NUCLEAR MATTER INCOMPRESSIBILITY: FROM VMC TO SKYRME–LANDAU PARAMETERIZATION

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The new Skyrme parameter set is determined by requiring that Variational Monte Carlo (VMC) calculations reproduce empirical values for properties of nuclear matter, such as binding energy per particle and saturation density. We found the new Landau parameter set by using the new Skyrme parameter set, the saturation density, and energy obtained from the new Skyrme parameter set for symmetric nuclear matter (SNM). Incompressibility of symmetric nuclear matter is also calculated by the described Skyrme–Landau Parameterization.

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1. Introduction

The knowledge about the nuclear incompressibility of infinite symmetric nuclear matter is very important for models of nuclear many-body systems. There is no infinite symmetric nuclear matter in nature but its empirical properties such as saturation density and saturation energy are well-established [1]. Incompressibility of nuclear matter has been studied experimentally and theoretically because of its importance in intermediate energy heavy-ion collisions, neutron star structure, and supernova explosion calculations [2, 3]. Correct determination of the nuclear matter incompressibility is important in order to extend our knowledge on the EOS, because incompressibility is directly related to the curvature of the EOS [2] at the saturation point \((E/A, \rho_0) = (-16 \text{ MeV}, 0.16 \text{ fm}^{-3})\), where \(E/A, \rho_0\) are the binding energy per particle of the nuclear matter and the nuclear matter density, respectively [4]. To experimentally determine the nuclear incompressibility is to measure the compressional-mode giant resonances (ISGMR), and the
isoscalar giant dipole resonance (ISGDR) [5]. In this study, nuclear matter equation of state [6–10] is determined using the VMC calculations at nuclear matter ground state condition. A new set of Skyrme parameters is determined by fitting the results obtained from VMC calculations to the Skyrme energy density functional by using Vautherin and Brink method [11]. Also, we have found the new Landau parameter set by using the new Skyrme parameter set and the saturation point \((E/A, \rho_0) = (-15.49 \text{ MeV}, 0.156 \text{ fm}^{-3})\), which were obtained from VMC simulations and the new Skyrme parameter set, respectively. Finally, we have calculated nuclear matter incompressibility using the new Landau parameter set.

2. Calculations

2.1. Interaction potential

The Hamiltonian operator with a two-body interaction potential \(V_{ij}\) can be written as

\[
H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} V_{ij}.
\]  

(1)

In this paper, we have used first four terms of Urbana potential

\[
V_{ij} = V^c + V^\sigma(\sigma_i \sigma_j) + V^\tau(\tau_i \tau_j) + V^{\sigma\tau}(\sigma_i \sigma_j)(\tau_i \tau_j)
\]  

(2)

which was proposed by Lagaris and Pandharipande [12]

\[
V_{ij} = V^c + V^\sigma(\sigma_i \sigma_j) + V^\tau(\tau_i \tau_j) + V^{\sigma\tau}(\sigma_i \sigma_j)(\tau_i \tau_j)
\]

\[
+ V^I S_{ij} + V^{I\tau} S_{ij}(\tau_i \tau_j) + V^b(L \cdot S)_{ij} + V^{b\tau}(L \cdot S)_{ij}(\tau_i \tau_j)
\]

\[
+ V^q L^2 + V^{q\sigma} L^2(\sigma_i \sigma_j) + V^{q\tau} L^2(\tau_i \tau_j)
\]

\[
+ V^{q\sigma\tau} L^2(\sigma_i \sigma_j)(\tau_i \tau_j) + V^{bb}(L \cdot S)^2 + V^{b\tau}(L \cdot S)(\tau_i \tau_j).
\]  

(3)

This is because: (i) The angular momentum operator does not considerably effect the binding energy because, the infinite nuclear matter is translationally invariant and has a fixed ratio of neutrons and protons. (ii) As the contributions of latter terms are much smaller than those of the first four, their effect is smaller than the statistical fluctuations inherent to the Monte Carlo technique so the inclusion of these terms was pointless.

In Eq. (3), \(V^c, V^\sigma, V^\tau\) and \(V^{\sigma\tau}\) depend only on the distance between the nucleons \(i\) and \(j\). In the Urbana potential, each term in Eq. (3) has three parts

\[
V^i = V^i_\pi + V^i_I + V^i_S
\]  

(4)

representing long-range \((V^i_\pi)\), intermediate-range \((V^i_I)\), and short-range \((V^i_S)\) interactions. The long-range part of the interaction \((V^i_\pi)\) is nonzero only for \(i = \sigma\tau\) and is given by
\[ V_\sigma^{\pi} = 3.488 \frac{e^{-\mu r}}{\mu r} \left( 1 - e^{cr^2} \right), \]  

(5)

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

\[ V_I^i(r) = I^i \left[ \left( 1 + \frac{3}{\mu r} + \frac{3}{(\mu r)^2} \right) e^{-\mu r} \left( 1 - e^{cr^2} \right) \right] \]  

(6)

and

\[ V_S^i(r) = \frac{S^i}{1 + e^{(r-R)/a}} \]  

(7)

respectively. Values of the potential strengths \( I^i \) and \( S^i \) and the parameters \( c, R, a \) were given by Lagaris and Pandharipande [12].

In order to produce correct saturation behaviour of the SNM, we use the phenomenological approach assuming the density-dependent term to be proportional to a short-ranged part of the Urbana potential, and we assume that the total interaction, including the many-body effects, is of the form of

\[ \nu_{14} + \text{TNI} = \nu_{\pi} + \nu_I + \nu_S + \nu_S(\alpha \rho)^\gamma, \]  

(8)

where \( \rho \) is the number density of nucleons. In the above equation, \( \alpha \) and \( \gamma \) are free parameters and adjusted so as to obtain the correct binding energy and saturation density of SNM.

2.2. VMC

We use a Monte Carlo method which is the same as the one described by Manisa [8] for nuclear matter. But, we have made our calculations only for symmetric nuclear matter.

We consider a cubic box of side \( L \) containing \( N \) nucleons with periodic boundary conditions to obtain the properties of bulk nuclear matter in the VMC calculations. The Jastrow-type wave function, which is the trial wave function, is used in the present study in the form of

\[ \Psi_j(\mathbf{R}) = \prod_{i<j} f_i(r_{ij}) \Phi, \]  

(9)

where \( \mathbf{R} \) is a \( 3N \) dimensional vector representing the coordinates of particles, \( f_i \) is the two-particle correlation function and \( \Phi \) is the many-particle wave function for the system of non-interacting particles. Jastrow suggests that this correlation function, in general, is an operator function [13]. However, in most applications, \( f_j \) is assumed to depend only on the interparticle distance, \( r_{ij} = |r_i - r_j| \).
We consider nucleons to be restricted to a cubic box of side $L$ with periodic boundary conditions, so that the wave number $k = 2\pi n/L$ and $n$ is an integer vector. Therefore, we can use plane waves $\phi(r) = e^{ikr}$ for the single-particle wave functions of the nucleons in bulk matter. In order to conserve the rotational invariance of bulk nuclear matter, we perform VMC calculations only for the numbers of neutrons and protons corresponding to completely filled energy shells. We assume that the space and spin parts of the wave function are separable. Under these conditions, choosing a many-particle trial wave function with

$$\Phi(R) = D^{P\uparrow}D^{P\downarrow}D^{N\uparrow}D^{N\downarrow}$$

is quite reasonable because the spin–isospin-dependent parts of the interaction potential are relatively weak. It is also well-known that the expectation value of the total energy is not very sensitive to small changes in the wave function. The determinants $D^{P\uparrow}$, $D^{P\downarrow}$, $D^{N\uparrow}$ and $D^{N\downarrow}$ in Eq. (10) are the Slater determinants of single-particle wave functions for corresponding spin–isospin state, then

$$D^s = \det\left(d^s_{ij}\right),$$

where

$$d^s_{ij} = \phi_j((r, s)_i).$$

The nuclear forces are short-ranged and saturate very quickly, thus the radial distribution function is not expected to have very long-range correlations, therefore, for the two-particle correlation function $f_j$ in Eq. (9), we use a function in the form of

$$f_j(r) = \left[1 + \frac{1}{1 + e^{(r_0 - r)/a}}\right]^t,$$

where $t$, $r_0$ and $a$ are variational parameters. We define a pseudo potential $u(r)$ for practical reasons such that $f_j(r_{ij}) = \exp(-u(r_{ij}))$, then our variational wave function becomes

$$\Psi_j = \exp\left(-\sum_{i<j} u(r_{ij})\right)D^{P\uparrow}D^{P\downarrow}D^{N\uparrow}D^{N\downarrow}.$$  

We sample the $3N$ dimensional space with the probability distribution

$$\frac{|\Psi(R)|^2}{\int dR|\Psi(R)|^2}$$

using a random walk created by the usual Metropolis method. The method given above is a slightly modified version of the VMC method for fermions defined by Ceperley et al. \[14\]. They have also discussed in detail the use of a trial wave function of this form.
The expectation value of any operator \( F \) is then simply the average value of the operator evaluated for the coordinates of the random walk with \( M \) moves
\[
\langle \hat{F} \rangle = \frac{\int d\mathbf{r} \Psi^*(\mathbf{r}) F(\mathbf{r}) \Psi(\mathbf{r})}{\int d\mathbf{r} |\Psi(\mathbf{r})|^2} \simeq \frac{1}{M} \sum_{i=1}^{M} F(\mathbf{r}_i). \tag{16}
\]

The system total energy is calculated as an average over a sufficiently long random walk. The contribution of the \( NN \) interactions to the total energy is calculated for interparticle separations up to a cut off distance of \( L/2 \). The pair-distribution function heals quickly and a reasonable approximation to include the contributions of the pairs farther apart is to assume that the density of particles is constant outside this interaction sphere, because the \( NN \) interaction is very short ranged [8].

<table>
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We must use fully occupied closed shells of plane waves for both neutrons and protons in order to preserve the isotropy of the system. Thus, the number of neutrons or protons must be chosen from the set \((2, 14, 38, 54, 66, 114, \ldots)\).

The total energies per nucleon obtained from the Monte Carlo calculations are presented in Table I. It can be seen from the table that we obtain saturation energy \(E_0 = -15.67\) MeV at saturation density \(\rho_0 = 0.158\) fm\(^{-3}\) \((k_F = 1.32\) fm\(^{-1}\)) from VMC calculations for SNM.

### 3. The new Skyrme parameter set for nuclear matter

The Skyrme energy density functional \(H(\vec{r})\), which is an algebraic function of the nucleon densities \(\rho_n(\rho_p)\), the kinetic energy \(\tau_n(\tau_p)\) and spin densities \(\vec{J}_n(\vec{J}_p)\), is given as follows \[11\]:

\[
H(\vec{r}) = \frac{\hbar^2}{2m} \tau(\vec{r}) + \frac{1}{2} t_0 \left[ \left( 1 + \frac{1}{2} x_0 \right) \rho^2 - \left( x_0 + \frac{1}{2} \right) \left( \rho_n^2 + \rho_p^2 \right) \right] + \frac{1}{4} (t_1 + t_2) \rho^2 \tau + \frac{1}{8} \rho \left( t_2 + t_1 \right) \left( \rho_n \tau_n - \rho_p \tau_p \right) + \frac{1}{16} (t_2 - 3t_1) \rho \nabla^2 \rho + \frac{1}{32} (3t_1 + t_2) \left( \rho_n \nabla^2 \rho_n + \rho_p \nabla^2 \rho_p \right) + \frac{1}{16} (t_1 - t_2) \left( \vec{J}_n^2 + \vec{J}_p^2 \right) + \frac{1}{4} t_3 \rho_n \rho_p \rho + H_C(\vec{r}) - \frac{1}{2} W_0 \left( \rho \nabla \cdot \vec{J} + \rho_n \nabla \cdot \vec{J}_n + \rho_p \nabla \cdot \vec{J}_p \right), \tag{17}
\]

where \(\rho_n + \rho_p = \rho\), \(\tau_n + \tau_p = \tau\) and \(\vec{J} = \vec{J}_n + \vec{J}_p\). In the above equation, \(t_0\), \(t_1\), \(t_2\), \(t_3\), \(x_0\) and \(W_0\) are Skyrme parameters. The direct part of the Coulomb interaction in \(H_C(\vec{r})\) is \(\frac{1}{2} V_C(\vec{r}) \rho_p(\vec{r})\), where

\[
V_C(\vec{r}) = \int \rho_p(\vec{r}) \left( \frac{e^2}{|\vec{r} - \vec{r'}|} \right) d^3 r'. \tag{18}
\]

Nuclear matter, which has a fixed ratio of neutrons and protons (ignoring the Coulomb forces), is a uniform hypothetical system with translational invariance. When the number of protons and neutrons is the same, the system is called symmetric nuclear matter. In symmetric nuclear matter case, we have

\[
\rho_n = \rho_p = \frac{1}{2} \rho, \quad \tau_n = \tau_p = \frac{1}{2} \tau, \quad \vec{J} - n = \vec{J}_p = 0 \tag{19}
\]

and \(\nabla \rho = \nabla \cdot \vec{J} = 0\), \(\rho = \left( \frac{2}{3\pi^2} \right) k_F^3\), \(\tau = \frac{3}{5} k_F^2\). Thus, from Eq. (17), one can get the binding energy per particle for symmetric nuclear matter

\[
\frac{E}{A} = \frac{H}{\rho} + \frac{3}{5} T_F + \frac{3}{8} t_0 \rho^2 + \frac{3}{80} \left( 3t_1 + 5t_2 \right) \rho k_F^2, \tag{20}
\]

where \(T_F = \hbar^2 k_F^2 / 2m\) is the kinetic energy of a particle at the Fermi surface.
Dutra et al. [15] present a detailed assessment of the ability of the 240 Skyrme interaction parameter sets in the literature to satisfy a series of criteria derived from macroscopic properties of nuclear matter in the vicinity of nuclear saturation density at zero temperature and their density dependence, derived by the liquid drop model in experiments with giant resonances and heavy-ion collisions. In our previous study [8], the properties of symmetric and asymmetric nuclear matter, which are the saturation energy, saturation density, incompressibility, pressure and asymmetry energy coefficient are calculated by the new Skyrme parameter set (SKAan-U14). The SKAan-U14 Skyrme parameter set is generated by fitting the energy results per nucleon, which contains 140 energy values obtained from Variational Monte Carlo (VMC) simulations, to the Skyrme energy density functional [16]. The obtained SKAan-U14 Skyrme parameter set is: \( t_0 = -424.75 \text{ MeV fm}^3 \),

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$t_1 = -1333.36$ MeV fm$^5$, $t_2 = -232.82$ MeV fm$^5$, $t_3 = 47807.61$ MeV fm$^6$, $x_0 = 0.96$, $x_1 = 0$, $x_2 = 0$, $x_3 = -0.51$ and $\alpha = 1.5$. In our other study [9], the equation of state (EOS) of pure neutron matter (PNM) and neutron-rich matter (NRM) for the realistic Urbana $V_{14}$ two nucleon interaction was obtained by using a Variational Monte Carlo (VMC) method.

In this study, we have focused on incompressibility: the symmetric nuclear matter Skyrme–Landau. In order to obtain the new Skyrme parameter set, we used the Skyrme energy density functional [11] different from Ref. [16] used in our previous study. The new Skyrme parameter set is generated by fitting the energy results per nucleon and contains 100 energy results obtained from VMC calculations to the Skyrme energy density functional. The new set obtained is: $t_0 = -561.9948614$ MeV fm$^3$, $t_1 = -0.185293342$ MeV fm$^5$, $t_2 = 1931.494108$ MeV fm$^5$, $t_3 = -5061.49105$ MeV fm$^6$, and $x_0 = 51506.8365$. Using these new parameters, we obtain saturation energy $E_0 = -15.49$ MeV at $\rho_0 = 0.156$ fm$^{-3}$ ($k_F = 1.32$ fm$^{-1}$) for SNM. These values are in a good agreement with VMC simulation results ($E_0 = -15.67$ MeV, $\rho_0 = 0.158$ fm$^{-3}$, $k_F = 1.32$ fm$^{-1}$) and with our expectations from semi-empirical mass formulas of known nuclei. Various semi-empirical mass formulas estimate the saturation point of the SNM to have an energy per particle between $-15$ and $-17$ MeV and Fermi momentum $k_F$ in the range of $1.29$–$1.44$ fm$^{-1}$ [17].

The obtained total energies per nucleon by the new Skyrme parameter set for SNM are presented in Table II. In Fig. 1, the binding energies ($E/A$)
of SNM obtained from VMC calculations along with the new Skyrme calculations are given. A comparison of VMC results used in fits and energy values calculated by the new Skyrme parameter set for SNM are also shown. It can be seen from the figure that values of binding energies obtained by the new Skyrme parameter set are in good agreement with the VMC calculations.

4. Incompressibility: Skyrme–Landau parameterization

In general, the Skyrme parameter sets are determined by requiring that Hartree–Fock (HF) calculations consistently reproduce empirical values for properties of nuclear matter, such as binding energy, saturation density, incompressibility, etc. [18]. It is useful to consider the Skyrme interaction for nuclear matter within the framework of the Landau theory [19, 20]. The most general Skyrme interaction for nuclear matter applications in Hartree–Fock (HF) approximation may be written as [18]

\[ v(\vec{k}, \vec{k}') = t_0(1 + x_0 P_\sigma) + \frac{1}{2} t_1(1 + x_1 P_\sigma) \left( k^2 + k'^2 \right) + t_2(1 + x_2 P_\sigma) \vec{k} \cdot \vec{k}' + \frac{1}{6} t_3 \rho + \frac{1}{2} t_4 \rho \left( k^2 + k'^2 \right), \]  

(21)

where the density-dependent terms represent the two-body reduction of three-body interactions as in Ref. [11]. This equation leads to non-zero Landau parameters. The Landau parameters may be identified immediately by noting in this case that \( k^2, k'^2 \) and \( \vec{k} \cdot \vec{k}' \) are equal to \( \frac{1}{2} k_F^2 (1 - \cos \theta) \). The parameters \( t_4, x_1 \) and \( x_2 \) are explicitly zero in Ref. [11]. Equation (21) allows the independent adjustment of \( E/A, k_F \) and six Landau parameters. The density-dependent term in Eq. (21) allows the independent determination of compressibility of nuclear matter, \( C \).

Using the SKaan-U14 Skyrme parameter set [8], we found a new Landau parameter set for nuclear matter in our previous study [21]. In this study, in order to obtain the Landau parameters, we use the following relations: the generalized Skyrme parameters in terms of the Landau parameters, of \( E/A \) and \( k_F \) [18]

\[ \rho t_0 = \rho N_0^{-1} \{(5/6) F_0 - (1/15) F_1\} - (9/5) T_{k_F} + 7E/A, \]
\[ \rho t_0 x_0 = -\rho N_0^{-1} \{ (2/3) F_0 + 2F'_0 + (2/3) F_1 + 2F'_1 \}, \]
\[ \rho k_F^2 t_1 = -\rho N_0^{-1} \{ (20/3) F_0 + F'_0 + G_0 + 3G'_0 + (2/3) F_1 \} - 2T_{k_F} - 10E/A, \]
\[ \rho k_F^2 t_1 x_1 = 2\rho N_0^{-1} \{ (2/3) F_0 + F'_0 + G_0 + (2/3) F_1 + 2F'_1 \}, \]
\[ \rho k_F^2 t_2 = \rho N_0^{-1} \{ F_0 - F'_0 - G_0 + 5G'_0 \}, \]
\[ \rho k_F^2 t_2 x_2 = \rho N_0^{-1} \{ 2F'_0 + 2G_0 - 4G'_0 \}, \]
\[ \rho^2 t_3 = \rho N_0^{-1} \{ F_0 + (14/5) F_1 \} + (18/5) T_{k_F} - 14E/A, \]
\[ \rho^2 k_F^2 t_4 = \rho N_0^{-1} \{ (5/3) F_0 - (2/3) F_1 \} - (2/3) T_{k_F} - (10/3) E/A, \]  

(22)
and the two constraints

\[ G_1 = -\{(2/3)F_0 + F_0' + G_0 + (2/3)F_1 + F_1'\}, \]
\[ G_1' = -\{(1/3)F_0 + G_0' + (1/3)F_1\}, \]  
(23)

where \( \rho = 2k_F^3/3\pi \).

Using the new Skyrme parameter set obtained from the VMC simulations, \( E/A = -15.49 \text{ MeV} \) and \( k_F = 1.32 \text{ fm}^{-1} \), we find the new Landau parameter set: \( F_0 = 5.055, \ F_0' = 3.011, \ G_0 = 2.324, \ G_0' = 4.402, \ F_1 = 12.053, \ F_1' = -8.379, \ G_1 = -8.361, \ G_1' = -10.104 \). These new Landau parameters provide demands of HF approximation

\[ (F_0 + F_0' + G_0 + G_0' + F_1 + F_1' + G_1 + G_1') = 0. \]  
(24)

The obtained new Landau parameters from the new Skyrme parameter set are given in Table III together with those obtained from the other Skyrme interactions. Detailed information on the density dependence of the Landau parameters can be found in Ref. [15].

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The compressibility of nuclear matter may be expressed simply in terms of these dimensionless Landau parameters as

\[ C = 6\frac{\hbar k_F^2}{2m} \frac{(1 + F_0)}{1 + F_1/3}. \]  
(25)

Using the obtained new Landau parameters from the new Skyrme parameter set, we found the incompressibility \( K = 273 \text{ MeV} \). Unfortunately, there is no sufficiently decisive experimental constraint available for nuclear matter incompressibility [24]. The incompressibility appears in some sophisticated mass formulas, however, it cannot be precisely determined from these
formulas, and quoted values in the literature have a wide range from 240 to 300 MeV with error estimates of $\pm 50$ MeV [25]. Considering the error bars in the quoted experimental values, the obtained incompressibility of nuclear matter by using the new Landau parameters might be acceptable.

5. Conclusion

The dependence of the total energy per nucleon on the density of nuclear matter is called the nuclear EOS. The EOS is of fundamental importance in the theories of nucleus–nucleus collisions at energies where the nuclear matter incompressibility $K$ comes into play as well as in the theories and supernova explosions.

Here, we have presented: (i) the results of a VMC simulation of the SNM using Urbana potential, (ii) a new Skyrme parameter set found to consistently reproduce empirical values of the saturation density and binding energy of nuclear matter obtained from VMC calculations, (iii) a new Landau parameter set for nuclear matter obtained for the new Skyrme parameter set, (iv) finally, nuclear matter incompressibility determined using the new Landau parameter set.

To sum up, in this paper, we have presented nuclear matter incompressibility using Skyrme–Landau parameterization with VMC calculations.

REFERENCES