Improved Trial Wave Functions for Nuclear Quantum Monte Carlo

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Outline

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

Quantum Monte Carlo

- **VMC:**

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

- **AFDMC:**

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

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

- 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.

Symmetrized Product Wave Function

- The symmetrized product is expensive to calculate and so an expansion truncated at linear order has been used in the past with good success.

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

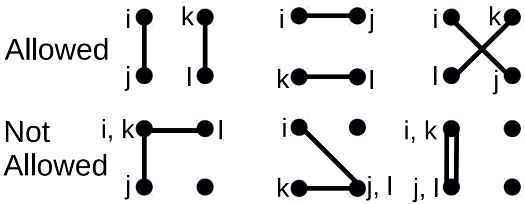
- We have taken this expansion to second order.

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

Independent Pair Quadratic Correlations

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

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



Results

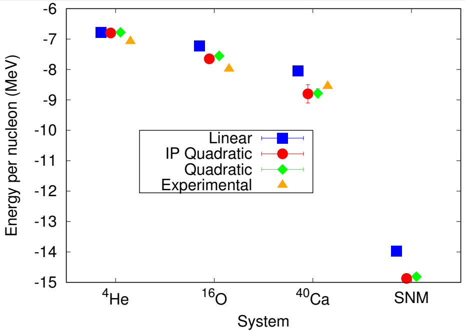
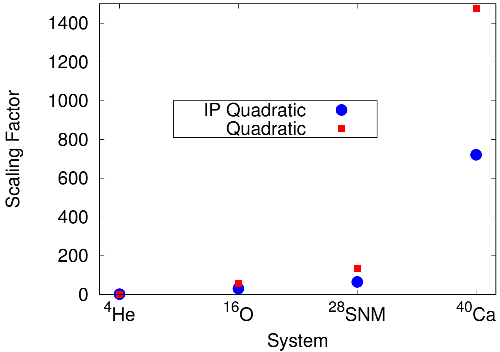


Table: Energy (*per nucleon) in MeV

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

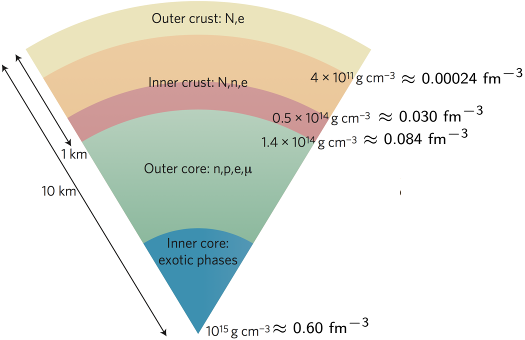


	^{4}He	^{16}O	SNM(28)	^{40}Ca
IP Quadratic	1.73	30.7	64.8	720.9
Quadratic	2.00	58.8	133.6	1473.9

Neutron Stars - Preliminary

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

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



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

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

- Both energies decreased, but the combination did not always.

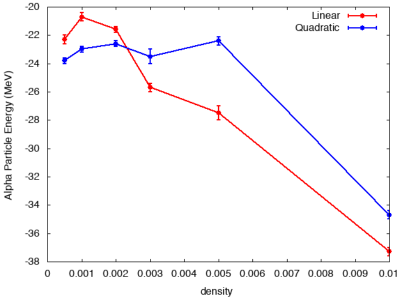


Table: Alpha energy in MeV

ρ (fm^{-3})	lin	ip
0.0005	-22.3(3)	-23.8(2)
0.001	-20.7(3)	-23.0(2)
0.002	-21.6(2)	-22.6(2)
0.003	-25.7(3)	-23.5(5)
0.005	-27.5(5)	-22.4(3)
0.01	-37.3(3)	-34.7(3)

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?

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

- 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.

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

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.

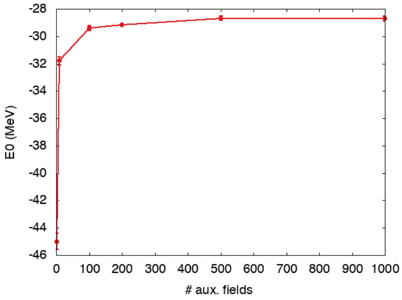


Table: ^{4}He energy with exp correlations. E_{linear}=-26.48(9) MeV.

# 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.

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

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