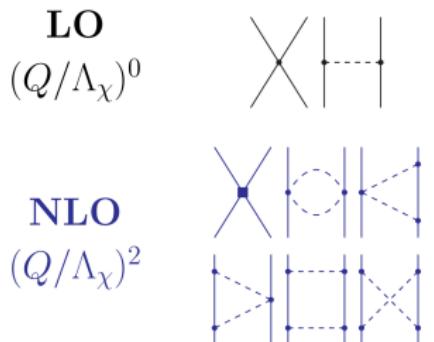
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Hamiltonian



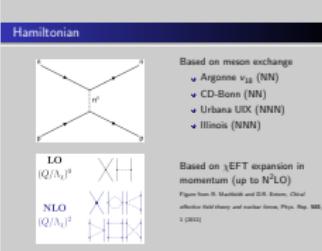
Based on meson exchange

- Argonne v₁₈ (NN)
- CD-Bonn (NN)
- Urbana UIX (NNN)
- Illinois (NNN)



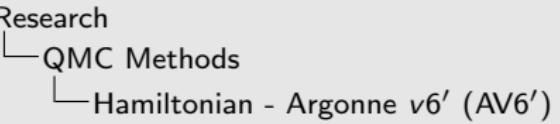
Based on χ EFT expansion in momentum (up to N²LO)

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



Hamiltonian - Argonne v6' (AV6')

2019-05-21



- 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

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

$$\begin{aligned}\mathcal{O}_{ij}^0 &= 1, \quad \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \quad S_{ij}, \quad S_{ij} \tau_i \cdot \tau_j \\ S_{ij} &= 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j\end{aligned}$$

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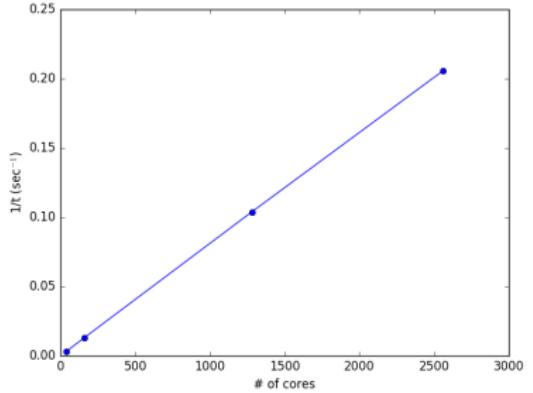
$$\mathcal{O}_{ij}^p = 1, \quad \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \quad S_{ij}, \quad S_{ij} \tau_i \cdot \tau_j$$

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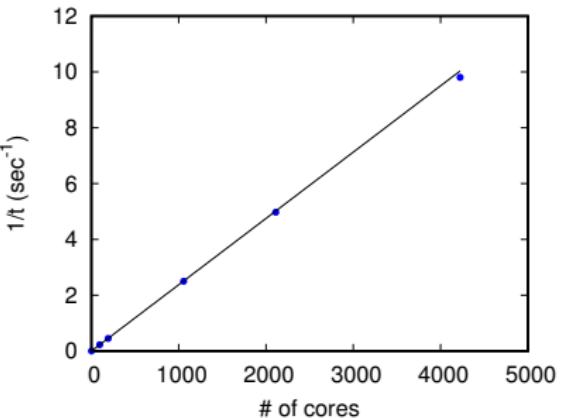
Scaling

- We have written our own AFDMC code.
- Not currently open source, but should be soon.
- Run on CPU made available through XSEDE allocations.

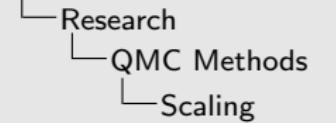
Time to propagate 10,000 walkers of ^{16}O for 100 steps.



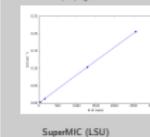
SuperMIC (LSU)



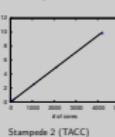
Stampede 2 (TACC)



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Time to propagate 10,000 walkers of ^{16}O for 100 steps.



SuperMIC (LSU)



Stampede 2 (TACC)

Trial Wave Function - 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.

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

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

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

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

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

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

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

2019-05-21

Research

Trial Wave Function

Spin Dependent Correlations

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

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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.

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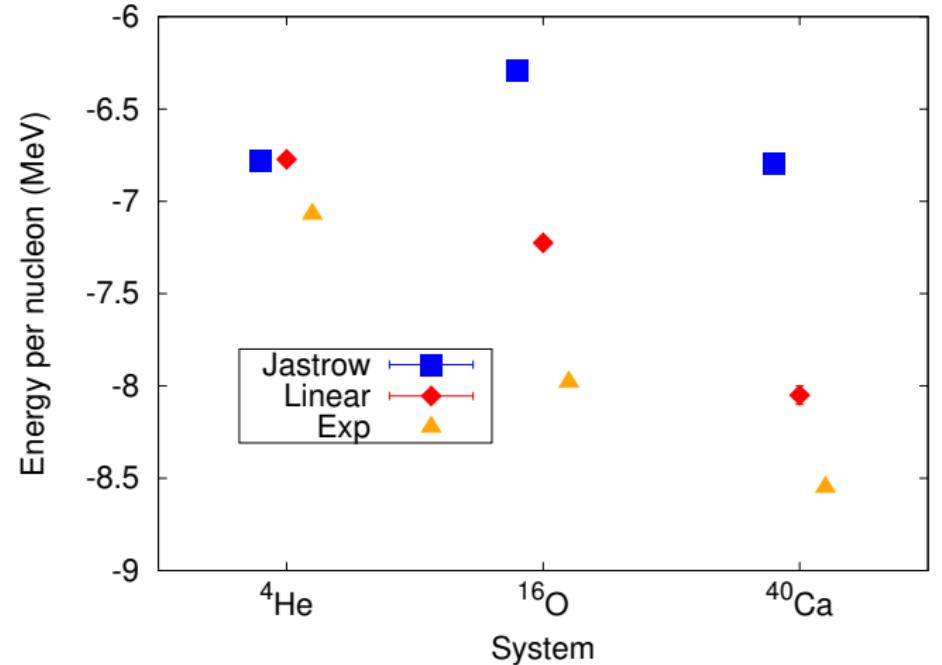
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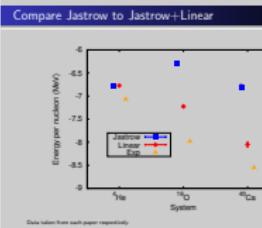
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Compare Jastrow to Jastrow+Linear



Data taken from each paper respectively.

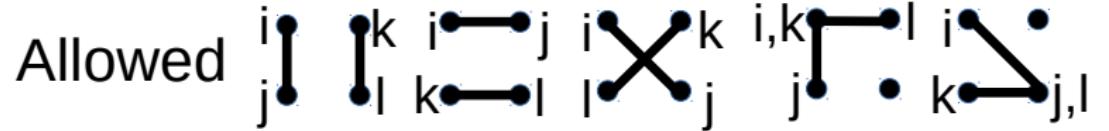


Compare Jastrow to Jastrow+Linear
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Symmetrized Product Wave Function

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

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



Symmetrized Product Wave Function

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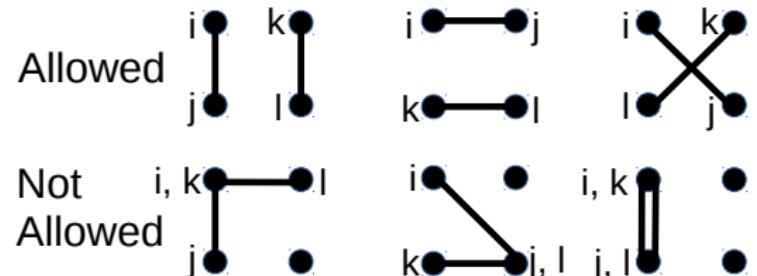
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Allowed						
Not Allowed						

Independent Pair Quadratic Correlations

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

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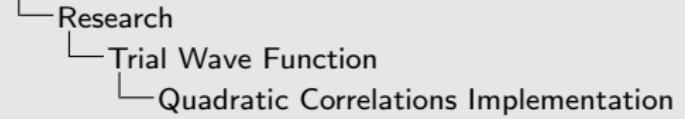
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$$|\psi_T\rangle = \left[\prod_{i < j} \epsilon(r_{ij}) \right] \left[1 + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \right. \\ \left. + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \sum_{k < l, ip} \epsilon(r_{kl}) \mathcal{O}_{kl}^q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

Allowed:

Not Allowed:

Quadratic Correlations Implementation



2019-05-21

- Much of my work was in working out the math and programming for implementing these correlations in an efficient way into the VMC and AFDMC code.
- More details of their implementation can be found in my dissertation, I will be focusing on the physical results.

Results - AFDMC

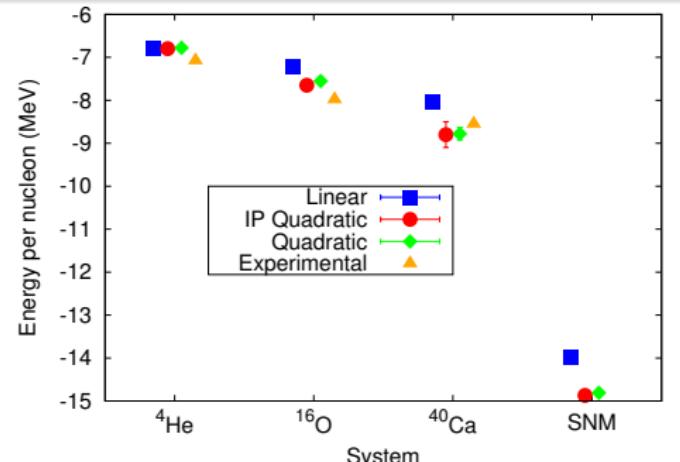
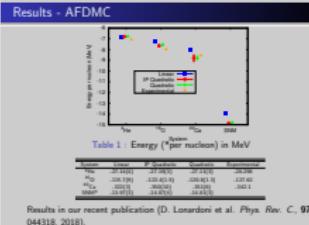


Table 1 : Energy (*per nucleon) in MeV

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)	

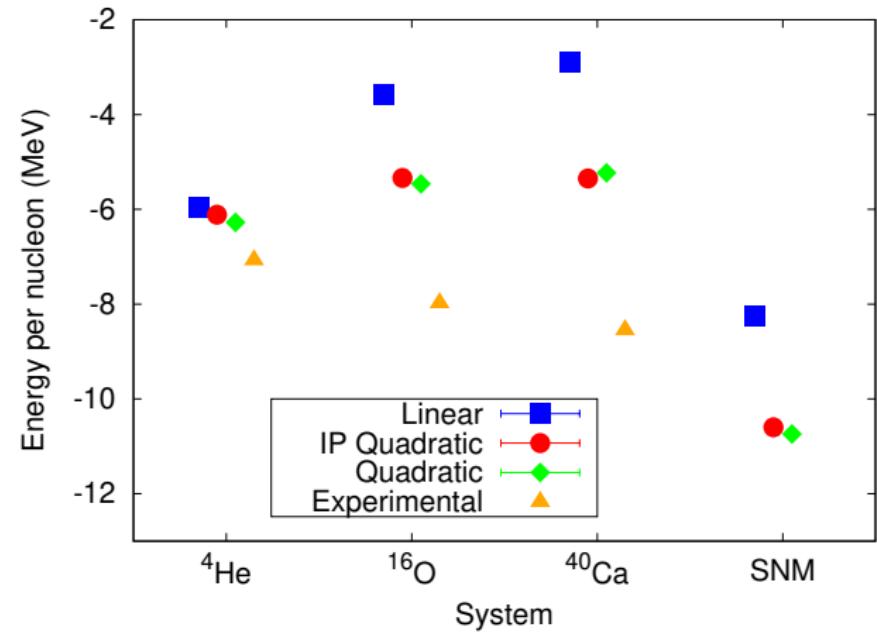
Results in our recent publication (D. Lonardoni et al. *Phys. Rev. C.*, **97**, 044318, 2018).



Results - VMC

Motivation
Research
Conclusion

QMC Methods
Trial Wave Function
Alpha Formation in NS

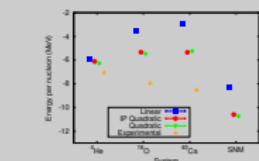


Dissertation Defense 31 / 44 [width=8cm]

└ Research
 └ Trial Wave Function
 └ Results - VMC

2019-05-21

Results - VMC



- Sanity check since AFDMC doesn't have upper bound constraint like VMC.
- ALL decreased in energy, even ^4He .

Results - χ EFT up to N²LO - Preliminary

Calculation	Correlations	⁴ He	¹⁶ 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)

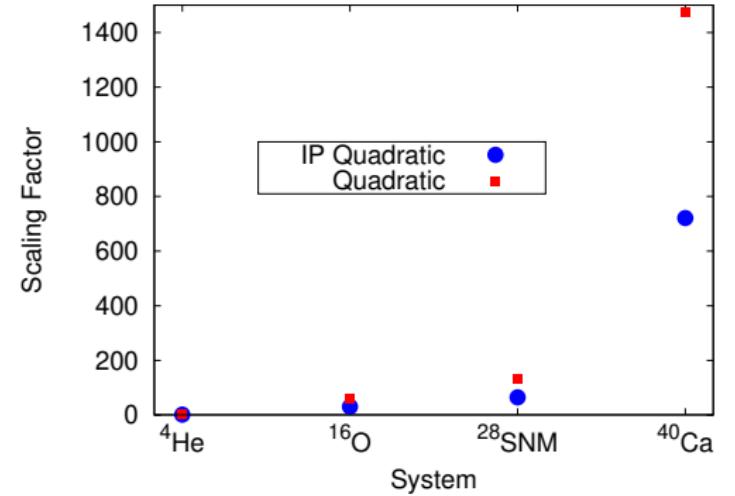
Note that the NN part of N²LO includes the spin-orbit interaction, which is not included in AV6' and which has been shown to decrease binding (S. Gandolfi et al. *Phys. Rev. C.*, **90**, 061306(R), 2014.).

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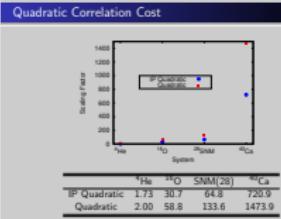
- N²LO with $R_0 = 1$ fm cutoff.
- All the energies are per particle, in MeV.
- All the wave functions have both two- and three-body correlations.
- Local chiral potential at N²LO for R0=1.0fm cutoff.
- ⁴He and SNM are done with the E1 parametrization.
- ¹⁶O is done with the Etau parametrization.
- ⁴He and ¹⁶O also contain the Coulomb.
- Re-optimized for ⁴He and ¹⁶O with quadratic.
- No re-optimization for SNM and only used growth energy.
- SNM with no correction for finite size effects.
- All DMC with constrained-path, no transient/unconstrained.

Quadratic Correlation Cost



	^4He	^{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

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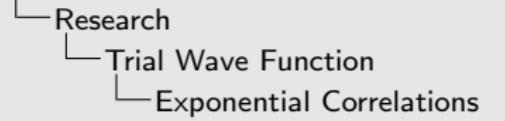


Exponential Correlations

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

- This looks just like the propagator and so we can **use the same trick** with the HS transformation.

$$\begin{aligned} G_{SD}(R'S', RS, \Delta\tau) &= \langle R'S' | e^{- \sum_{p=2}^6 \sum_{i < j} v_p(r_{ij}) \mathcal{O}_{ij}^p \Delta\tau} | RS \rangle \\ &= \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n \Delta\tau} x_n} O_n \end{aligned}$$



2019-05-21

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Exponential Correlations - Preliminary

- Problems with statistical errors related to the sampling.
- Calculating the potential energy with exponential correlations and the rest with linear correlations.

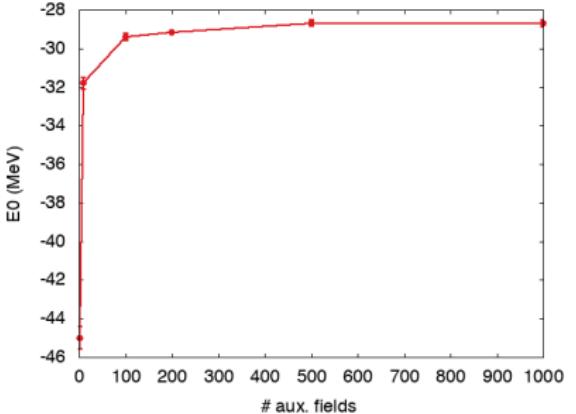


Table 2 : ${}^4\text{He}$ energy with exp correlations. $E_{\text{linear}} = -26.48(9)$ MeV.

# fields	E (MeV)
1	-45.0(6)
10	-31.8(3)
100	-29.4(2)
200	-29.15(8)
500	-28.68(18)
1000	-28.7(2)

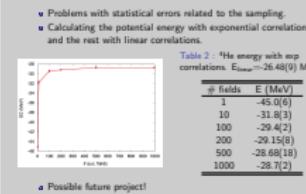
- Possible future project!

2019-05-21

Research

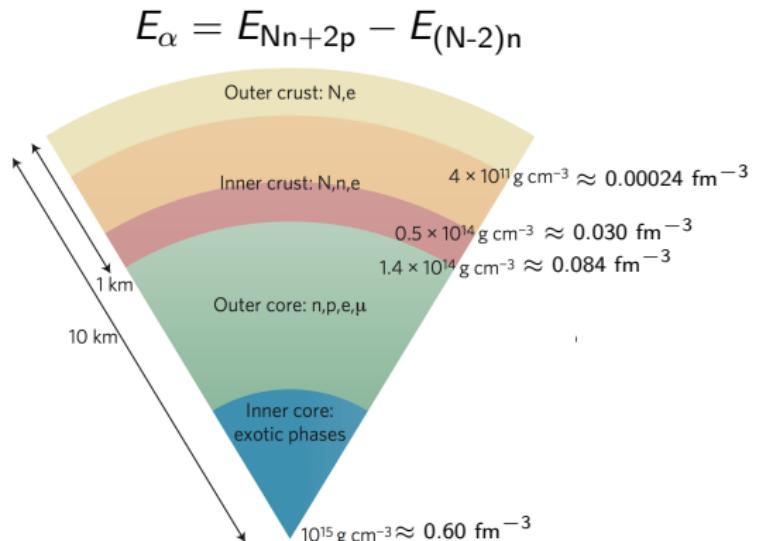
Trial Wave Function

Exponential Correlations - Preliminary

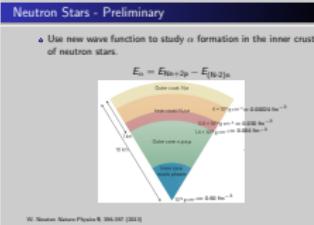


Neutron Stars - Preliminary

- Use new wave function to study α formation in the inner crust of neutron stars.



W. Newton *Nature Physics* **9**, 396-397 (2013)



Alpha Particle Clustering in Mostly Neutron Matter - Preliminary

- If alpha particles form in nearly neutron matter then we should be able to estimate their energy by

$$E_\alpha = E_{14n+2p} - E_{12n}$$

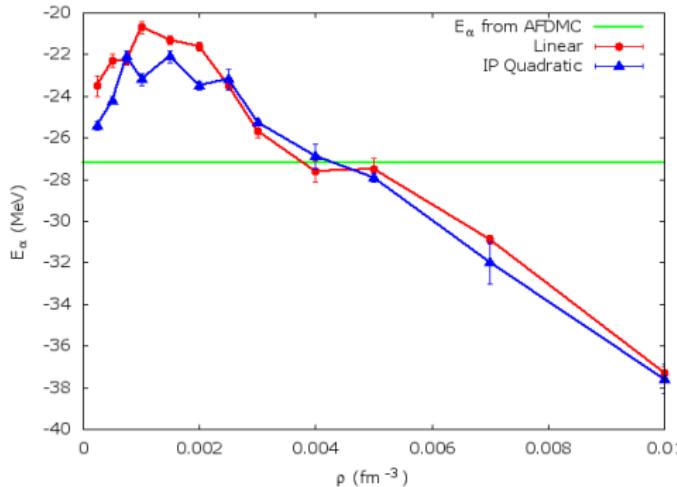
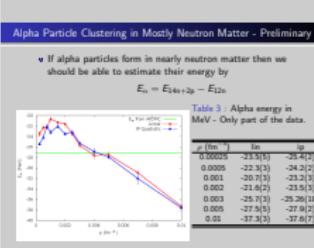


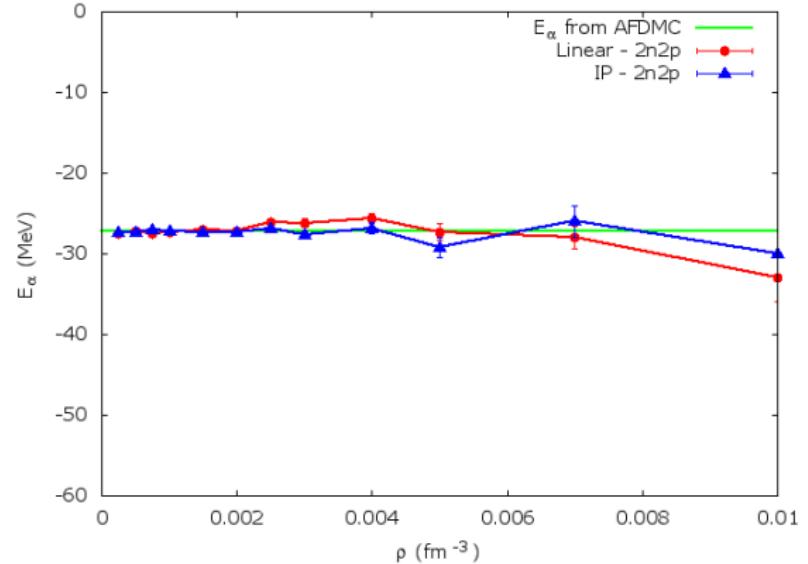
Table 3 : Alpha energy in MeV - Only part of the data.

ρ (fm $^{-3}$)	lin	ip
0.00025	-23.5(5)	-25.4(2)
0.0005	-22.3(3)	-24.2(2)
0.001	-20.7(3)	-23.2(3)
0.002	-21.6(2)	-23.5(3)
0.003	-25.7(3)	-25.26(18)
0.005	-27.5(5)	-27.9(2)
0.01	-37.3(3)	-37.6(7)

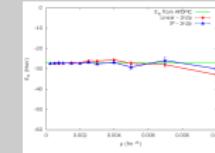
- Green line is what would be expected for an α alone (see next slide for α alone).
- Dissolution at about 0.0025 is about what we would expect from other papers.



2 Protons + 2 Neutrons Only



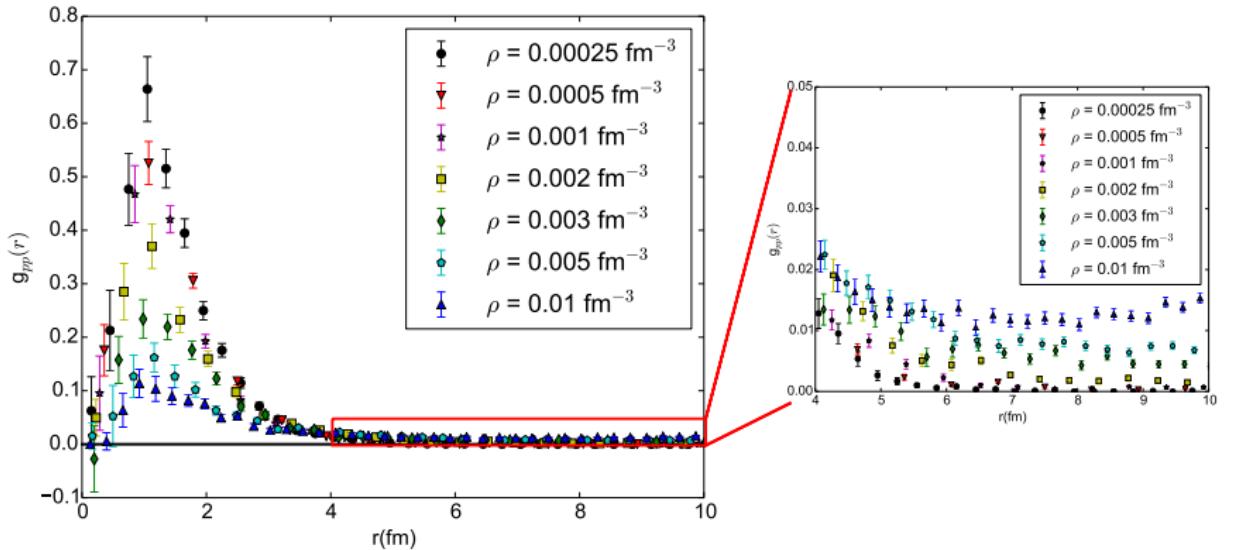
The remaining energy could be due to the α interacting with the excess neutrons.



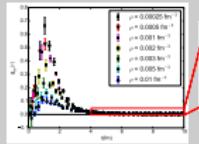
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Check for Clustering - Pair Correlation Function

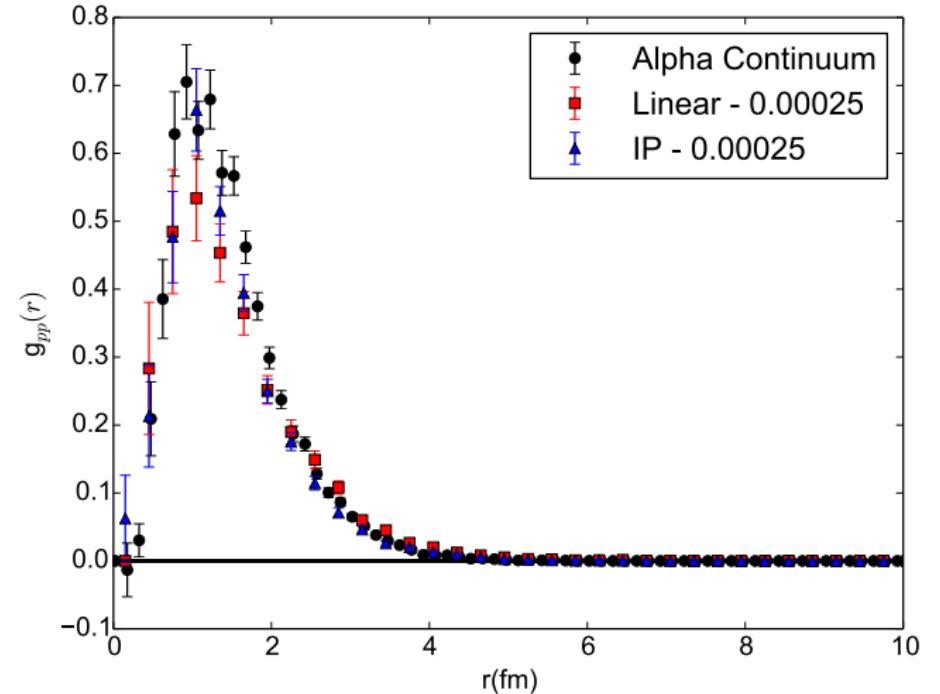
$$g_{pp}(r) = \frac{1}{4\pi r^2} \langle \Psi | \sum_{i < j} \hat{p}_i \hat{p}_j \delta(r - r_{ij}) | \Psi \rangle$$



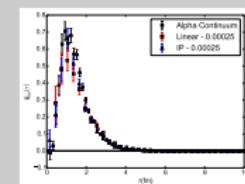
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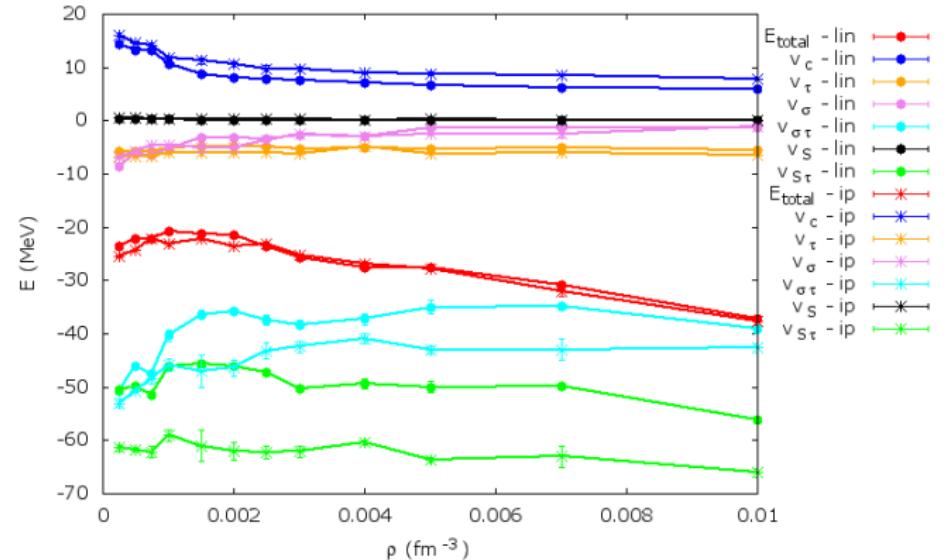
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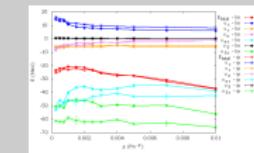
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Clustering - Other Insights



The tensor-tau and sigma-tau (from One Pion Exchange) are most affected by improved correlations.

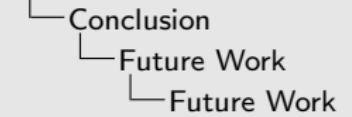


The tensor-tau and sigma-tau (from One Pion Exchange) are most affected by improved correlations.

- This is for the $14n2p$ calculation at 0.00025 (I think).
- Terms that supplied most binding were most affected by the improved correlations.
- This holds true for other systems as well i.e. $16O$.

Future Work

- Investigate alpha clustering with a pfaffian pairing wave function.
- Further improve the efficiency and accuracy of the trial wave function with the exponential correlations.
- Do a full investigation of both improved wave functions with the more sophisticated χ EFT potentials.

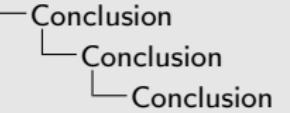


2019-05-21

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Conclusion

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- AFDMC calculations need improved correlations for larger systems.
- I have improved the correlations, however, more efficient techniques are needed.
 - One possibility is to use the HS transformation with the exponential correlations.
- We can use AFDMC to study clustering in nearly neutron matter.
 - It appears that, at least at low density, the improved wave function correlations are important.

Thank You

Advisor: Kevin Schmidt

Collaborators: Stefano Gandolfi (LANL), Joe Carlson (LANL),
and Diego Lonardoni (MSU-FRIB and LANL), Lucas Madeira
(ASU and IFSC/USP), Rong Chen (ASU)

Committee: Igor Shovkovy, Oliver Beckstein, Ricardo Alarcón



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Extra Slides

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2019-05-21

└ Extra Slides

Monte Carlo Integration

2019-05-21

└ Monte Carlo Integration

- We often want to solve multidimensional integrals.

$$I = \int g(\mathbf{R}) d\mathbf{R}$$

- We can rewrite this in terms of a probability distribution $P(\mathbf{R})$.

$$I = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R}$$

- This looks like an expectation value of $f(\mathbf{R})$. If the \mathbf{R}_n 's are pulled from $P(\mathbf{R})$ then we can write this in discrete form as

$$I = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n) \approx \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n)$$

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Metropolis Algorithm

The Metropolis algorithm is a Markov Chain method that does not depend on history except for the previous point.

- ① Start at a random position, \mathbf{R} .
- ② Propose a move to a new position \mathbf{R}' , pulled from a distribution $T(\mathbf{R}'|\mathbf{R})$, where T could be a Gaussian centered on the current position.
- ③ One possible condition for accepting the move is given by enforcing detailed balance.

$$A(\mathbf{R}'|\mathbf{R}) = \min \left(1, \frac{P(\mathbf{R}') T(\mathbf{R}|\mathbf{R}')}{P(\mathbf{R}) T(\mathbf{R}'|\mathbf{R})} \right)$$

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χ EFT vs. AV6' with AFDMC

2019-05-21

└ χ EFT vs. AV6' with AFDMC

Table 4 : Energy per nucleon in MeV calculated with AFDMC with AV6'
and χ EFT up to N²LO compared to experimental data where available.

Corr	Potential	⁴ He	¹⁶ O	SNM
Linear	AV6'	-6.79(1)	-7.23(6)	-13.97(3)
	N ² LO	-6.89(2)	-5.74(4)	-9.5(1)
IP Quad	AV6'	-6.798(8)	-7.65(9)	-14.87(4)
	N ² LO	—	-7.3(2)	-12.5(1)
Quad	AV6'	-6.778(8)	-7.55(8)	-14.81(3)
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χ EFT vs. AV6' with VMC

Table 5 : Energy per nucleon in MeV calculated with VMC with AV6' and χ EFT up to N²LO.

Corr	Potential	⁴ He	¹⁶ O	SNM
Linear	AV6'	-5.96(1)	-3.581(3)	-8.25(4)
	N ² LO	-5.86(1)	-1.08(1)	1.56(5)
IP Quad	AV6'	-6.113(8)	-5.338(3)	-10.60(3)
	N ² LO	—	-4.03(4)	—
Quad	AV6'	-6.275(5)	-5.463(3)	-10.74(2)
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└ Exponential Correlations - Problems

- When taking numerical derivatives the order of A matrix eigenvectors (given by n) can change. This means that each term in the derivative can have each eigenvector matched with a different auxiliary field.

$$\exp \left(\sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right) = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-x_n^2/2} e^{\sqrt{\lambda_n} x_n O_n}$$

- To fix this we can define the operators O_n in terms of the square roots of the A matrices. This gives an operator that sums over the eigenvector order.

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Exponential Correlations - Problems

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└ Exponential Correlations - Problems

- Just Almost like before

$$\begin{aligned} \exp \left(\sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right) = & \exp \left(\frac{1}{2} \sum_{i\alpha, j\beta} \sigma_{i\alpha} \sum_{k\gamma} (A_{i\alpha, k\gamma}^\sigma)^{1/2} (A_{k\gamma, j\beta}^\sigma)^{1/2} \sigma_{j\beta} \right. \\ & + \frac{1}{2} \sum_{i\alpha, j\beta} \sigma_{i\alpha} \sum_{k\gamma} (A_{i\alpha, k\gamma}^{\sigma\tau})^{1/2} (A_{k\gamma, j\beta}^{\sigma\tau})^{1/2} \sigma_{j\beta} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \\ & \left. + \frac{1}{2} \sum_{i,j} \sum_k (A_{i,k}^\tau)^{1/2} (A_{k,j}^\tau)^{1/2} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \right) \end{aligned}$$

u ~~done~~ Almost like before

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$$\begin{aligned} \exp\left(\sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p\right) &= \exp\left(\frac{1}{2} \sum_{k\delta=1}^{3A} (\mathcal{O}_{k\delta}^\sigma)^2 \right. \\ &\quad \left. + \frac{1}{2} \sum_{\gamma=1}^3 \sum_{k\delta=1}^{3A} (\mathcal{O}_{k\delta,\gamma}^{\sigma\tau})^2 + \frac{1}{2} \sum_{\gamma=1}^3 \sum_{k=1}^A (\mathcal{O}_{k,\gamma}^\tau)^2 \right) \\ \mathcal{O}_{k\delta}^\sigma &= \sum_{i\alpha} \sum_n \sigma_{i\alpha} \psi_{n,i\alpha}^\sigma (\lambda_n^\sigma)^{1/2} \psi_{n,k\delta}^\sigma \\ \mathcal{O}_{k\delta,\gamma}^{\sigma\tau} &= \sum_{i\alpha} \sum_n \tau_{i\gamma} \sigma_{i\alpha} \psi_{n,i\alpha}^{\sigma\tau} (\lambda_n^{\sigma\tau})^{1/2} \psi_{n,k\delta}^{\sigma\tau} \\ \mathcal{O}_{k\delta}^\tau &= \sum_i \sum_n \tau_{i\gamma} \psi_{n,i}^\tau (\lambda_n^\tau)^{1/2} \psi_{n,k\delta}^\tau \end{aligned}$$

Exponential Correlations - Problems

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$$\mathcal{O}_{k\delta}^\tau = \sum_i \sum_n \tau_{i\gamma} \psi_{n,i}^\tau (\lambda_n^\tau)^{1/2} \psi_{n,k\delta}^\tau$$

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└ Exponential Correlations - Problems

2019-05-21

└ Two-Body Operator Updates

$$S = \begin{pmatrix} \langle \alpha_1 | \mathbf{r}_1, s_1 \rangle & \langle \alpha_1 | \mathbf{r}_2, s_2 \rangle & \dots & \langle \alpha_1 | \mathbf{r}_A, s_A \rangle \\ \langle \alpha_2 | \mathbf{r}_1, s_1 \rangle & \langle \alpha_2 | \mathbf{r}_2, s_2 \rangle & \dots & \langle \alpha_2 | \mathbf{r}_A, s_A \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \alpha_A | \mathbf{r}_1, s_1 \rangle & \langle \alpha_A | \mathbf{r}_2, s_2 \rangle & \dots & \langle \alpha_A | \mathbf{r}_A, s_A \rangle \end{pmatrix}$$

$$S_{\alpha i} = \langle \alpha | \mathbf{r}_i, s_i \rangle = \sum_{\gamma=1}^4 \langle \alpha | \mathbf{r}_i \chi_{\gamma} \rangle \langle \chi_{\gamma} | s_i \rangle.$$

This is for an uncorrelated Slater Determinant.

- $|\chi_{\gamma}\rangle$ are the $|n \uparrow\rangle$, $|n \downarrow\rangle$, etc.

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When correlation operators are included we employ the identity

$$\det(S^{-1}S') = \frac{\det S'}{\det S} \quad \text{or} \quad \det(S^{-1}S'') = \frac{\det S''}{\det S}$$

where

$$S^{-1}S'' = \begin{pmatrix} 1 & 0 & \dots & \langle \alpha_1 | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \dots & \langle \alpha_1 | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle & \dots & 0 & 0 \\ 0 & 1 & \dots & \langle \alpha_2 | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \dots & \langle \alpha_2 | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \langle \alpha_A | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \dots & \langle \alpha_A | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle & \dots & 0 & 1 \end{pmatrix}$$

and

$$\det S^{-1}S'' = \det \begin{pmatrix} \langle \alpha_i | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \langle \alpha_i | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle \\ \langle \alpha_j | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \langle \alpha_j | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle \end{pmatrix}$$

Two-Body Operator Updates

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Two-Body Operator Updates

2019-05-21

Two-Body Operator Updates

In practice this is done by calculating

$$\frac{\langle \Phi | \mathcal{O}_{ij} | RS \rangle}{\langle \Phi | RS \rangle} = \sum_{\gamma=1}^4 \sum_{\delta=1}^4 d_{2b}(\chi_\gamma, \chi_\delta, ij) \langle \chi_\gamma \chi_\delta | \mathcal{O}_{ij} | s_i s_j \rangle,$$

where

$$d_{2b}(\chi_\gamma, \chi_\delta, ij) = \frac{\langle \Phi | R, s_1, \dots, s_{i-1}, \chi_\gamma, s_{i+1}, \dots, s_{j-1}, \chi_\delta, s_{j+1}, \dots, s_A \rangle}{\langle \Phi | RS \rangle}.$$

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Two-Body Operator Updates

To reduce the number of calculations in the inner loops we precalculate the matrix elements

$$P_{\chi_\gamma,ij} = \sum_{\alpha} S_{j\alpha}^{-1} S_{\alpha i} (s_i \leftarrow \chi_\gamma),$$

$$P_{\chi_\delta,ij} = \sum_{\alpha} S'_{j\alpha}^{-1} S'_{\alpha i} (s_j \leftarrow \chi_\delta).$$

The d_{2b} distribution can then be written as

$$d_{2b}(\chi_\gamma, \chi_\delta, ij) = \det \begin{pmatrix} P_{\chi_\gamma,ii} & P_{\chi_\gamma,ij} \\ P_{\chi_\delta,ji} & P_{\chi_\delta,jj} \end{pmatrix}$$

The d_{2b} can be precalculated and multiplied by each operator expectation value $\langle \chi_\gamma \chi_\delta | \mathcal{O}_{ij} | s_i s_j \rangle$.

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Two-Body Operator Updates - Scaling

2019-05-21

└ Two-Body Operator Updates - Scaling

Calculation	Functional Form	Scaling
Ψ (linear)	$1 + \mathcal{O}_{ij}^c$	$O(A^2)$
Ψ (quadratic)	$1 + \mathcal{O}_{ij}^c + \mathcal{O}_{ij}^c \mathcal{O}_{kl}^c$	$O(A^4)$
$\langle H \rangle$ (linear)	$(1 + \mathcal{O}_{ij}^c) \mathcal{O}_{mn}^p$	$O(A^4)$
$\langle H \rangle$ (quadratic)	$(1 + \mathcal{O}_{ij}^c + \mathcal{O}_{ij}^c \mathcal{O}_{kl}^c) \mathcal{O}_{mn}^p$	$O(A^6)$

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Forward Walking

- Mixed estimators contain bias from Ψ_T

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

$$\langle \mathcal{O} \rangle_{mixed} = \frac{\langle \Psi_T | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle}$$
- Some of this can be removed with a “forward walking” scheme
$$\langle \mathcal{O} \rangle_p = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle} = \frac{\langle \Psi_T | \frac{\Psi(\tau)}{\Psi_T} \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi_T | \frac{\Psi(\tau)}{\Psi_T} | \Psi(\tau) \rangle}$$

$$= \frac{\sum_i \mathcal{O}_i W_i}{\sum_i W_i}$$

i are the random samples (walkers).

Forward Walking

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└ Forward Walking

EXPLAIN HOW THE PARAMETARS ARE VARIED IN VMC.

Start with basics and then really try to understand it.

See thesis from Casula, New QMC approaches for the simulation
of electronic systems: a first application to aromatic molecules and
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2019-05-21

└ VMC - Parameter Variation

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FINISH THIS! Maybe call it the BCS wave function, which we calculate as a pfaffian of paired orbitals.

2019-05-21

└ Pfaffian Wave Function

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WHY ARE CLUSTERS IMPORTANT? ARE THEY NORMALLY
DONE WITH SOME MODEL, NOT AB INITIO LIKE WE ARE
DOING? ARE THEY LEAST WRITTEN IN TERMS OF P,
N, AND ALPHA DEGREES OF FREEDOM? WE ARE ONLY
USING N AND P.