

VARIATIONAL MONTE CARLO CALCULATIONS OF ENERGY PER PARTICLE OF NUCLEAR MATTER

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Abstract-In this paper, symmetrical nuclear matter has been investigated. Total, kinetic and potential energies per particle were obtained for nuclear matter by Variational Monte Carlo method. We have observed that the results are in good agreement with those obtained by various authors who used different potentials and techniques.

Key words : nuclear matter, nucleon-nucleon interactions, Monte Carlo method.

1. INTRODUCTION

Monte Carlo (MC) method is used for simulating the classical many-particle systems by introducing artificial dynamics based on “random numbers”. The Variational Monte Carlo (VMC) method was first used by Macmillan [1] for simple bose systems, such as atomic helium liquids, where the interaction potentials depend only on interparticle distance. These methods were extended in order to study simple fermion systems [2,3]. However, nuclear matter can not be regarded as a simple system because of the strong dependence of the nucleon-nucleon interactions on the spin and isospin orientations [4]. (MC) methods were also developed to investigate nuclear interactions in some nucleus with a few nucleon systems [5,6].

Quantum Monte Carlo method has been developed to calculate the properties of quantum many-body systems. The ways which are used in the method is basically same as for classical systems. The direct simulations in the classical many-body system have been proved the only way to get thoroughly reliable information about many-body effects, particularly as the systems get more complex. Quantum systems can be reduced to classical systems in certain limits (e.g. at high temperature) hence if it is needed to simulate the classical systems, one needs simulation to calculate the properties of quantum systems. [7]. In this paper we will introduce how the variational quantum Monte Carlo method can be applied to the symmetrical nuclear matter and how the physical properties of the system under consideration can be calculated.

2. JASTROW THEORY, VARIATIONAL WAVE FUNCTION AND METROPOLIS ALGORITHM

In variational Monte Carlo method the ground state wave function $\Psi_0(\vec{R})$ is approximated by a variational wave function $\Psi_V(\vec{R})$ with many variational parameters, which are determined by minimizing $\langle H \rangle$. A common choice of Ψ_V for simple fermion systems contains a product of two and three-body correlation functions $f(r_{ij})$ and $F(r_{ij}, r_{jk}, r_{ki})$ and Slater determinant [8] :

$$\Psi_V(\vec{R}) = \left[\prod_{i \langle j \langle k} F(r_{ij}, r_{jk}, r_{ki}) \right] \left[\prod_{i \langle j} f(r_{ij}) \right] \Phi. \quad (1)$$

This Ψ_V reduces to the Hartree-Fock form when the correlation functions $f = F = 1$. When the three-body correlation $F=1$, but pair correlation $f \neq 1$, one obtains the Jastrow form. We will base our calculations on a wave function of the form

$$\Psi_j(\vec{R}) = \prod_{i \langle j} f_j(r_{ij}) \Phi. \quad (2)$$

Where Φ is the many particle wave function for the system of non-interacting particles and \vec{R} is a 3N dimensional vector representing the coordinates of particles, while f_j is the two particle correlation function. Jastrow suggested that this correlation function in general can be an operator function [9]. However in most applications of f_j it is assumed to depend only on the interparticle distance $r_{ij} = |r_i - r_j|$. In order to simulate the nuclear matter, we will consider a system of N nucleons confined in a cube of side L with periodic boundary conditions. Therefore for the single particle wave functions we can use the plane waves

$$\phi(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \quad (3)$$

where $\vec{k} = 2\pi\vec{n} / L$ and n is an integer vector. Because of the symmetry of ground state we can use real plane waves

$$\phi(\vec{r}) = \begin{cases} \cos\left(\frac{2\pi}{L} \vec{n} \cdot \vec{r}\right) \\ \sin\left(\frac{2\pi}{L} \vec{n} \cdot \vec{r}\right) \end{cases} \quad (4)$$

instead of complex plane waves in eq.(3). Under these conditions the many particle wave function in eq.(2) becomes

$$\Phi(R) = \prod_{s=1}^g \bar{D}^s \quad (5)$$

where D^s is the slater determinant of single particle wave functions

$$d_{ij}^s = \phi_j((\vec{r}, s)_i), \quad \bar{D}^s = \det(d_{ij}^s). \quad (6)$$

For the two particle correlation function f_j in eq.(2) we chose a function similar to the Woods-Saxon potential

$$f_j(r) = \left[\frac{1}{1 + e^{(r_0-r)/a}} \right]^l. \quad (7)$$

Here we define the pseudo potential $u(r)$ for practical reasons as

$$f_j(r_{ij}) = \exp(-u(r_{ij})) \quad u(r_{ij}) = -\ln(f_j(r_{ij})) \quad (8)$$

then our variational wave function becomes

$$\Psi_j = \exp\left(-\sum_{i(j)} u(r_{ij})\right) \times \prod_{s=1}^g \bar{D}^s. \quad (9)$$

The method of sampling the wave function is identical to that used for classical ensembles [10]. The only complication that arises is the evaluation of the determinant. Initial coordinates are chosen for each particle; typically they are either on a lattice or are a result of a previous Monte Carlo calculations. The particles are then moved one by one to new trial positions. Suppose particle 1 is being moved. Then its new trial position r_{new} is $\bar{r}_1 + \bar{\xi}$, where $\bar{\xi}$ is a random vector uniformly distributed in a cube of side Δ centered at the origin. The new position for particle 1 is accepted with a probability equal to

$$P = \min\left[1, \left|\Psi(\bar{r}_y) / \Psi(\bar{r}_1)\right|^2\right]. \quad (10)$$

If the absolute value of the wave function at the new position is larger than that was at the old, the new coordinates are automatically accepted. This random walk is Markovian and by the usual argument [1] the set of coordinates generated by a sufficiently long calculation is an unbiased sample drawn from the probability distribution $|\Psi(R)|^2 / \int dR |\Psi(R)|^2$.

The expectation value of any operator F is simply the average value of the operator evaluated for the coordinates of the random walk with M moves

$$\langle \hat{F} \rangle = \frac{\int d\bar{r} \Psi^*(\bar{r}) F(\bar{r}) \Psi(\bar{r})}{\int d\bar{r} |\Psi(\bar{r})|^2} \cong \frac{1}{M} \sum_{i=1}^M F(\bar{r}_i). \quad (11)$$

The most effective way to handle this wave function is to calculate the inverses of the matrices D^s at the beginning of the random walk and then update them as the particles are moving. This inverse is needed to compute the Metropolis acceptance ratio [eq.(10)] and the variational energy. Let \bar{D}^s be the inverse of the transpose of D^s of Eq.(6). Then, the equation

$$\sum_{j=1}^I \bar{D}_{ij}^s D_{kj}^s = \delta_{ik} . \quad (12)$$

can be defined. Note that the first index always represents an orbital, the second a particle. Now the determinant of a matrix is equal to the scalar product of any column (row) of the matrix with the same column (row) of the matrix of cofactors. Let particle 1 (with spin s) be moved to a new trial position. Since only one particle is being moved; only one column of the matrix D^s will change, and the required ratio of wave functions is easily evaluated. Since \bar{D}^s is proportional to the matrix of cofactors, the ratio of determinants is

$$\sum_{j=1}^I \bar{D}_{j1}^s \Phi_j(r_{new}) = q, \quad \frac{\Psi(R_{new})}{\Psi(R)} = q \exp\left(-\sum_{j=2}^N u(r_{newj}) - u(r_{1j})\right). \quad (13)$$

If the move is accepted all of the elements of \bar{D}^s will be needed to be changed

$$\bar{D}_{ji}^s = \begin{cases} \bar{D}_{ji}^s / q & i = 1 \\ \bar{D}_{ji}^s - \bar{D}_{j1}^s \sum_{k=1}^I \frac{\bar{D}_{kj}^s \Phi_k(r_{new})}{q} & i \neq 1 \end{cases} \quad (14)$$

3. NUCLEON-NUCLEON INTERACTION POTENTIALS

The simplest model of a nucleus is a collection of point nucleons that obey the nonrelativistic Schrödinger equation and interact through a two-body potential that fits nucleon-nucleon scattering data and the properties of the deuteron. Any assumed two-body potential implies a curve of energy per particle versus density for nuclear matter. The saturation point of this curve must agree with the empirical one if the potential used in the calculation represents that of the nucleus well. Therefore it is essential to have a method for reliably calculating by using an assumed potential and the binding energy of nuclear matter as a function of density. Only if this calculation can be done accurately does it make sense to compare the calculated saturation point with the empirical one and hence to accept or reject the potential [11]. Therefore the starting point for nuclear matter calculation is a two-body potential that models the nucleon-nucleon interaction [12]. We have used the Urbana V_{14} potential for the nucleon-nucleon interaction. This potential, due to Lagaris and Pandharipande, was obtained by fitting the phase shift data from low energy nucleon-nucleon scattering experiments and the properties of deuteron [13]. Urbana potential contains 14 operator components and it has the form

$$\begin{aligned} V_{ij} = & v^c + v^\sigma (\sigma_i \cdot \sigma_j) + v^\tau (\tau_i \cdot \tau_j) + v^{\sigma\tau} (\sigma_i \cdot \sigma_j)(\tau_i \cdot \tau_j) \\ & + v^t S_{ij} + v^{t\tau} S_{ij} (\tau_i \cdot \tau_j) + v^b (\mathbf{L} \cdot \mathbf{S})_{ij} + v^{b\tau} (\mathbf{L} \cdot \mathbf{S})_{ij} (\tau_i \cdot \tau_j) \\ & + v^q L^2 + v^{q\sigma} L^2 (\sigma_i \cdot \sigma_j) + v^{q\tau} L^2 (\tau_i \cdot \tau_j) + v^{q\sigma\tau} L^2 (\sigma_i \cdot \sigma_j)(\tau_i \cdot \tau_j) \\ & + v^{bb} (\mathbf{L} \cdot \mathbf{S})^2 + v^{bb\tau} (\mathbf{L} \cdot \mathbf{S})^2 (\tau_i \cdot \tau_j). \end{aligned} \quad (15)$$

3.1. Expectation Values of Potential and Kinetic Energy

The variational parameters r_0 , a and t in Eq.(7) will be obtained from the minimization of the total variational energy E_j

$$E_j = \frac{\langle \Psi_j | H | \Psi_j \rangle}{\langle \Psi_j | \Psi_j \rangle}, \quad \mathbf{H} = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i < j} V_{ij}. \quad (16)$$

where \mathbf{H} is the expectation value of Hamiltonian operator in the ground state of the system. Here $(-\hbar^2 \nabla_i^2 / 2m)$ is the kinetic energy operator of the i -th particle and V_{ij} is the potential energy operator between the pair i and j . For the moment it is sufficient to know that this potential depends only on the distance between the particles i and j and on their spin isospin orientations. Therefore it is easy to calculate the expectation value for the potential energy per nucleon

$$\langle V_1 \rangle = \frac{\int dR \Psi^*(R) V_1(R) \Psi(R)}{\int dR \Psi^*(R) \Psi(R)}, \quad \langle V_1 \rangle \cong \frac{1}{2M} \sum_i V_1(R_i) \quad (17)$$

where $V_1(R_i)$ is the total potential energy in the i -th step of the random walk due to the interactions between the moving particle and all other particles contained in a sphere of radius $L/2$. In this manner of calculation each interaction is considered twice and therefore there is factor of $1/2$ in Eq. (17). As we consider only the particles contained in a sphere of radius $L/2$, the contribution of the particles outside this sphere should be added to our estimation of the potential energy [4]. This contribution calculated with the assumption that the radial distribution function equals unity outside this sphere. Thus the contribution is

$$V_{>L/2} = \frac{1}{2} \int_{L/2}^{\infty} \rho V(r) 4\pi r^2 dr \quad (18)$$

where ρ is the number density of the matter. The expectation value of the total kinetic energy is given by

$$\langle T \rangle = \frac{\int dR \Psi^*(R) T(R) \Psi(R)}{\int dR \Psi^*(R) \Psi(R)}. \quad (19)$$

Using the variational wave function from Eq.(9) and inverse matrices from Eq.(14) average kinetic energy for the first particle is expressed as[4]

$$\begin{aligned} \langle T_1 \rangle = \frac{\hbar^2}{2m} \frac{1}{M} \sum \left\{ \sum_{j=1}^I \bar{d}_{j1}^s \bar{\nabla}_1^2 \varphi(r_1) - 2 \sum_{j=1}^I \bar{d}_{j1}^s \bar{\nabla}_1 \varphi(r_1) \sum_{j=2}^N \bar{\nabla}_1 u(r_{1j}) \right. \\ \left. - \sum_{j=2}^N \bar{\nabla}_1^2 u(r_{1j}) + \left(\sum_{j=2}^N \bar{\nabla}_1 u(r_{1j}) \right)^2 \right\} \end{aligned} \quad (20)$$

The expectation value for the kinetic energy of particle 1 can also be expressed as [14,15]

$$\langle T_1 \rangle = \frac{\hbar^2}{2m} \frac{\int dR (\nabla_1 \Psi^*) (\nabla_1 \Psi)}{\int dR \Psi^* \Psi} \quad (21)$$

using the Monte Carlo method and inverse matrices we get

$$\begin{aligned} \langle T_1 \rangle = \frac{\hbar^2}{2m} \frac{1}{M} \sum \left\{ \left(\sum_{j=1}^I \bar{d}_{j1}^s \bar{\nabla}_1 \varphi(r_1) \right)^2 + \left(\sum_{j=2}^N \bar{\nabla}_1 u(r_{1j}) \right)^2 \right. \\ \left. - 2 \left(\sum_{j=1}^I \bar{d}_{j1}^s \bar{\nabla}_1 \varphi(r_1) \right) \left(\sum_{j=2}^N \bar{\nabla}_1 u(r_{1j}) \right) \right\} \end{aligned} \quad (22)$$

The variance of the previous form goes to zero as the wave function approaches an eigen state of the Hamiltonian. These two forms for the kinetic energy give the same result if the configuration space is adequately sampled. Therefore the alternative form for the kinetic energy is used to control whether the configuration space is sufficiently sampled.

4. APPLICATION OF VARIATIONAL MONTE CARLO METHOD TO NUCLEAR MATTER

The 14 operator components in Eq.(15) are necessary to have a good fit to the experimental data. However, the first four terms are much stronger and due to the symmetrical nature of the nuclear matter the terms depending on the relative angular momentum operator \mathbf{L} do not considerably effect the binding energy of the nuclear matter. Therefore in our calculations we have used only the first four terms of the Urbana potential, that is the two nucleon interaction used in our calculations,

$$V_{ij} = V^c + V^\sigma (\sigma_i \cdot \sigma_j) + V^\tau (\tau_i \cdot \tau_j) + V^{\sigma\tau} (\sigma_i \cdot \sigma_j) (\tau_i \cdot \tau_j), \quad (23)$$

where V^c , V^σ , V^τ and $V^{\sigma\tau}$ depend only on the distance between the nucleons i and j . Each term in Eq. (23) has three parts

$$V^i = V_\pi^i + V_I^i + V_S^i \quad (24)$$

representing long-range (V_π^i), intermediate-range (V_I^i), and short range (V_S^i) interactions. (V_π^i) is nonzero only for $i = \sigma\tau$ and is given by

$$V_\pi^{\sigma\tau}(r) = 3.488 \frac{e^{-\mu r}}{\mu r} (1 - e^{-cr^2}) \quad (25)$$

where $\mu = 0.7 \text{ fm}^{-1}$ is the inverse Compton wavelength for pions. The intermediate and short range parts are, respectively,

$$V_I^i(r) = I^i \left[\left(1 + \frac{3}{\mu r} + \frac{3}{(\mu r)^2} \right) \frac{e^{-\mu r}}{\mu r} (1 - e^{-cr^2}) \right]^2, \quad V_S^i(r) = \frac{S^i}{1 + e^{(r-R)/a}}. \quad (26)$$

Values of the potential strengths I^i and S^i and the parameters c , R , a are given in Table I.

Table I. Parameters of the Urbana V_{14} nucleon-nucleon potential.

I	I^i	S^i
c	-5.7030	2575.3
σ	0.7628	-366.56
τ	0.8892	-466.56
$\sigma\tau$	-0.2790	40281
$c=0.2\text{fm}^{-2}, R=0.5\text{fm}, a=0.2\text{fm}$		

We have incorporated three and more body interactions into our calculations with the assumption that the strength of the short range part of the potential

$$V_S^I(r) = \frac{S^i}{1 + e^{(r-R)/a}} [1 + \alpha(\rho)^\beta]. \quad (27)$$

The parameters α and β in the above equation is adjusted so as to obtain a binding energy close to the observed value of $E=-16 \text{ MeV}$.

Table II. Total, potential and kinetic energy per nucleon for the nuclear matter as a function of density

$\rho(fm^{-3})$ Density	Tot.Energy (MeV)	Pot.Energy (MeV)	Kin.Energy (MeV)	$\rho(fm^{-3})$ Density	Tot.Energy (MeV)	Pot.Energy (MeV)	Kin.Energy (MeV)
0.01	0.51657	-3.56805	4.08764	0.21	-13.58950	-49.30824	41.19925
0.02	0.12196	-6.57212	6.72132	0.22	-12.90494	-50.61014	43.65940
0.03	-1.75476	-10.55439	8.88308	0.23	-10.74015	-53.97984	49.68146
0.04	-3.07755	-14.01034	11.10621	0.24	-9.84579	-49.51716	46.61423
0.05	-4.59480	-17.03785	12.73923	0.25	-8.18015	-50.43835	49.71531
0.06	-6.00842	-20.79842	15.24023	0.26	-6.18196	-49.45341	51.25565
0.07	-7.50641	-23.96694	17.09342	0.27	-3.69219	-49.72471	54.55634
0.08	-8.74660	-26.68039	18.77688	0.28	-0.98018	-50.02049	58.11602
0.09	-10.12231	-29.40210	20.35867	0.29	2.22632	-44.64206	56.50796
0.10	-11.26877	-32.10169	22.17168	0.30	5.60101	-44.55496	60.37118
0.11	-12.48090	-34.82090	23.96136	0.31	8.93460	-43.08104	62.81800
0.12	-13.38560	-36.52438	25.06420	0.32	13.29550	-42.08761	66.78393
0.13	-14.22610	-38.59986	26.62366	0.33	32.89046	-60.85293	105.75378
0.14	-14.93340	-41.18732	28.84771	0.34	24.40687	-27.52648	64.56423
0.15	-15.34160	-42.84453	30.45917	0.35	28.02116	-26.52689	67.81017
0.16	-15.59880	-44.36715	32.10475	0.36	33.16407	-29.32822	76.39621
0.17	-15.66470	-46.05091	34.11980	0.37	40.27195	-19.55187	74.37996
0.18	-15.55380	-48.39241	36.98577	0.38	46.01228	-23.07687	84.30776
0.19	-15.17280	-48.53123	37.93499	0.39	53.76104	-8.00477	77.65702
0.20	-14.65840	-50.14799	40.51069	0.40	59.98947	-6.18824	82.75149

Table III. Equilibrium density, binding energy and Fermi momentum were obtained by various authors with different potentials and techniques for nuclear matter.

$\rho(fm^{-3})$ Equilibrium Density	$E(\rho)(MeV)$ Binding Energy	$k_F(fm^{-1})$ Fermi Momentum	Used Method	Reference
0.24217	-17.2	1.53	Reid v_6 Potential	Day (1978) [11]
0.1589	-16.0	1.33	Urbana v_{14} Potential	Lagaris and Pandharipande (1981) [13]
0.18553	-15.0	1.4	Walecka Model	Horowitz and Serot (1983) [17]
0.27695	-17.8	1.6	Paris Potential	Day and Wiringa (1985) [18]
0.16114	-16.237	1.33	Thomas-Fermi Model	Myers and Swiatecki (1998) [19]
0.192	-13.74	1.42	Urbana v_{14} Potential	Atav and Oğul (2000) [4]
0.1696	-15.59	1.35	Urbana v_{14} Potential	This Study

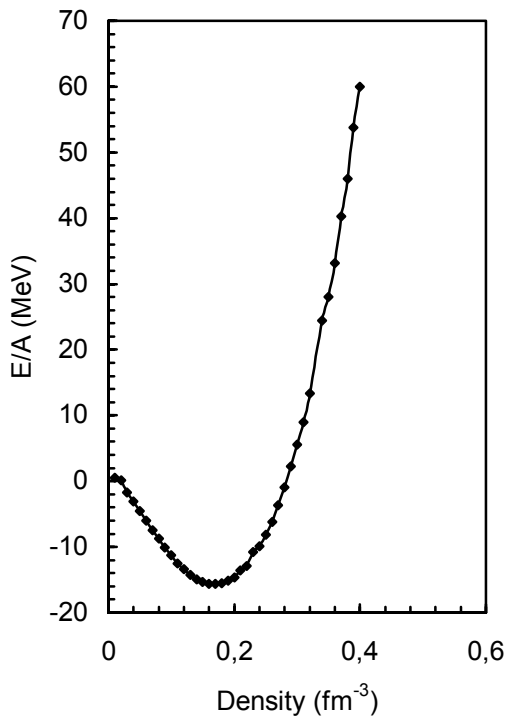


Figure I. Binding energy per nucleon for the nuclear matter as a function of density.

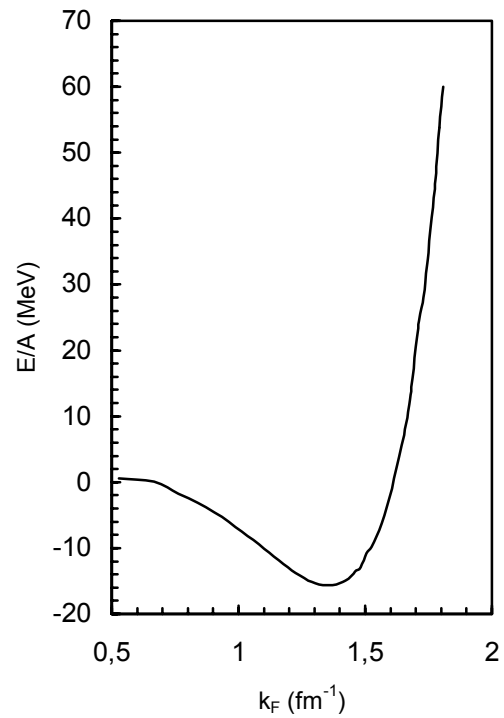


Figure II. Binding energy per nucleon for the nuclear matter as a function of Fermi momentum.

5. CONCLUSIONS

Nuclear matters are hypothetical systems of nucleons interacting without Coulomb forces. Symmetrical nuclear matter is composed of equal numbers of neutrons and protons. It is translationally invariant with a fixed ratio of protons and neutrons. In the ground state of the nuclear matter 4 nucleons can go into each spatial state so the degeneration number g for nuclear matter is 4. The goal of nuclear matter theory is to obtain empirically known bulk properties, such as the binding energy, equilibrium density, symmetry energy, incompressibility, etc., starting from the underlying two-body interactions [12]. In this paper we have interested in the ground states of the symmetrical nuclear matter and as mentioned before we will consider a system of N nucleons confined in a cube of side L with periodic boundaries.

It is well known that three and more body interactions are very important in dense systems like nuclear matter. Using only the two-body interactions gives very large equilibrium densities for nuclear matter [8]. Therefore three and more body interactions somehow should be incorporated into our calculations. In order to simulate three and more particle interactions, the strongly repulsive short range part of the Urbana potential was assumed to depend on $[1 + \alpha(\rho)^\beta]$. For symmetrical nuclear matter, we have obtained the kinetic, potential and total energies per nucleon at densities between $\rho = 0.01 \text{ fm}^{-3}$ and $\rho = 0.40 \text{ fm}^{-3}$ with 0.01 fm^{-3} steps. Equilibrium

density of nuclear matter was obtained to be $\rho_0 = 0.169 \text{ fm}^{-3}$ and the corresponding Fermi momentum $k_F = 1.35 \text{ fm}^{-1}$, where the binding energy per nucleon for the nuclear matter is obtained to be $E(\rho_0) = -15.59 \text{ MeV}$. Binding energy per nucleon for the nuclear matter as a function of density and Fermi momentum are given in Figure I and Figure II respectively. Table II shows the results, and Table III compares our results with those obtained by other authors with different techniques and potentials. It can be seen from this table that our results are closer to the observed values than all the other.

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