# Nuclear Quantum Monte Carlo at SUU

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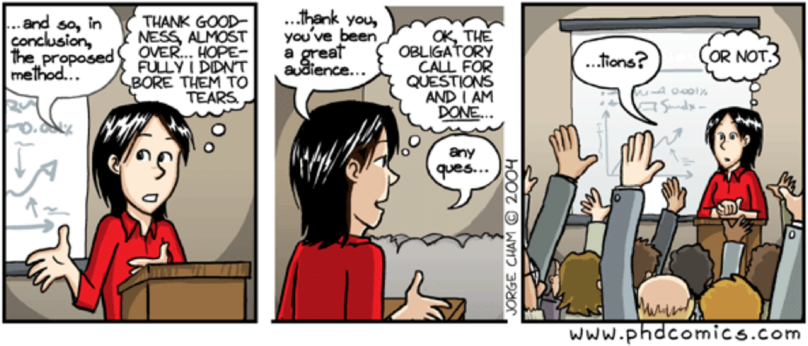
Cedar City, UT

# Outline

- What problems I work on + background
- Method I use to solve problems
- Specific work I've done
- Results I've gotten
- Future work/Conclusion

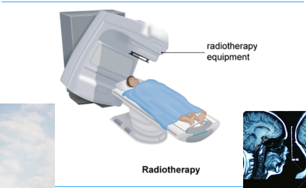
# Questions

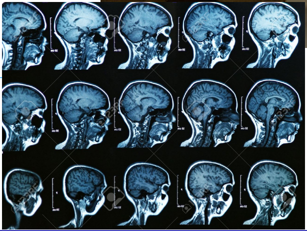

...and so, in conclusion, the proposed method...
THANK GOODNESS, ALMOST OVER... HOPEFULLY I DIDN'T BORE THEM TO TEARS.
...thank you, you've been a great audience...
OK, THE OBLIGATORY CALL FOR QUESTIONS AND I AM DONE...
any ques...
JORGE CHAM © 2004
...tions?
OR NOT.
www.phdcomics.com

# Why Nuclear Physics?

- Nuclear physics has been an important topic to study for over a century
  - Nuclear energy
  - Radiotherapy to kill cancer cells
  - Nuclear Magnetic Resonance (MRI imaging)
  - Radioactive dating

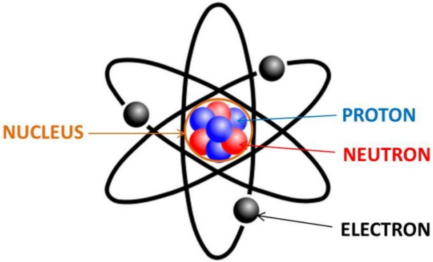
to name a few ...



# Why Nuclear Physics?

- Much of this was done without a good understanding of how nuclear particles interact with each other.
- My research has to do with understanding that fundamental interaction between nuclear particles (called nucleons).



# Nuclear Problem

- We want to solve for the ground state energy of nuclei. This is also called the **binding energy**, $B$.

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- Quantum Mechanics tells us that this energy is equal to

$$E_0 = -B = \int d\mathbf{r}_1 \dots d\mathbf{r}_A \Psi_0^*(\mathbf{r}_1, \dots, \mathbf{r}_A)\hat{H}\Psi_0(\mathbf{r}_1, \dots, \mathbf{r}_A)$$

But let's break this down a bit.

# Nuclear Problem

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- $\hat{H}$ is called the Hamiltonian. This is just a fancy way of saying the thing that tells us what the energy is. For the EM force it's something like

$$H_{\text{EM}} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} k \frac{q_1 q_2}{r_{ij}}$$

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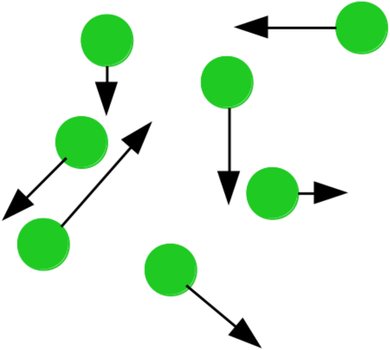
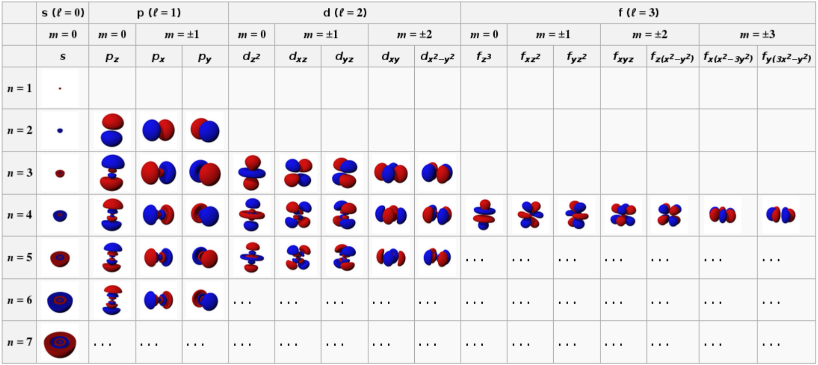
- The last part, $\Psi_0$, is called the wave function, and it deserves it's own slide.

# Wave Function

- Ingredients to describe the state of a classical system:
  - Position and momentum (velocity) of each particle.
- If we knew those things for every particle we could (classically) predict everything in the universe.



- Quantum Mechanics tells us that particles don't have just a single position, but they can be in multiple places at the same time. The probability of finding a particle in a given place is given by the square of the **wave function**, $|\Psi(\mathbf{R})|^2$.
- You've probably seen this idea before:



# Wave Functions

- The state that has the lowest energy is called the **ground state**.
- All we need to do now is plug in the ground state $\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_A)$, the nuclear Hamiltonian $\hat{H}$, and solve the integral…that's it!

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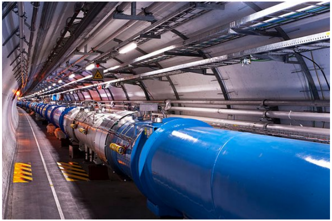
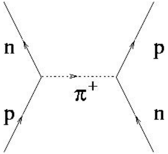
- There are only a couple of small problems:
  - We don't actually know a great way to write $\hat{H}$ for nuclear physics.
  - We don't know what the ground state is.
  - The integrals are too big and complicated for our computers to solve using normal numerical integration methods.

# Solving the Problems - $\hat{H}$

- Two methods we use to get approximations to $\hat{H}$:
  - **Phenomenological Approach:** Make an educated guess and then smash particles together and fit the guess to the data.



  - **Quantum Field Theory Approach:** Make approximations to the "true" theory to determine what the interaction will look like.



# Solving the Problems - $\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_A)$

- One guess for the wave function would be to find "single particle" states and put each particle in one of those;

$$\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_A) = \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\ldots\phi_A(\mathbf{r}_A)^1$$

[1] We technically antisymmetrize this with respect to particle exchange.

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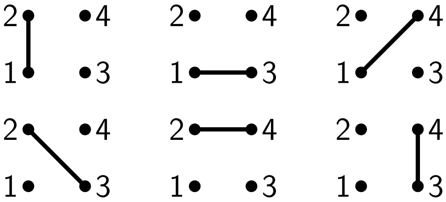
- This is a good start but notice that the particles don’t interact in this wave function. Let’s force this in.

$$\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_A) = \left[1 + \sum_{i<j} \mathcal{O}_{ij}\right] \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$

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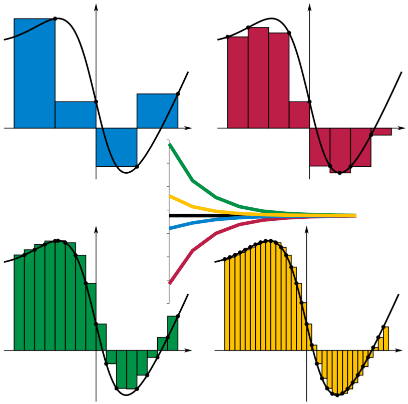
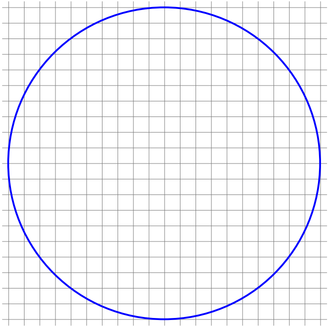
# Solve the Problems - Monte Carlo Integration



- At 1000 samples per dimension that's $10^{15}$, $10^{51}$, and $10^{123}$ samples just to calculate the intergral for $^4$He, $^{16}$O, and $^{40}$Ca respectively.
- That's infeasible! We need something else.

# Solve the Problems - Monte Carlo Integration

- Let's try the Monte Carlo method. Monte Carlo uses random samples instead of a defined number of grid points. Let's integrate to find the area of a circle.



$$A_{\text{circle}} = \sum_i \sum_j dx_i dy_j$$

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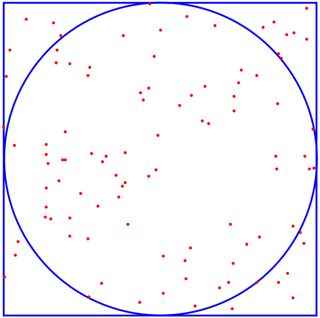


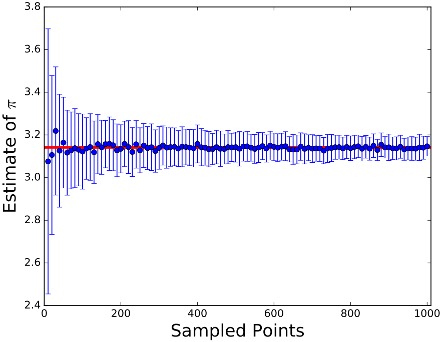
$$\frac{A_{\text{circle}}}{A_{\text{box}}} = \frac{\#\text{ points in the circle}}{\#\text{ points in the box (total)}}$$

# Monte Carlo Example

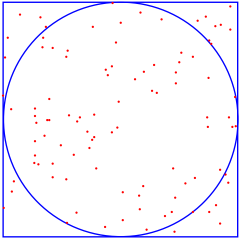
- You can estimate $\pi = 3.14159$ using the method above.

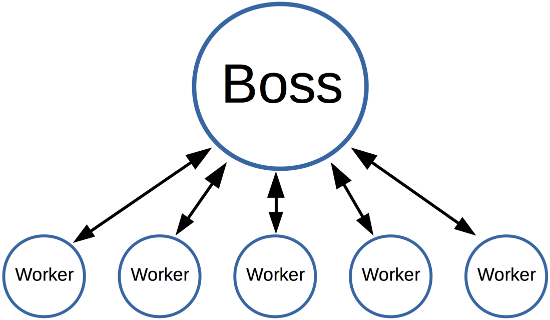
$$\frac{A_{\text{circle}}}{A_{\text{box}}} = \frac{\pi r^2}{(2r)(2r)} = \frac{\pi}{4} = \frac{\#\text{ points in the circle}}{\#\text{ points in the box (total)}}$$

$$\pi = 4\frac{\#\text{ points in the circle}}{\#\text{ points in the box (total)}}$$



# Monte Carlo on a Supercomputer






$$E = \int \Psi^*(\mathbf{R}) H \Psi(\mathbf{R}) d\mathbf{r_1} d\mathbf{r_2} \ldots d\mathbf{r_N}$$

$\Psi^*(\mathbf{R}) H \Psi(\mathbf{R})$ at each point

- We call our "guess" for the wave function the **trial wave function**, $\Psi_T(\mathbf{R})$.
- It is a combination of the ground state and higher energy states.

$$\Psi_T(\mathbf{R}) = c_0\Psi_0(\mathbf{R}) + \sum_n c_n\Psi_n(\mathbf{R})$$

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$$\Psi_T(\mathbf{R}) = c_0\Psi_0(\mathbf{R}) + \sum_n c_n\Psi_n(\mathbf{R})$$

$$E_V = \int \Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R}) d\mathbf{r_1} d\mathbf{r_2} \dots d\mathbf{r_N} \geq E_0$$

- This idea is called the **variational principle**.
- It's very powerful because it guarantees an upper bound on the ground state energy.

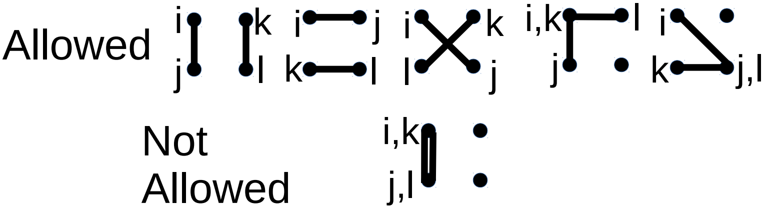
# Monte Carlo in Nuclear Physics

$$E_V = \int \Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R}) d\mathbf{r_1} d\mathbf{r_2} \dots d\mathbf{r_N}$$

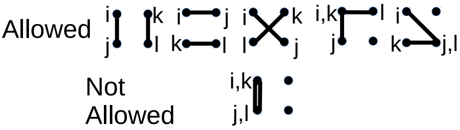
- Guess $\Psi_T(\mathbf{R})$
- Get a good guess for $\hat{H}$ from somebody else
- Put it on a supercomputer
- Change $\Psi_T(\mathbf{R})$ until you get the lowest energy you can (Variational Monte Carlo)

- In the past the wave function we use only "correlates" 2 nucleons at a time. I added correlations that correlated 4 nucleons at a time.

$$\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_A) = \left[ 1 + \sum_{i<j} \mathcal{O}_{ij} + \sum_{i<j} \sum_{\substack{k<l \\ ij \neq kl}} \mathcal{O}_{ij}\mathcal{O}_{kl} \right] \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_A)$$



# Improved Trial Wave Function - Quadratic Correlations




- Calculation time can be saved by just looking at **independent pairs** since they capture most of the physics.

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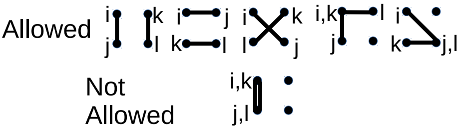
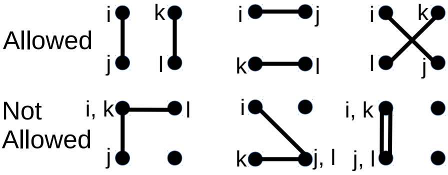



- Calculation time can be saved by just looking at **independent pairs** since they capture most of the physics.

$$\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_A) = \left[1 + \sum_{i<j}\mathcal{O}_{ij} + \sum_{i<j}\sum_{\substack{k<l\\ ij\neq kl}}\mathcal{O}_{ij}\mathcal{O}_{kl}\right]\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_A)$$



# Results

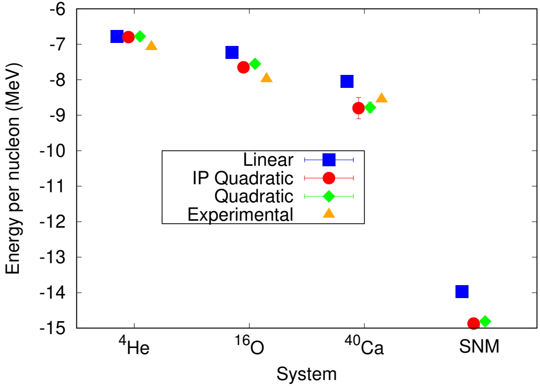
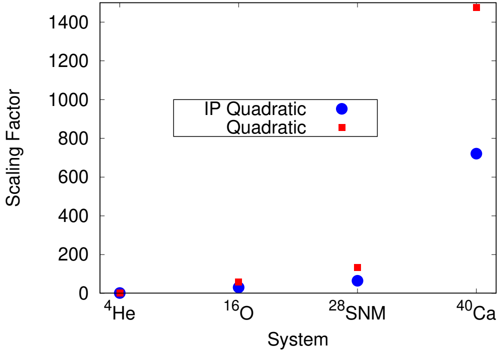



Table: Energy (*per nucleon) in MeV

| 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

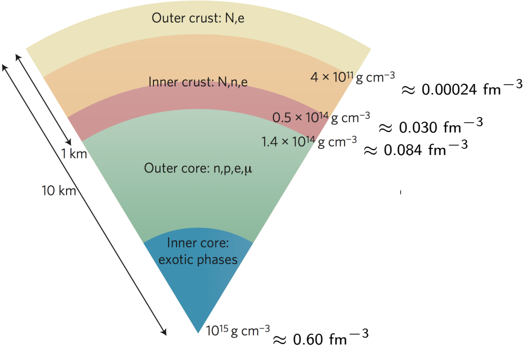



| | $^4$He | $^{16}$O | SNM(28) | $^{40}$Ca |
|---|---|---|---|---|
| IP Quadratic | 1.73 | 30.7 | 64.8 | 720.9 |
| Quadratic | 2.00 | 58.8 | 133.6 | 1473.9 |

# Neutron Stars - Preliminary

- Use new wave function to study $\alpha$ 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

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

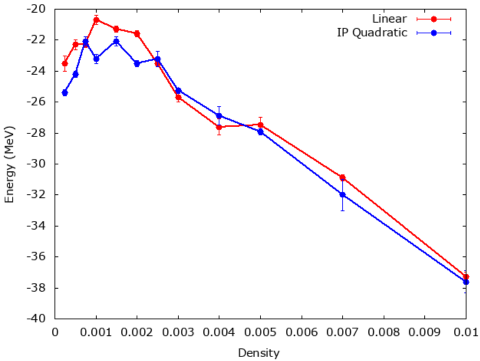
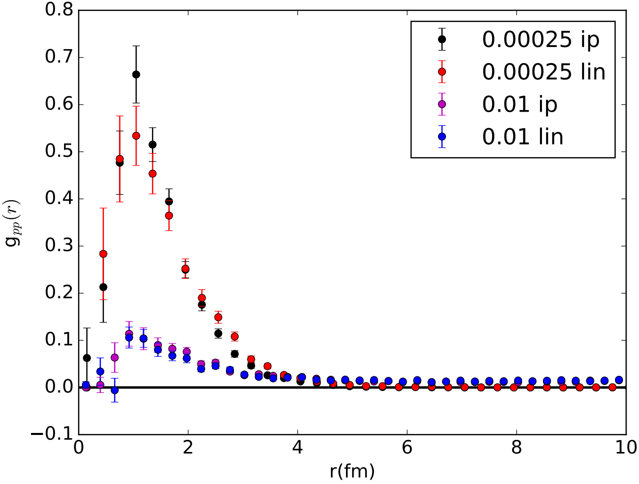



Table: Alpha energy in MeV

| $\rho$ (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) |

# Pair Correlation Function - Preliminary

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



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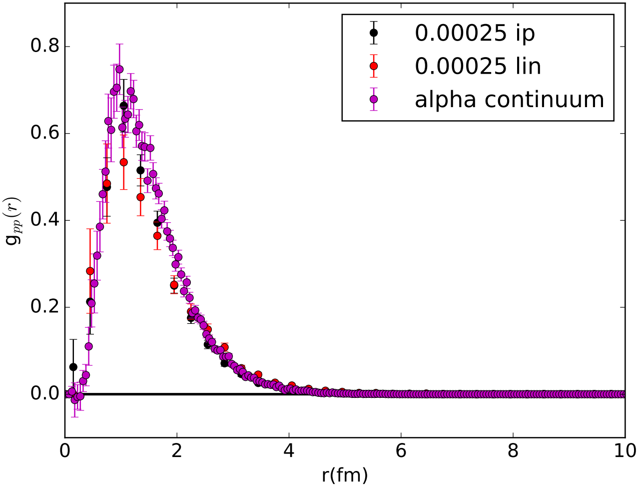
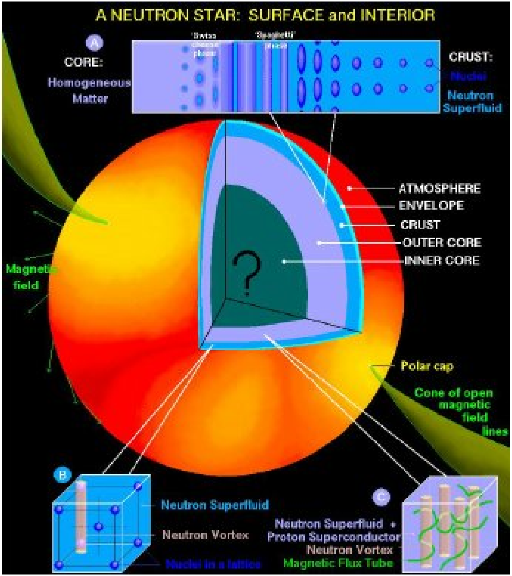
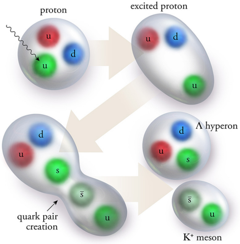
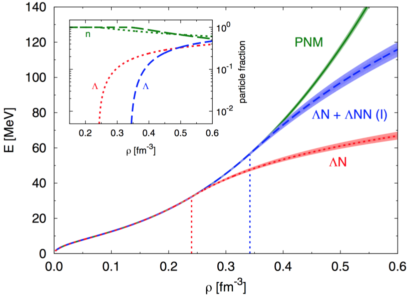


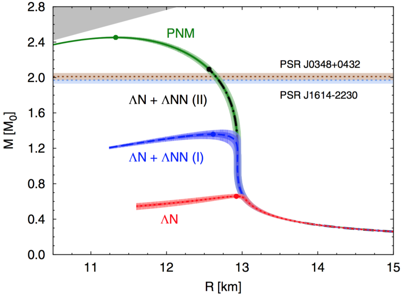
# Future Work

- Other improvements to trial wave function
- Neutron star equation of state, $E(\rho)$
  - Using $\chi$EFT 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
- Any interesting physics, especially with applications to computation


A NEUTRON STAR: SURFACE and INTERIOR
A
CORE:
Homogeneous
Matter
CRUST:
Neutron
Superfluid
ATMOSPHERE
ENVELOPE
CRUST
OUTER CORE
INNER CORE
?
Magnetic
field
Polar cap
Cone of open
magnetic
field
lines
B
Neutron Superfluid
Neutron Vortex
C
Neutron Superfluid +
Proton Superconductor
Neutron Vortex
Magnetic Flux Tube




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

# Conclusion/Summary

- Quantum Monte Carlo is a powerful method for studying nuclear systems.
- We need to improve the wave function to study larger, more interesting systems.
- There are a variety of interesting problems that would be fun to do in collaboration with SUU students and faculty.

# Thanks

PhD Advisor: Kevin Schmidt (ASU)
Collaborators: Stefano Gandolfi (LANL) and Joe Carlson (LANL)

# Picture References

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