Oral Comprehensive Exam/Prospectus: Improved Trial Wave Function for Quantum Monte Carlo Calculations of Nuclear Systems

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Outline

1. Motivation
2. Research
   - Quantum Monte Carlo
   - Trial Wave Function
   - Results
3. Conclusion
   - Conclusion
4. Prospectus
   - Exponential Correlations
   - Clustering in Nuclear Matter
   - Outlook

Background

- $\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \Psi^*(\mathbf{R}) H \Psi(\mathbf{R}) d\mathbf{R}$
- One of the earliest approximate interactions came from Yukawa[1].

$$V_Y(r) = -g^2 \frac{e^{-\lambda r}}{r}$$

- The inclusion of NN and NNN terms into this many body Hamiltonian, which could depend on spin and isospin, makes this calculation grow in complexity.

[1] H. Yukawa. "On the Interaction of Elementary Particles. I.". In: *Proc. Phys. Math. Soc. Japan.* 3rd ser. 17 (1935), p. 48.

Background

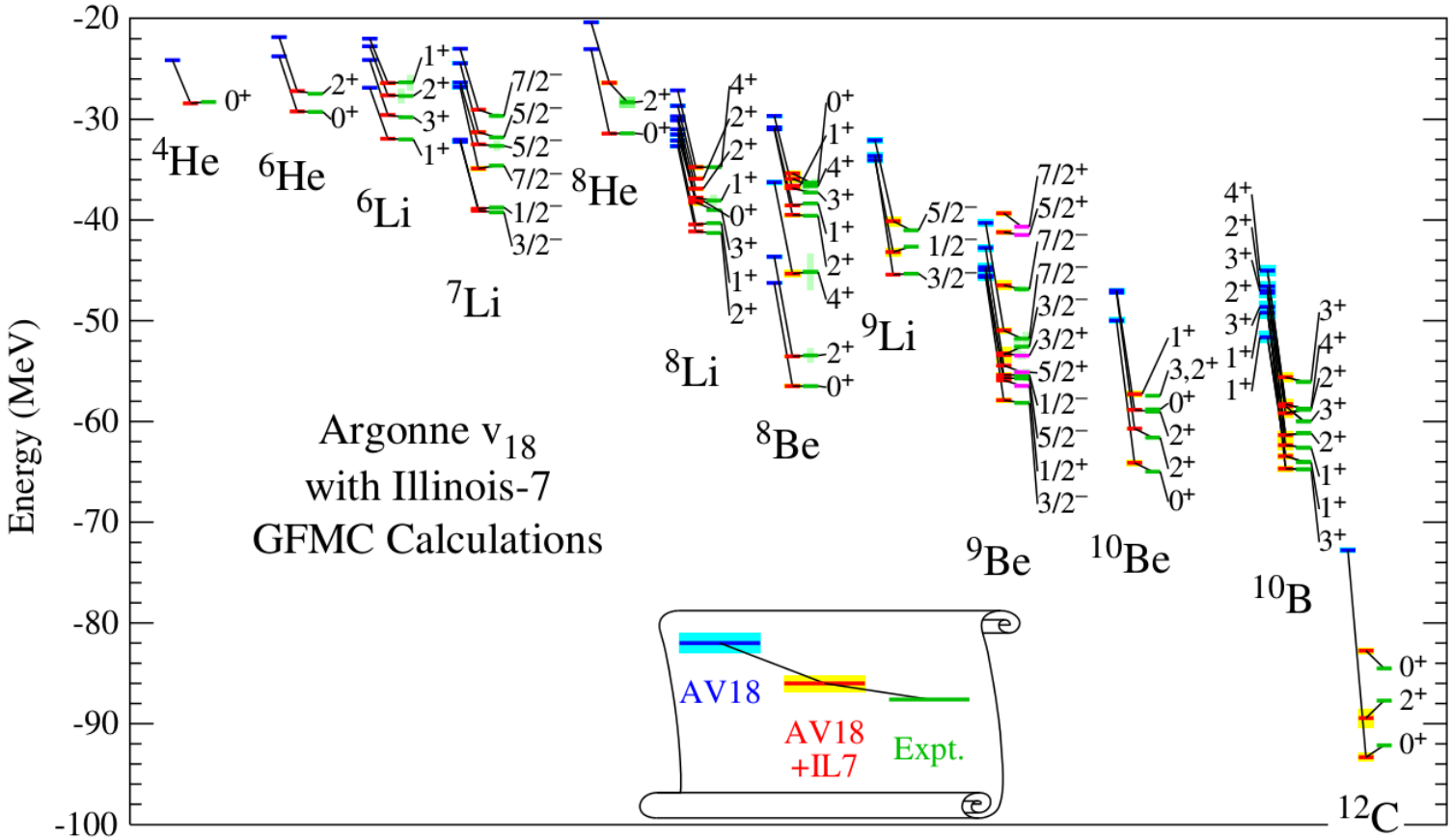
- Approximate basis set methods:
  - No-core shell model[2]
  - Coupled-cluster[3]
- Compatibility with local and non-local (velocity dependent) potentials
- Two issues that these methods have
  - Truncation of basis set
  - Poor scaling with basis set size

[2] Bruce R. Barrett, Petr Navrátil, and James P. Vary. "*Ab initio* no core shell model". In: *Prog. Part. Nucl. Phys.* 69 (2013), pp. 131–181.

[3] G Hagen et al. "Coupled-cluster computations of atomic nuclei". In: *Rep. Prog. Phys.* 77.9 (2014), p. 096302.

Background

- GFMC can get results for nuclei up to ^{12}C.



Background

- We use the phenomenological potential AV6′, which is a subset of the AV18[4] potential used in GFMC before.

$$v_{ij} = \sum_{p=1,6} v(r_{ij}) \mathcal{O}_{ij}^{p}$$

$$\mathcal{O}_{ij}^{p=1,6} = 1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j), S_{ij}, S_{ij}(\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)$$

$$S_{ij} = 3(\boldsymbol{\sigma}_i \cdot \mathbf{r_{ij}})(\boldsymbol{\sigma}_j \cdot \mathbf{r_{ij}}) - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

[4] R.B. Wiringa, V. G. J. Stoks, and R. Schiavilla. "Accurate Nucleon-Nucleon Potential with Charge-Independent Breaking". In: *Phys. Rev. C* 51 (1995), pp. 38–51.

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

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

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 can be a Gaussian centered on the current position.
3. The probability of accepting the move is given by

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

4. The move is accepted if $A \geq u$ where u is a uniform random number between 0 and 1.

Variational Monte Carlo

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

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

- To use what we learned above 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 $\Psi_T(\mathbf{R})\Psi_T^{-1}(\mathbf{R})$.

$$P(\mathbf{R}) = \frac{|\Psi_T(\mathbf{R})|^2}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}$$

$$E_L(\mathbf{R}) = \frac{\Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R})}{\Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})}$$

- 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 $E_V \geq E_0$.

Variational Monte Carlo - Implementation

1. Generate N configurations (walkers) distributed randomly.
2. Loop over each walker and do the following
   1. Calculate $P(\mathbf{R}) = |\langle \Psi_T | \mathbf{R} \rangle|^2$
   2. Propose a move $\mathbf{R}' = \mathbf{R} + \Delta\xi$, where ξ could be a vector of random variable from a Gaussian.
   3. Calculate $P(\mathbf{R}') = |\langle \Psi_T | \mathbf{R}' \rangle|^2$
   4. Calculate the probability of acceptance $A = \min\left(1, \frac{P(\mathbf{R}')}{P(\mathbf{R})}\right)$
   5. If accepted then $\mathbf{R} \rightarrow \mathbf{R}'$, else the next position in the Markov Chain for that walker is the same as the last, namely $\mathbf{R}$
3. Calculate observables and repeat steps 2 until energy is minimized or uncertainties are low enough.

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

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

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

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

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

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 ξ is a uniform random number from $[0, 1]$.

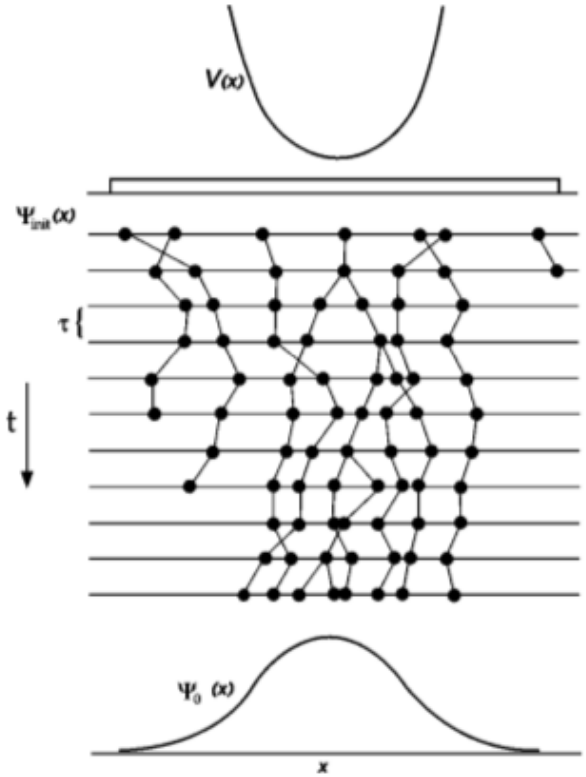


Figure: Reprinted from W.M.C. Foulkes et al. *Rev. Mod. Phys.*, 73:33-83, 2001.

Diffusion Monte Carlo - Implementation

1. Start with N configurations (walkers) from VMC
2. Loop over each walker and do the following
   1. Propose a move, $\mathbf{R}' = \mathbf{R} + \chi$, where χ is a vector of random numbers from the shifted Gaussian $\exp\left(\frac{m}{2\hbar^2\Delta\tau}\left(\mathbf{R}' - \mathbf{R} + 2\frac{\nabla\Psi_I(\mathbf{R}')}{\Psi_I(\mathbf{R}')}\right)^2\right)$.
   2. The move is then accepted with the probability $A(\mathbf{R}' \leftarrow \mathbf{R}) = \min\left(1, \frac{\Psi_T^2(\mathbf{R}')}{\Psi_T^2(\mathbf{R})}\right)$.
   3. Calculate the weight $w(\mathbf{R}') = \exp\left(-\left(E_L(\mathbf{R}') + E_L(\mathbf{R}) - 2E_0\right)\Delta\tau/2\right)$.
   4. Do branching.
   5. Calculate and collect the observables and uncertainties needed and increase the imaginary time by $\Delta\tau$.
3. Repeat from step 2 to 6 until the uncertainties are small enough.

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

- 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^σ, $9A$ for $O_{n\alpha}^{\sigma\tau}$, and $3A$ for $O_{n\alpha}^{\tau}$), the spin-isospin dependent part of the propagator becomes

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

Slater Determinant

- The simplest wave function for a many-fermion system is a Slater determinant.

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

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

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

where $\langle RS|\phi\rangle$ is the Slater determinant described above.

Full Trial Wave Function

- A completely cluster decomposable ($|\Phi_A + \Phi_B\rangle = |\Phi_A\rangle\,|\Phi_B\rangle$) set of spin-isospin dependent correlations could be an exponential

$$|\psi_T\rangle = \prod_{i<j} f_c(r_{ij}) e^{\sum_p f_p(r_{ij})\mathcal{O}_{ij}^p} |\phi\rangle\,.$$

- However, a symmetrized product wave function captures almost the same physics.

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

Quadratic Correlations

- If we assume the correlations are small we can expand this exponential to first order.

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

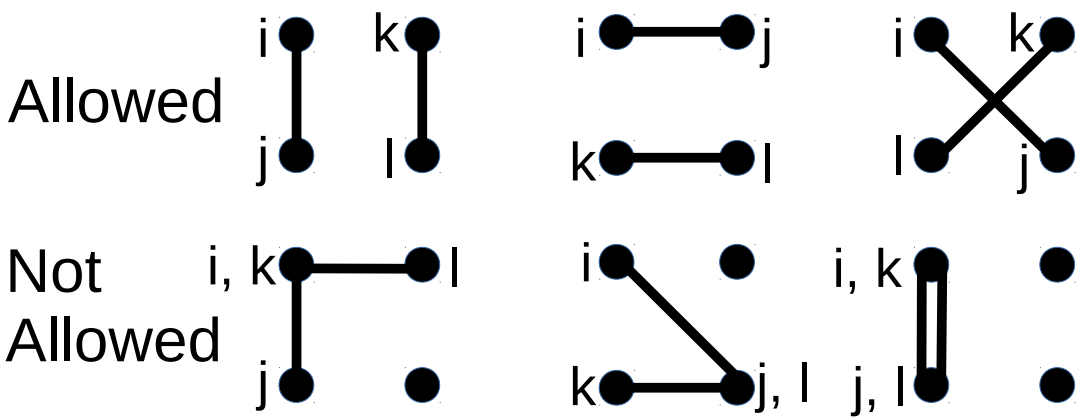
- By expanding the product you can write this as

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

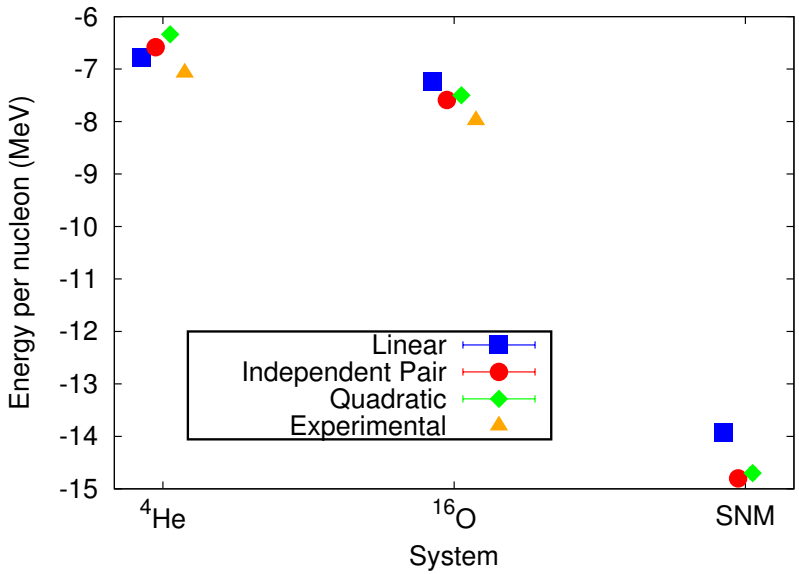
Independent Pair Correlations

- Or it can be expanded to get independent pair terms

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



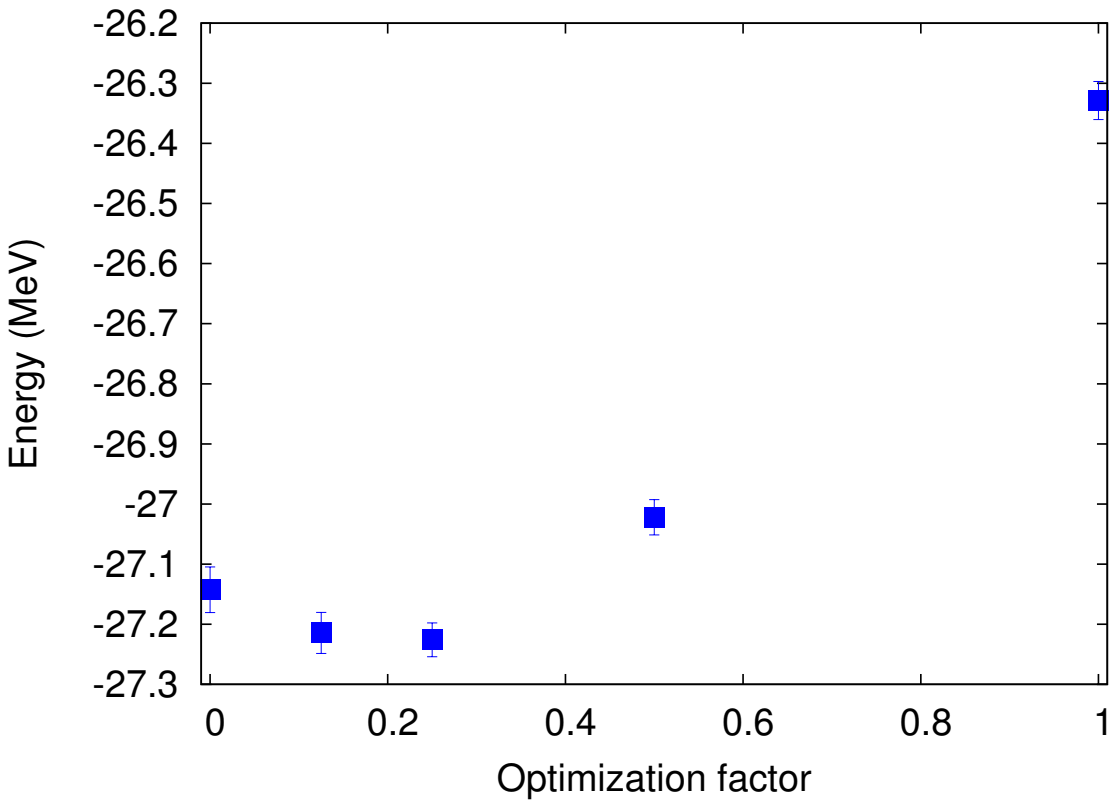
Results



	Linear	IndPair	Quadratic	Expt.
^{4}He	-27.17(4)	-26.33(3)	-25.35(3)	-28.295
^{16}O	-115.7(9)	-121.5(1.5)	-120.0(1.4)	-127.619
SNM($\rho = 0.16$ fm^{-1})	-13.92(6)	-14.80(7)	-14.70(11)	

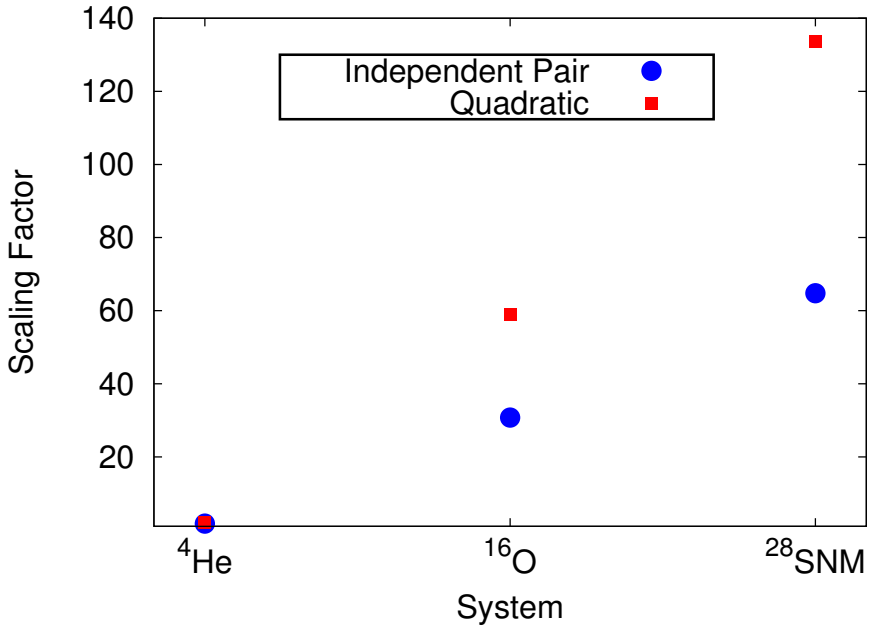
Energies (per nucleon) in MeV, SNM was done with 28 particles with periodic boundary conditions.

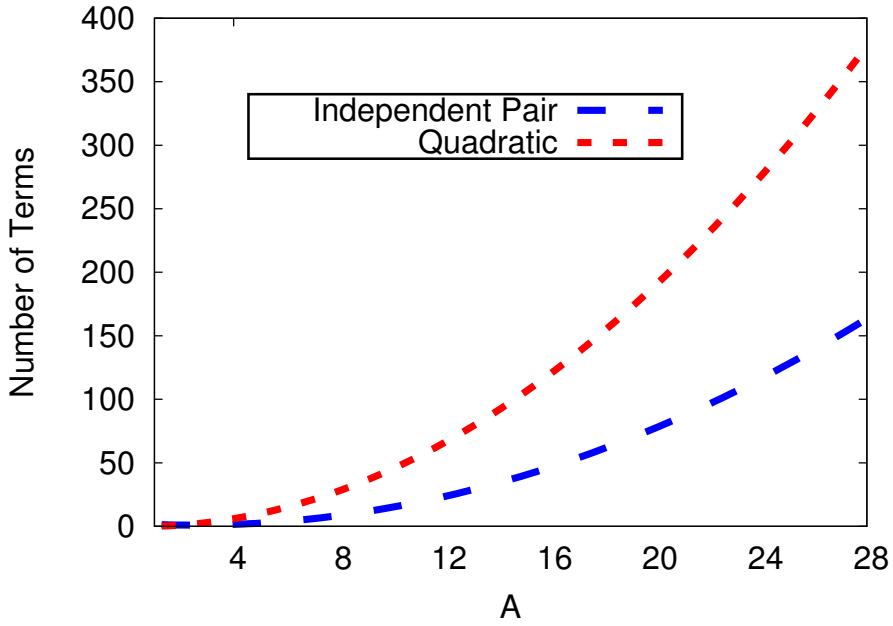
Results



Optimization of quadratic β parameter for ^{4}He with independent pair correlations.

Results





	^{4}He	^{16}O	SNM(28)
Independent Pair	1.73	30.7	64.8
Quadratic	2.00	58.8	133.6

Conclusion

- We have added independent pair and full quadratic correlations to the already linearly correlated wave function.
- The addition of these operators decreases the energy for each system.
- Though there was not a large difference between independent pair and full quadratic correlations the scaling was about twice as good for independent pair correlations.

End of Comprehensive

Questions?

Outlook

- I will apply these calculations to other medium mass nuclei.
  - ^{40}Ca
  - Other isotopes of Oxygen
  - Open shell nuclei
- This work will then be published.
  - Draft by the end of the summer.
- When this project is done I plan to move on to one or more additional projects.

Exponential Correlations

- Another way to improve the trial wave function is to start with the exponential correlations and use the Hubbard-Stratanovich transformation to sample them, just like we do for the spin-isospin part of the propagator in AFDMC.

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

Exponential Correlations

- Compare what we have for the potential (without the Jastrow part) to what we have for the Green's function.

$$\langle \psi_T | RS \rangle = \langle \phi | \, e^{\sum_p \sum_{i<j} f_p(r_{ij}) \mathcal{O}_{ij}^p} \, | RS \rangle$$

$$G_{SD}(R'S', RS, \Delta\tau) = \left\langle R'S' \right| e^{\sum_p \sum_{i<j} u_p(r_{ij}) \mathcal{O}_{ij}^p \Delta\tau} \left| RS \right\rangle$$

- The only differences between these are the different function u and f, and the $\Delta\tau$. Then the correlations in the trial wave function can be written as

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

Exponential Correlations

- To improve the variance of sampling the average of with samples x and $-x$ is taken.
- This improved wave function will allow us to study larger nuclear system like neutron-rich nuclei created by the r-process.

Particle Clustering in Nuclear Matter

- When a nucleus has an even number of n and p each n pairs with a p, and this decreases the energy of the system.
- However two n and two p can pair together to form an α-particle.
- At low densities quartetting is more energetically favorable than pairing[5].
- I want to show that we can see this clustering.
- I also want to do calculations at different densities to study how these clusters dissolve as a function of density.

[5] P. Schuck et al. "Alpha-Particle Condensation in Nuclear Systems". In: *J. Phys.: Conf. Ser.* 413 (2013), p. 012009.

Neutron Star

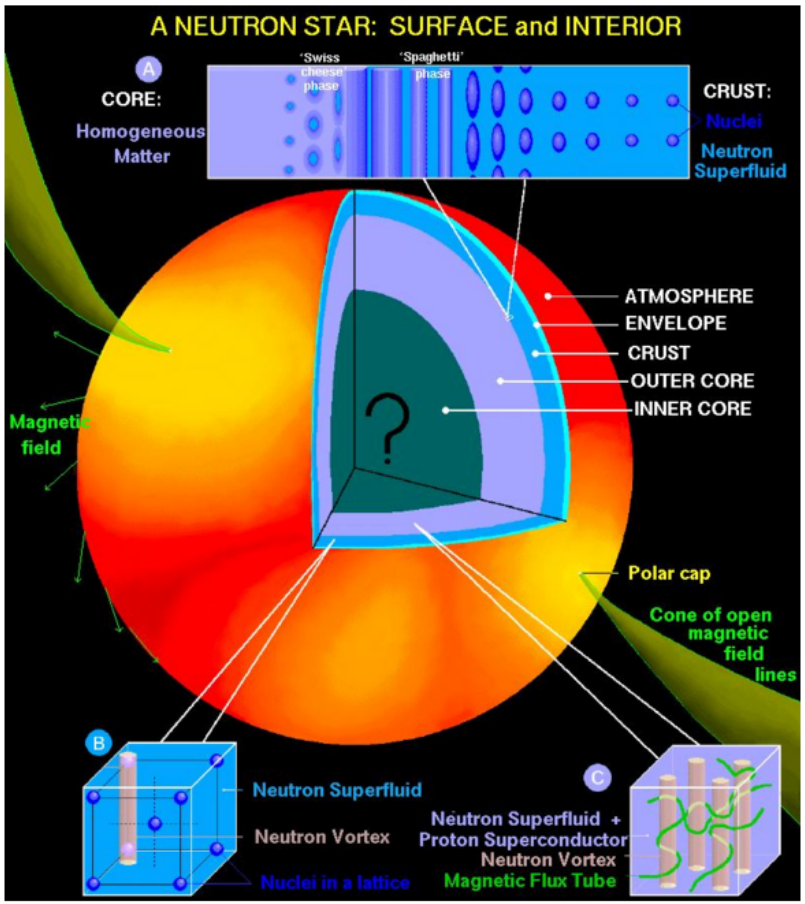


Figure: Reprinted from Dany Page et al. *Annu. Rev. Nucl. Part. Sci.*, 56:327-374, 2006.

Particle Clustering in Nuclear Matter

- Calculate the energy/particle ($E_{14n}/14$) of pure neutron matter with 14 particles in a periodic box and compare with 14 neutrons plus 2 protons ($E_{14n2p}/16$).
- If there is quartetting there should be a shift in the energy.

$$E_{14n2p}/16 \approx (E_{12n} + E_{\alpha})/16$$

- If neutron matter had energy $E_n/N \approx 15\text{MeV}$ and the alpha $E_{\alpha} \approx -28\text{MeV}$ this would be

$$E_{14n2p}/16 \approx \left(15\frac{\text{MeV}}{part} \cdot 12 - 28\text{MeV}\right)/16 = 4\text{MeV}$$

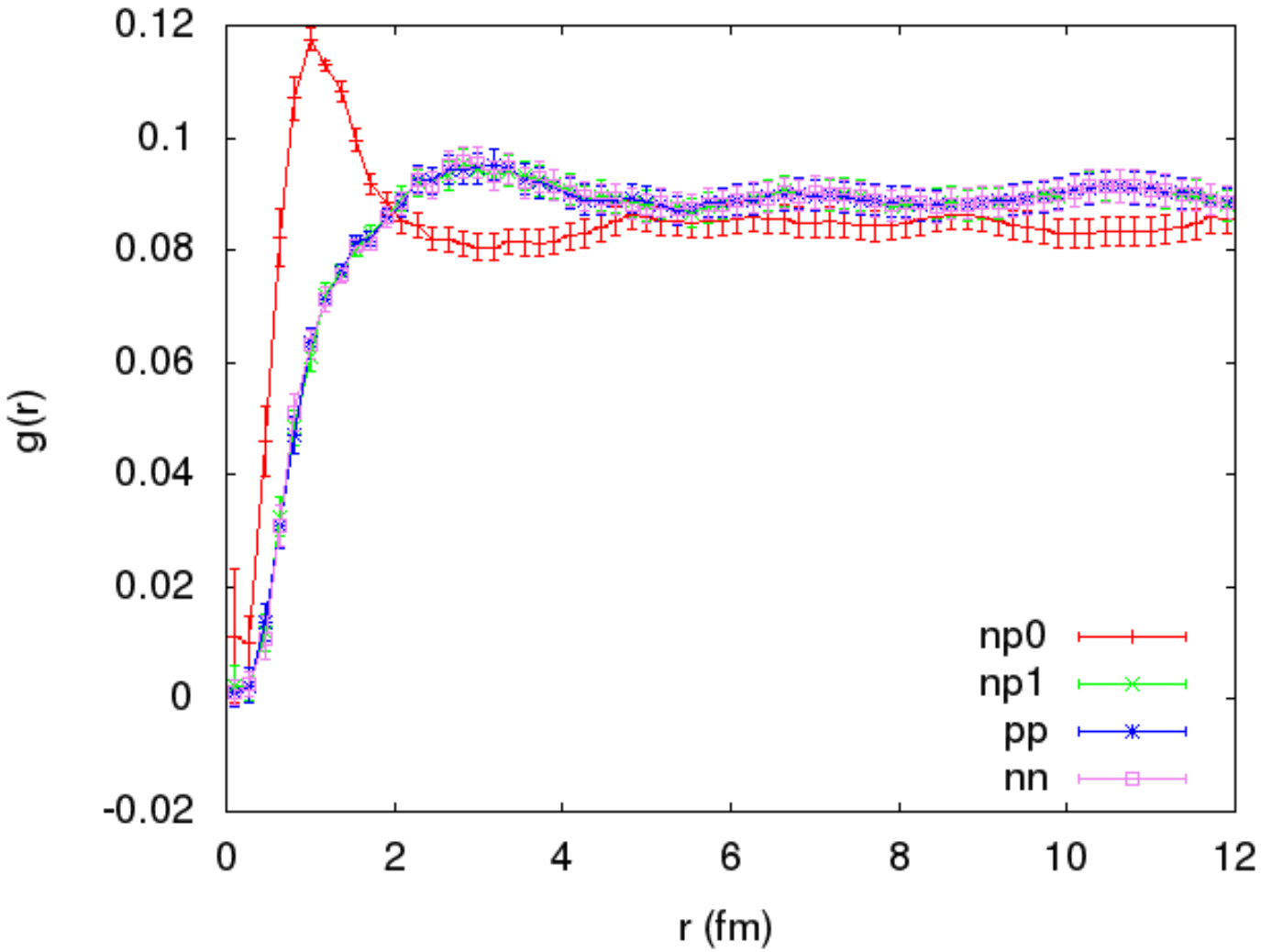
Pair Distribution Functions

- Pair Distribution Functions

$$g(\mathbf{r}) = \frac{2V}{N^2} \left\langle \sum_{i<j} \delta^3 \left(\mathbf{r} - \mathbf{r}_i + \mathbf{r}_j \right) \right\rangle$$

- This tells us the probability that a particle is within some distance of another particle.

Pair Distribution Functions for SNM



Timetable

Summer 17	Submit draft for quadratic correlations paper
Fall 17	"Complete" exponential correlations project
Spring 18	"Complete" alpha clustering project
Summer 18	Submit a draft of alpha clustering paper
Fall 18	Start writing dissertation
Spring 19	Finish dissertation and defense

Available Resources

- Current XSEDE Allocation: 100,000 hours on LSU SuperMIC
  - Quadratic Correlations: 100,000 hours
- Future XSEDE Allocation: 480,000 hours on LSU SuperMIC
  - Exponential Correlations: 240,000 hours
  - Alpha Clustering: 240,000 hours

Dissertation Breakdown

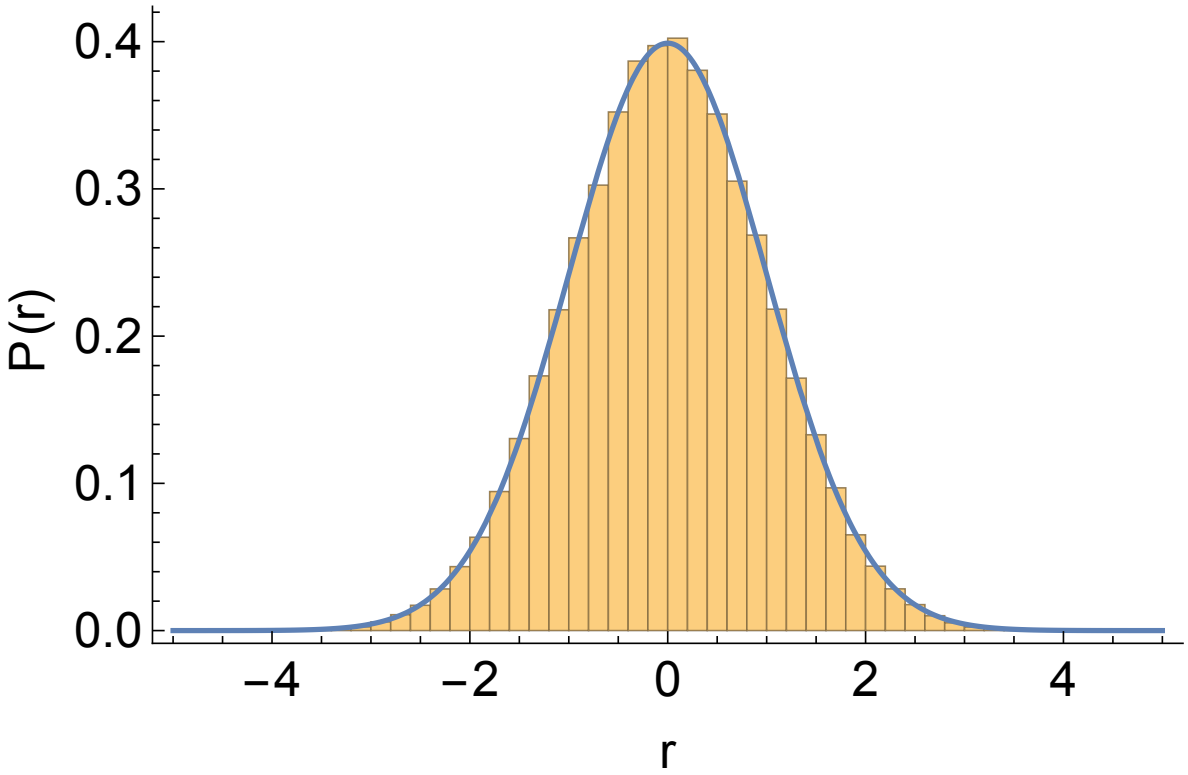
1. Introduction
2. Methods
    1. Variational Monte Carlo
    2. Diffusion Monte Carlo
    3. Auxiliary Field Diffusion Monte Carlo
    4. Hamiltonian
3. Trial Wave Function
    1. Expand the Symmetric Product Wave Function
    2. Exponential Wave Function
    3. Comparing Trial Wave Functions
4. Alpha Clustering in Nuclear Matter
    1. Theory
    2. Results
5. Conclusion

End of Prospectus

Questions?

Sampling $P(\mathbf{R})$

- We need to draw samples from a probability density. If this is an function with an invertible CDF this is easy to do.



$$r = \mathrm{CDF}^{-1}(\xi)$$

- If not then we need to use other methods to sample the distribution.