Nuclear Quantum Monte Carlo at SUU

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- Explain what kind of problem you are trying to solve
    - Mix in a brief introduction to Quantum Mechanics
- Explain how the problem is solved.
- Explain what you have done **and** what students could do with you in the future.

Outline

- Quantum Monte Carlo methods
- Improved trial wave function
- Alpha formation in nearly neutron matter - preliminary
- Another Improved trial wave function - preliminary
- Future work/Conclusion

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- Fix frame total slide numbering in footer, it's right in pdinterview.pdf
- Start with a brief description of the atom, as described by Rutherford.
- Compare EM force to nuclear force and show some of the crude models, explaining why we have the crude models. Mention that it actually depends on other QM properties like spin, etc.
  - Talk about e- orbitals and how QM was able to describe the periodic table maybe.
- Brief explanation of how QM works and a wave function
- Schrödinger equation is the way to solve nuclear physics problems.
- Show the integral that you're solving.
- How QMC work to solve these kinds of problems.
- What you've done.
- What you think would be good to do in the future WITH SUU STUDENTS. Including non-nuclear computational

Nuclear Physics Problem

- We all have this picture in our head of an atom: dense nucleus in the center that we mostly ignore except for it's protons charges and a bunch of electrons zipping around around it.

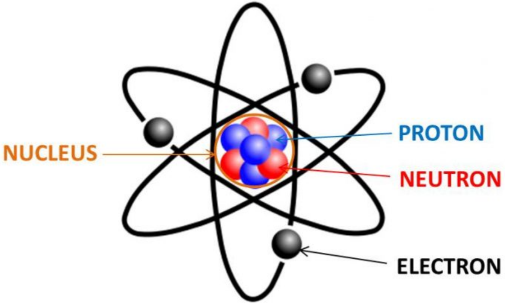
Nuclear Physics Problem

- We all have this picture in our head of an atom: dense nucleus in the center that we mostly ignore except for it's protons charges and a bunch of electrons zipping around around it.
- We know how the calculate interactions between the electrons, and between the electrons and protons.

Nuclear Physics Problem

- We all have this picture in our head of an atom: dense nucleus in the center that we mostly ignore except for it's protons charges and a bunch of electrons zipping around around it.

- What about the nucleons (neutrons and protons), how do they interact with eachother and with electrons?



Picture References

Atomic model, accessed 1 mar 2019: http://www.whoinventedfirst.com/who-discovered-the-atom/

Quantum Monte Carlo

- **VMC:**

$$E_V = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

- **AFDMC:**

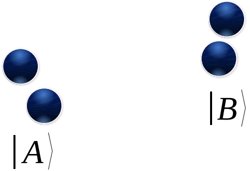
$$\langle \mathbf{R}_N | \Psi_T(\tau) \rangle = \int d\mathbf{R}_1 \ldots d\mathbf{R}_N \left[\prod_{i=1}^{N} G(\mathbf{R}_i, \mathbf{R}_{i-1}, \Delta\tau) \right] \langle \mathbf{R}_0 | \Psi_T(0) \rangle$$

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

- Ψ_T is calculated in practically every part of the calculation and plays an important role in guiding the propagation and diffusion of the calculation to the ground state.

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.

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

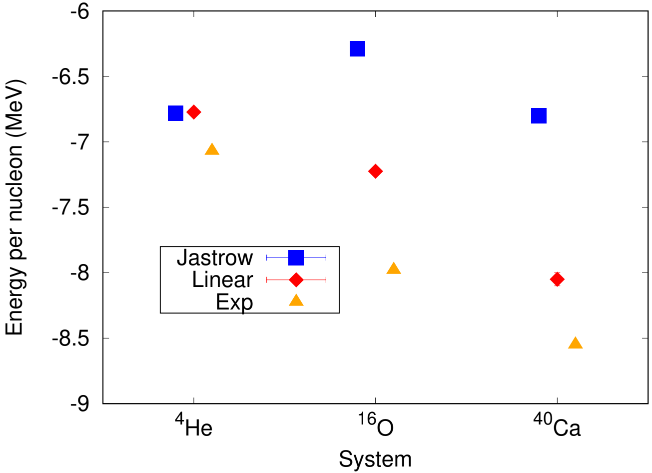
S. Gandolfi et al. *Phys. Rev. Lett.*, **99**, 022507, 2007.

- 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



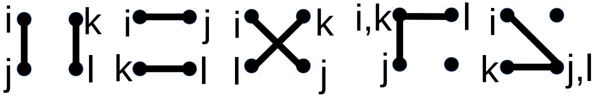
Data taken from each paper respectively.

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



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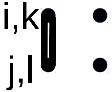
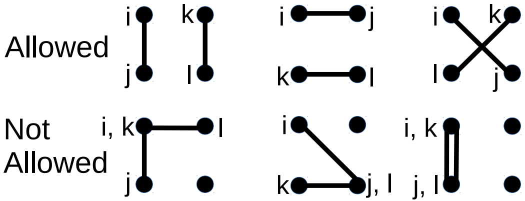


Independent Pair Quadratic Correlations

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

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



Results

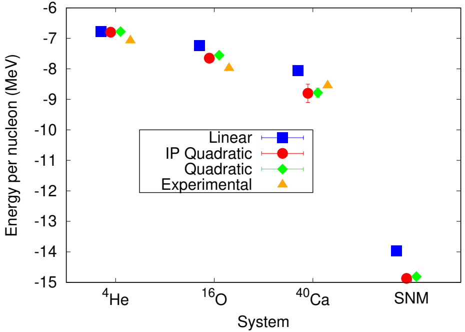
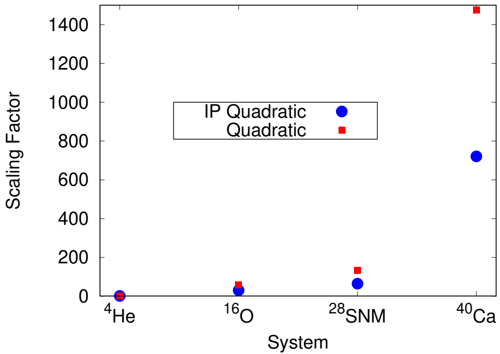


Table : Energy (*per nucleon) in MeV

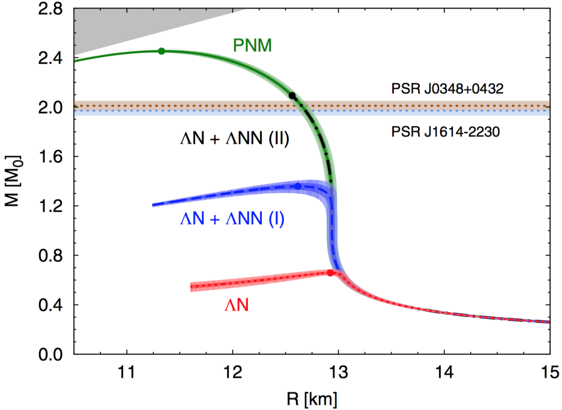
System	Linear	IP Quadratic	Quadratic	Experimental
^{4}He	-27.14(4)	-27.19(3)	-27.11(3)	-28.296
^{16}O	-115.7(9)	-122.4(1.5)	-120.8(1.3)	-127.62
^{40}Ca	-322(3)	-350(10)	-351(6)	-342.1
SNM*	-13.97(3)	-14.87(4)	-14.81(3)	

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

Quadratic Correlation Cost



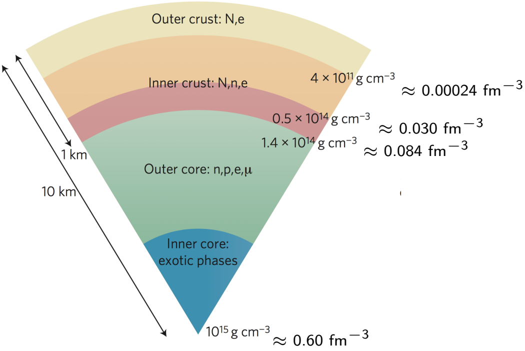
	^{4}He	^{16}O	SNM(28)	^{40}Ca
IP Quadratic	1.73	30.7	64.8	720.9
Quadratic	2.00	58.8	133.6	1473.9



Diego Lonardoni et al. *Phys. Rev. Lett.*, **114**, 092301, 2015.

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

$$E_\alpha = E_{\text{Nn+2p}} - E_{\text{(N-2)n}}$$



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

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

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

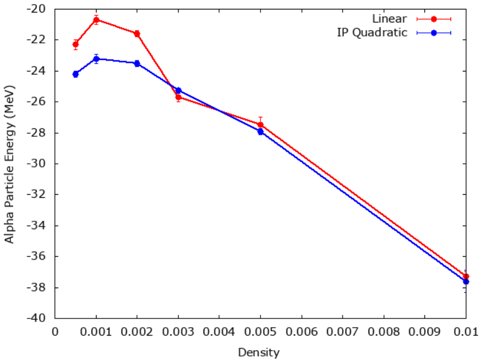
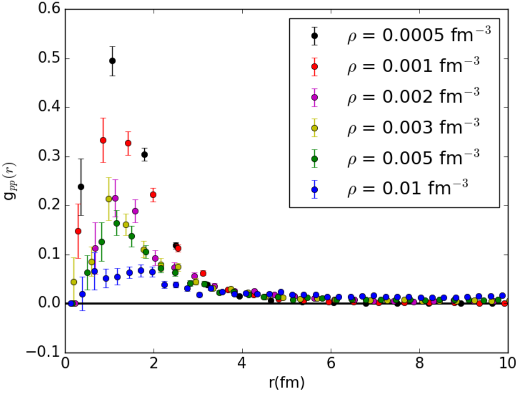


Table : Alpha energy in MeV

ρ (fm^{-3})	lin	ip
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)

Pair Correlation Function - Preliminary

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



Exponential Correlations - Preliminary

- The quadratic correlations improved the trial wave function, but with a large computational cost. Can we do better with the exponential correlations?

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

- We don't know how to calculate the exponential of two-body operators. But we have already tackled this exact problem with the spin sampling in AFDMC by using the Hubbard-Stratanovich transformation.

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

Exponential Correlations - Preliminary

- Following the same procedure used in AFDMC spin sampling we can write the exponential correlations as

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}^p_{ij}\right) = \exp\left(\frac{1}{2}\sum_{n=1}^{15A}(O_n)^2\,\lambda^\sigma_n\right),$$

where the $3A$ O^σ_n, $9A$ $O^{\sigma\tau}_{n\alpha}$, and $3A$ $O^\tau_{n\alpha}$ single particle operators are

$$O^\sigma_n = \sum_{j,\beta}\sigma_{j,\beta}\psi^\sigma_{n,j,\beta}$$

$$O^{\sigma\tau}_{n\alpha} = \sum_{j,\beta}\tau_{j,\alpha}\sigma_{j,\beta}\psi^{\sigma\tau}_{n,j,\beta}$$

$$O^\tau_{n\alpha} = \sum_{j}\tau_{j,\alpha}\psi^\tau_{n,j}.$$

Exponential Correlations - Preliminary

- Using the Hubbard-Stratanovich transformation this can then be written as

$$\exp\left(\frac{1}{2}\sum_{n=1}^{15A}(O_n)^2\,\lambda_n^\sigma\right) = \prod_{n=1}^{15A}\frac{1}{\sqrt{2\pi}}\int dx_n e^{-x_n^2/2} e^{\sqrt{\lambda_n}x_n O_n}, \tag{1}$$

and the auxiliary fields can be sampled to be

$$\Psi_T(R,S) = \langle RS|\prod_{n=1}^{15A}\frac{1}{N}\sum_{\{x_n\}}^{N}\frac{1}{\sqrt{2\pi}}e^{\sqrt{\lambda_n}x_n O_n}\,|\Phi\rangle\,. \tag{2}$$

Exponential Correlations - Preliminary

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

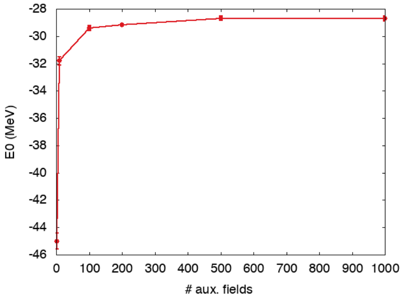


Table : ^{4}He energy with exp correlations. E_{linear}=-26.48(9) MeV.

# 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)

- Currently looking into this problem.

Future Work

- Neutron star equation of state
  - Using χEFT interaction
  - Understanding the hyperon problem
- Understand what is happening at higher nuclear densities
- Other interesting projects that push our understanding and application of nuclear physics

Summary/Conclusion

- We have improved the previously used two-body spin-isospin correlations.
- The improved trial wave functions appear to make a significant difference in the energy of the calculations, but currently cost too much to use for large systems.
- We have shown that our calculation can see what are probably alpha particles forming in mostly neutron matter around the density of neutron star crusts. These calculations appear to be even better when improved correlations are used.

Thanks

Advisor: Kevin Schmidt (ASU)
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