Variational Theory of Nuclear Matter at Finite Temperature

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Work done with :
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Objectives

Ab initio reliable Many Body Method to calculate the Equation of State of Dense Matter at Finite Temperature

Argonne v18

- Fit to NN scattering phase shifts in vacuum.
- Operator dependent

$$v_{\mathrm{Av18}} = v^{\mathrm{p}} \mathcal{O}^{\mathrm{p}}$$

Wiringa, Stoks and Schiavilla - Phys. Rev. C (1995)

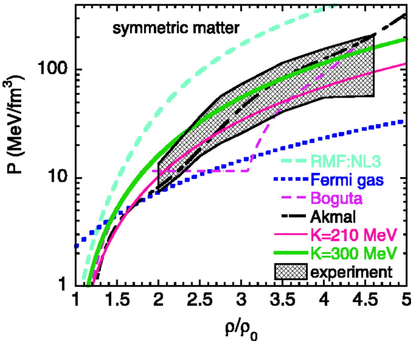
Urbana IX

- Fit to the binding energy of triton and the saturation density of nuclear matter
- $V_{\mathrm{UIX}} = V^R + V^{2\pi}$

Pudliner, Pandharipande, Carlson, and Wiringa, Phys. Rev. Lett. (1995)

Objectives

Ab initio reliable Many Body Method to calculate the Equation of State of Dense Matter at Finite Temperature



Danielewicz, Lacey, Lynch Science **298** 1592 (2002)

- Variational Chain Summation method
- Zero Temperature $\longrightarrow$ Akmal-Pandharipande-Ravenhall EOS

Akmal, Pandharipande Phys. Rev. C (1997), Akaml, Pandharipande and Ravenhall Phys. Rev. C (1998)

Objectives

Ab initio reliable Many Body Method to calculate the Equation of State of Dense Matter at Finite Temperature

Finite Temperature VCS

- Identify the relevant variational principle at $T \neq 0$ which can be used to constrain the free energy
  $\longrightarrow$ Gibbs-Bogoliubov variational principle
- Recast this principle so that we can use the powerful technology of VCS
- Resolve the problem of orthogonality corrections
  $\longrightarrow$ The wavefunctions used in VCS are not mutually orthogonal

Ansatz for the Wavefunctions

$$\Psi_l(1,2,\ldots,N) = \mathcal{S}\left(\prod_{i<j}\mathcal{F}_{ij}\right)\Phi_l(1,2,\ldots,N)$$

Eigenstate of the Interacting System

Long Range Part(Free Fermi Gas Wavefunction)

Short Range Part(Pair Correlation Operator)

Long Range Part

- Simple Slater determinant
- The single particle spectrum is different from the non-interacting case

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m^\star} + U(\rho, T)$$

Ansatz for the Wavefunctions

$$\Psi_l(1,2,\ldots,N) = \mathcal{S}\left(\prod_{i<j}\mathcal{F}_{ij}\right)\Phi_l(1,2,\ldots,N)$$

Eigenstate of the Interacting System

Long Range Part(Free Fermi Gas Wavefunction)

Short Range Part(Pair Correlation Operator)

Short Range Part

- Product of pair correlation operators
- The pair correlation operators mimic the operator dependence of the potential

$$\mathcal{F}_{ij} = \sum_{p} f^{\mathrm{p}}(r_{ij})\mathcal{O}_{ij}^{\mathrm{p}}$$

Finite Temperature

Variational Principle at $T \neq 0$

$$F < F_v = \langle H \rangle_v - TS_v$$

$$\langle \cdot \rangle_v = \mathrm{Tr}\left[\frac{e^{-\beta H_v}\cdot}{\mathrm{Tr}(e^{-\beta H_v}\cdot)}\right]$$

$$S_v = \text{Entropy due to } H_v$$

- We can choose $H_v = E_l^v |\Psi_l\rangle\langle\Psi_l|$ and $E_l^v = \sum_l \epsilon(k) n_l(k)$
- Then the entropy is :

$$S_v = -\sum_k \bar{n}(k) \ln \bar{n}(k) + (1 - \bar{n}(k)) \ln(1 - \bar{n}(k))$$

- Use VCS is to calculate $\langle \Psi_l | H | \Psi_l \rangle$

Schmidt and Pandharipande Phys. Lett. B (1979), Friedman and Pandharipande Nucl. Phys A (1981)

Finite Temperature

Variational Principle at $T \neq 0$

$$F < F_v = \langle H \rangle_v - TS_v$$

$$\begin{aligned} \langle \cdot \rangle_v &= \mathrm{Tr}\left[\frac{e^{-\beta H_v} \cdot}{\mathrm{Tr}(e^{-\beta H_v} \cdot)} \right] \\ S_v &= \text{Entropy due to } H_v \end{aligned}$$

- The above inequality will hold iff the Ψ_I's are ORTHONORMAL
- Unfortunately, the Ψ_I's are NOT ORTHONORMAL

$$\langle \Psi_I | \Psi_I' \rangle \neq 0$$

Orthogonality Corrections

Orthonormalization :

$$|\Theta_I\rangle = |\Psi_I\rangle - \frac{1}{2}\sum_{I} |\Psi_{I'}\rangle\langle\Psi_{I'}|\Psi_I\rangle + \dots$$

$$\longrightarrow \langle\Theta_I|H|\Theta_I\rangle = \langle\Psi_I|H|\Psi_I\rangle - \frac{1}{2}\sum_{I}\langle\Psi_I|H|\Psi_{I'}\rangle\langle\Psi_{I'}|\Psi_I\rangle + \dots$$

- No good methods to calculate the Orthogonality Corrections (OFF DIAGONAL MATRIX ELEMENTS)
- VCS can be used only for DIAGONAL MATRIX ELEMENTS

Orthogonality Corrections

Orthonormalization :

$$|\Theta_I\rangle = |\Psi_I\rangle - \frac{1}{2}\sum_{I} |\Psi_{I'}\rangle\langle\Psi_{I'}|\Psi_I\rangle + \dots$$

$$\longrightarrow \langle\Theta_I|H|\Theta_I\rangle = \langle\Psi_I|H|\Psi_I\rangle - \frac{1}{2}\sum_{I}\langle\Psi_I|H|\Psi_{I'}\rangle\langle\Psi_{I'}|\Psi_I\rangle + \dots$$

It can be shown that :

The orthogonality correction to the Free Energy VANISH in the Thermodynamic Limit

Mukherjee and Pandharipande Phys. Rev. C (2007)

Best estimate for the Free Energy

$$F = \langle \Psi_l | H | \Psi_l \rangle_v - TS_v + E_{\text{corrections}} (\text{not ortho. cor.})$$

- Quasiparticle Hamiltonian

$$\begin{aligned} H_v &= \sum_l E_l^v |\Theta\rangle\langle\Theta| \\ E_l^v &= \sum_k \epsilon(k) n_l(k) \end{aligned}$$

- Quasiparticle Spectrum

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m^\star} + U(\rho, T)$$

- (Quasiparticle) Entropy

$$S_v = -\sum_k \bar{n}(k) \ln \bar{n}(k) + (1 - \bar{n}(k)) \ln(1 - \bar{n}(k)))$$

Best estimate for the Free Energy

$$F = \langle \Psi_l | H | \Psi_l \rangle_v - TS_v + E_{\text{corrections}}(\text{not ortho. cor.})$$

$$\Psi_l(1,2,\ldots,N) = \mathcal{S}\left(\prod_{i<j}\mathcal{F}_{ij}\right)\Phi_l(1,2,\ldots,N)$$

Eigenstate of the Interacting System

Long Range Part(Free Fermi Gas Wavefunction)

Short Range Part(Pair Correlation Operator)

1. The expectation value of the Hamiltonian is expanded into cluster integrals
2. The pair correlation operator $\mathcal{F}$ is found by minimizing the two body cluster
3. The wavefunction has 4 variational parameters $m^\star, d_c, d_t$ and α
4. The full matrix element is calculated by resumming the cluster expansion

Best estimate for the Free Energy

$$F = \langle \Psi_I | H | \Psi_I \rangle_v - TS_v + E_{\text{corrections}} (\text{not ortho. cor.})$$

There are 3 other corrections added to the Free energy :

1. Relativistic corrections
2. Estimate of the perturbative corrections
3. A correction term added to the zero temperature EOS to get the correct saturation energy

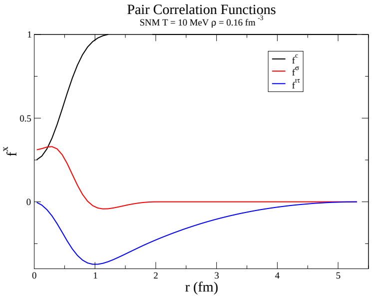
Limitations

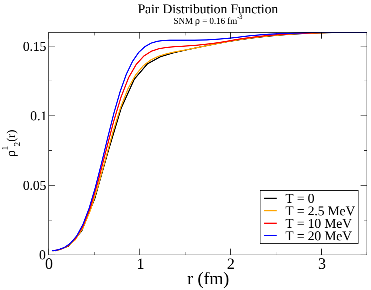
- Non uniform matter
- Only nucleonic degrees of freedom are included
- Pairing
- Thermal pions

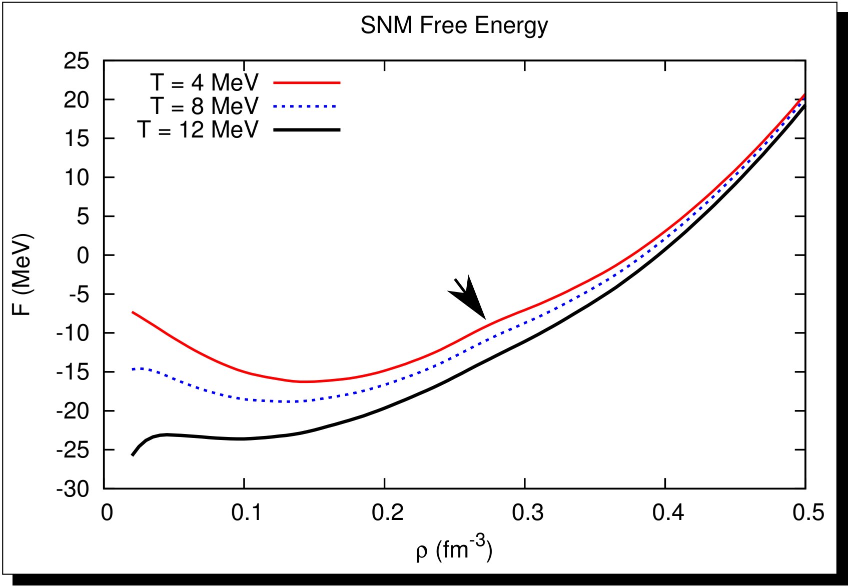
Best estimate for the Free Energy

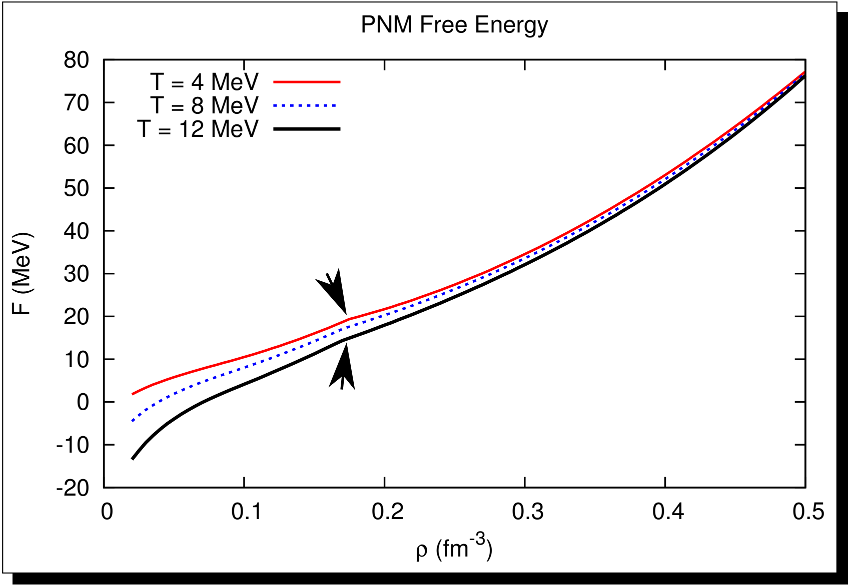
$$F = \langle \Psi_I | H | \Psi_I \rangle_v - TS_v + E_{\text{corrections}} (\text{not ortho. cor.})$$

- The optimal variational parameters are found by minimizing only the variational part of the free energy
- An extra penalty term is added during the minimization to make sure that the sum rules (mass and charge) are reasonably well satisfied



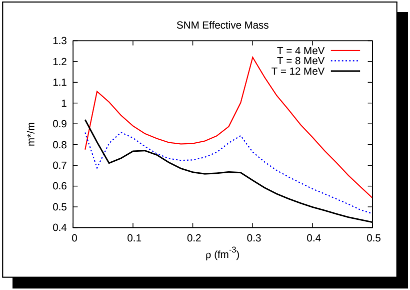



SNM Free Energy
T = 4 MeV
T = 8 MeV
T = 12 MeV
F (MeV)
25
20
15
10
5
0
-5
-10
-15
-20
-25
-30
0
0.1
0.2
0.3
0.4
0.5
ρ (fm-3)



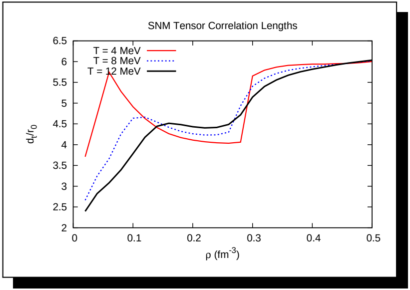
PNM Free Energy
T = 4 MeV
T = 8 MeV
T = 12 MeV
F (MeV)
ρ (fm^{-3})
80
70
60
50
40
30
20
10
0
-10
-20
0
0.1
0.2
0.3
0.4
0.5

Spin-Isospin (π^0 condensation) phase transition

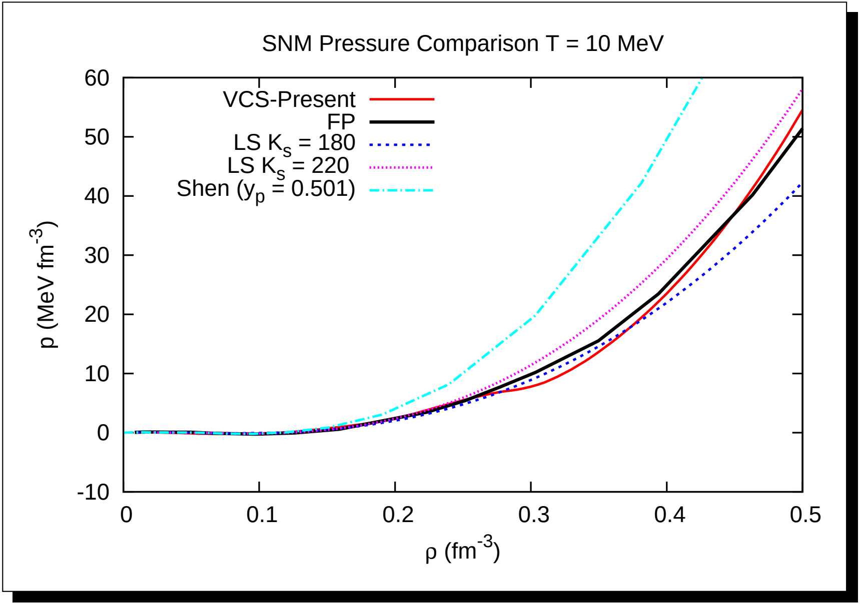


- The effective mass $m^{\star}$ show an enhancement across the phase transition

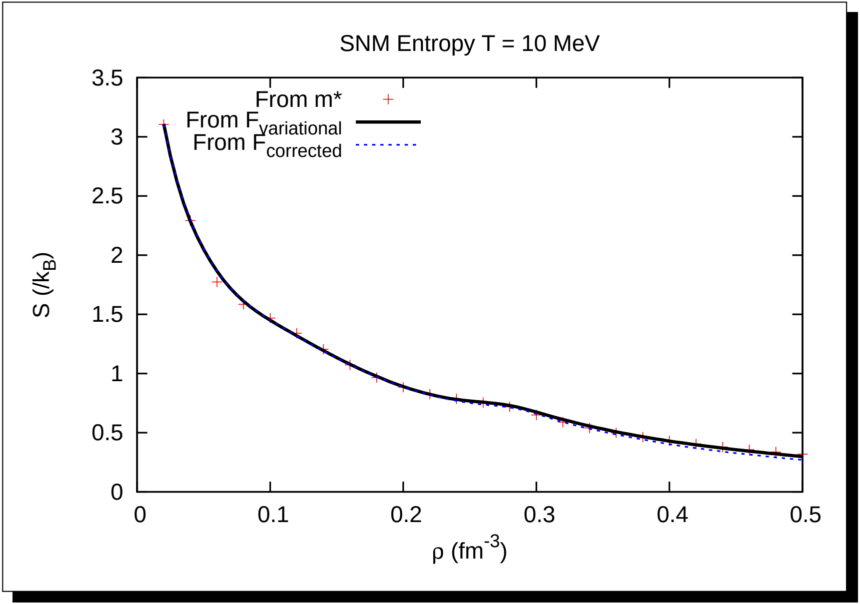
- The tensor correlation length d_t is the length at which the pair correlation operators in the tensor channel vanish



Comparison with other calculations



Thermodynamic Consistency



(Near) Future Work

- VCS can be used only for Pure Neutron Matter and Symmetric Nuclear Matter
- Asymmetric Nuclear Matter :

$$E_{\text{potential}}(\delta) = (1-\delta^2)E_{\text{potential}}(0) + \delta^2 E_{\text{potential}}(1)$$

- Single particle spectrum and effective mass at zero temperature and comparison with the finite temperature spectrum