NUCLEON–NUCLEON CORRELATIONS AND THE ISOSPIN AND SPIN SYMMETRY ENERGY*

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Using the Hellmann–Feynman theorem, we calculate the potential and kinetic energy contributions to the binding energy of symmetric nuclear matter, neutron matter and polarized neutron matter. These energies are used to analyze the symmetry energy of nuclear matter and the spin symmetry energy of neutron matter. The analysis is performed within the Brueckner–Hartree–Fock approach using the Argonne V18 realistic potential plus the Urbana IX three-body force. The kinetic energy difference between the correlated system and the underlying Fermi sea is used to estimate the importance of nucleon–nucleon correlations in the different systems concluding that at a given density, symmetric nuclear matter is more correlated than neutron matter, and that this is more correlated than polarized neutron matter. Our microscopic results show no indication of a ferromagnetic transition in neutron matter.

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1. Introduction

The complexity of the nucleon–nucleon interaction and, therefore, the corresponding one of nucleon–nucleon correlations is reflected in the richness of the structure and excitation spectra of nuclei along the nuclide chart. One of the central issues of nuclear physics has been always to reach a microscopic understanding of nuclei using realistic forces. From the very beginning, it was evident that these realistic forces have a complicated operatorial structure which depends on the spin–isospin state of the interacting nucleons, and contain a tensor component that couples the spatial and the spin degrees of freedom [1]. A good point to start is the microscopic study of symmetric nuclear matter and neutron matter [2–4] which has important consequences in the determination of neutron star interiors [5–8]. At the same time, phenomenological approaches based on effective interactions have been able to reproduce satisfactorily the binding energies of nuclei in large regions of the nuclide chart [9] and also the properties of interior of neutron stars [10]. Many of such interactions are built to describe nuclei close to the stability valley and, therefore, predictions far away from these conditions should be taken with care. Skyrme ones are the most common and suitable ones among them [11]. However, in spite of the large amount of constraints, there is still a large dispersion on the results when using different effective forces. Therefore, fully microscopic approaches with realistic interactions look as a safe and necessary procedure.

Microscopic approaches start from realistic nucleon–nucleon (NN) interactions that should be able to reproduce the scattering and bound state properties of the free two-nucleon system. The in-medium correlations are then built using many-body techniques that incorporate the effects of the nuclear medium. In this paper, we present results obtained in the lowest order of Brueckner–Bethe–Golstone formalism, the so-called Brueckner–Hartree–Fock approximation [2, 3]. It should be noticed that other microscopic many-body approaches have recently had a substantial progress with a general good agreement between them [12]. One should mention here the achievements using Self-Consistent Green's Function [13–15], the Quantum Monte Carlo developments [16–18], the recent calculations in correlated basis functions [19], and the progress using the so-called chiral forces based on effective field theories [15, 20].

Unfortunately, whatever realistic two-nucleon force (2NF) is used in a microscopic nuclear many-body calculation, the saturation properties of nuclear matter fail to be reproduced. Saturation densities are too large and saturation energies too attractive. Three-nucleon forces (3NF) are then expected to take care of this limitation. Three-body forces are also necessary in light nuclei, whose binding energies are not reproduced when computed with 2NF only. In the few-body case, however, the theory based on 2NF only, underbinds experimental data, whereas nuclear matter is generally overbound. Consequently, 3NFs are expected to provide further attraction in light systems (or small densities) and repulsion for the infinite system (at higher densities) [21]. In the calculations reported in this paper, we employ the Argonne V18 (Av18) $2N$ potential [22] supplemented with the Urbana IX three-body force [23] which for the use in the BHF calculations was reduced to a two-body density-dependent force by averaging over the third nucleon in the medium [24].

The NN interactions produce NN correlations in the nuclear wave function which strongly departs from the mean-field wave function. For a uniform system, the mean-field wave function is described by a Slater determinant built with plane waves which occupy all the momenta up to the Fermi level, *i.e.*, the free Fermi sea (FFS). To learn on the nature of the NN correlations, one can study their effects on several quantities. A first quantity affected by the NN correlations is the energy itself. A first qualitative measurement of the importance of the NN correlations is provided by the difference between the BHF and the HF energies. The latter is simply calculated as the expectation value of the Hamiltonian on the FFS (E_{HF}). NN correlations also affect the momentum distribution, which in the HF approach is a step function, $\Theta(k_{\mathrm{F}} - k)$. The NN correlations modify $n(k)$, by depleting the occupation below k_{F} and populating momenta above k_{F}. Therefore, the difference between $n(k)$ for the correlated system and the step function provides another measure of NN correlations [25–27]. In principle, the standard BHF approximation for the energy does not give access to $n(k)$. However, one can always have an estimate of the modification of $n(k)$ by comparing the kinetic energies associated to the respective momentum distributions. Another indicator, closely related to the previous one, is the difference of the expectation values of the interaction in the FFS and the correlated system.

On the other hand, to learn on the dependence of the NN correlations on the isospin and spin degrees of freedom, we study the spin–isospin channel decomposition of the expectation value of the interaction energy, and their contribution to the symmetry energy of nuclear matter which is defined as the difference between the energy per particle of neutron matter and symmetric nuclear matter [28]. Finally, we get a further insight into the spin dependence by considering the spin symmetry energy of neutron matter defined as the difference between the energy per particle of polarized and non-polarized neutron matter [30].

2. Kinetic and potential energies in the BHF approach

In the BHF approach, the ground-state energy is evaluated in terms of the so-called hole-line expansion, where the diagrams are grouped according to the number of hole lines. The expansion is derived in terms of the in-medium two-body scattering G-matrix. The G-matrix sums an infinite set of diagrams of the perturbative expansion, and takes into account the effect of the Pauli operator as well as the in-medium potential felt by the nucleons in the intermediate states. The G-matrix shows a regular behavior even for strong short-range repulsions, present in most of the realistic interactions and represents the effective interaction between two nucleons in the presence of the nuclear medium. In the BHF approach, the energy is given by the sum of the kinetic energy of the free Fermi sea and the sum of *two-hole-line* diagrams including the effect of two-body correlations through the G-matrix [2–4]. In principle, the contribution from *three-hole-line* diagrams (which account for the effect of three-body correlations) is minimized when the so-called continuous prescription for the in-medium potential is used [31]. We adopt this prescription in all the calculations reported in this paper.

The BHF approximation gives the correction to the energy of the FFS, but does not give direct access to the separate contributions of the kinetic and potential energies. However, one can use the Hellmann–Feynman theorem to estimate the ground state expectation values of both contributions from the derivative of the total energy with respect to a properly introduced parameter. Writing the nuclear Hamiltonian as $H = T + V$, and defining a λ-dependent Hamiltonian $H(\lambda) = T + \lambda V$, the expectation value of the potential energy in the ground state can be obtained as

$$\langle V \rangle = \frac{\langle \Psi_{\rm gs} \mid V \mid \Psi_{\rm gs} \rangle}{\langle \Psi_{\rm gs} \mid \Psi_{\rm gs} \rangle} = \left(\frac{{\rm d}E(\lambda)}{{\rm d}\lambda} \right)_{\lambda=1} , \tag{1}$$

where $E(\lambda)$ is the energy of the ground-state corresponding to $H(\lambda)$. It has been shown that, when one evaluates $E(\lambda)$ in the BHF approximation, Eq. (1) provides a good estimate of the potential energy [32,33]. The kinetic energy $\langle \Psi_{\rm gs} \mid T \mid \Psi_{\rm gs} \rangle$ can then be obtained by subtracting $\langle \Psi_{\rm gs} \mid V \mid \Psi_{\rm gs} \rangle$ from the total energy.

The Hellmann–Feynman theorem also permits to analyze the different terms of the nuclear force by evaluating their explicit contributions. In fact, the Av18 potential has 18 components of the form of $v_p(r_{ij}) O^p_{ij}$ with

$$\begin{aligned} O_{ij}^{p=1,18} \; = \; & 1, \quad \vec{\tau}_i \cdot \vec{\tau}_j, \quad \vec{\sigma}_1 \cdot \sigma_j, \quad (\vec{\sigma}_i \cdot \vec{\sigma}_j)(\vec{\tau}_i \cdot \vec{\tau}_j), \quad S_{ij}, \quad S_{ij}(\vec{\tau}_i \cdot \vec{\tau}_j) , \\ & \vec{L} \cdot \vec{S}, \quad \vec{L} \cdot \vec{S}(\vec{\tau}_i \cdot \vec{\tau}_j), \quad L^2, \quad L^2(\vec{\tau}_i \cdot \vec{\tau}_j), \quad L^2(\vec{\sigma}_1 \cdot \sigma_j) , \\ & L^2(\vec{\sigma}_1 \cdot \sigma_j)(\vec{\tau}_i \cdot \vec{\tau}_j), \quad \left(\vec{L} \cdot \vec{S}\right)^2, \quad \left(\vec{L} \cdot \vec{S}\right)^2 (\vec{\tau}_i \cdot \vec{\tau}_j), \quad T_{ij} , \\ & (\vec{\sigma}_1 \cdot \sigma_j) T_{ij}, \quad S_{ij} T_{ij}, \quad (\tau_{z_i} + \tau_{z_j}) , \end{aligned} \tag{2}$$

where S_{ij} is the usual tensor operator, $\vec{L}$ the relative orbital angular momentum, $\vec{S}$ the total spin of the nucleon pair, and $T_{ij} = 3\tau_{z_i}\tau_{z_j} - \tau_i\tau_j$ the isotensor operator defined analogously to S_{ij}. Note that the last four operators break the charge independence of the nuclear interaction. As we have mentioned above, the Urbana IX three-body force is reduced to an effective density-dependent two-body interaction when used in the BHF approach. This force is built with three components of the type $u_p(r_{ij},\rho)O^p_{ij}$, where

$$O^{p=1,3}_{ij} = 1\,, \quad (\vec{\sigma}_i \cdot \vec{\sigma}_j)\,(\vec{\tau}_i \cdot \vec{\tau}_j)\;, \quad S_{ij}\,(\vec{\tau}_i \cdot \vec{\tau}_j) \tag{3}$$

introducing additional central, $\sigma\tau$, and tensor terms [24].

3. Symmetric nuclear matter and neutron matter

We start our discussion by comparing the HF and the BHF energies, reported in Table I, at $\rho = 0.187$ fm^{-3} which is the saturation density in our calculation, including three-body forces. For SNM, $\langle E\rangle_{\mathrm{HF}}$ is repulsive and one needs the NN correlations provided by the G-matrix to obtain the attractive $\langle E\rangle_{\mathrm{BHF}}$. Notice that the difference between E_{BHF} and E_{HF} is smaller for neutron matter than for nuclear matter. Besides, the kinetic energy is larger in the correlated system than in the underlying FFS, indicating a modification of $n(k)$ with respect to the FFS. Again, this difference is larger for symmetric nuclear matter than for neutron matter. The same is true for the difference between $\langle V\rangle_{\mathrm{HF}}$ and $\langle V\rangle$ in the interacting systems. These results point to the fact that neutron matter is less correlated than symmetric nuclear matter. The absence of certain isospin channels and partial waves, due to the Pauli exclusion principle, provides a simple explanation for this behavior. Looking at the symmetry energy, the HF estimation provides 8.836 MeV in front of 34.3 MeV in the BHF approach. However, the balance of kinetic and interaction energy of the symmetry energy is completely different. In fact, due to the larger increase in kinetic energy in symmetric nuclear matter when correlations are taken into account, with respect to the neutron matter, it turns out that the kinetic energy contribution is rather small, or even negative at this density. Most of these differences are explained by looking at the contribution of the tensor–isospin component of the Av18 potential. In fact, $\langle S_{ij}(\vec{\tau}_i \cdot \vec{\tau}_j)\rangle_{\mathrm{HF}} = 0$, both for SNM and NM, while $\langle S_{ij}(\vec{\tau}_i \cdot \vec{\tau}_j)\rangle = -37.59$ MeV in SNM and $\langle S_{ij}(\vec{\tau}_i \cdot \vec{\tau}_j)\rangle = -4.98$ MeV in NM [28, 29]. Table II shows the spin (S)- and isospin (T)-channel decomposition of the interaction energy, in the HF and taking correlations into account. For neutron matter, the channels with $T = 0$ are not active. The main contribution to the interaction energy is provided by the spin channel $S = 1$, where the tensor is active. It is precisely the channel $(S = 1, T = 0)$, the one that gives by large the most important contribution to the symmetry energy.

TABLE I

Kinetic, $\langle T\rangle$, and potential, $\langle V\rangle$, energy contributions to the total energy per particle of symmetric nuclear (SNM) and neutron matter (NM) at $\rho = 0.187$ fm^{-3}. Results in the HF approximation are also shown. Units are given in MeV.

	$E_{\rm SNM}$	$E_{\rm NM}$	$E_{\rm sym}$
$\langle E\rangle_{\rm HF}$	46.108	54.944	8.836
$\langle E\rangle_{\rm BHF}$	-15.230	19.070	34.300
$\langle T\rangle_{\rm FS}$	24.529	38.911	14.382
$\langle V\rangle_{\rm HF}$	21.578	16.033	-5.545
$\langle T\rangle$	54.294	53.321	-0.973
$\langle V\rangle$	-69.524	-34.251	35.273

TABLE II

Spin (S)- and isospin (T)-channel decomposition of the potential energy contributions to the energy of nuclear and neutron matter at $\rho = 0.187$ fm^{-3}. The results in the HF approximation are also shown. Units are given in MeV.

(S,T)	$V^{\rm HF}_{\rm SNM}$	$V_{\rm SNM}$	$V^{\rm HF}_{\rm NM}$	$V_{\rm NM}$	$E^{\rm HF}_{\rm sym}$	$E_{\rm sym}$
(0,0)	6.205	5.600	0	0	-6.205	-5.600
(0,1)	0.076	-23.064	3.428	-29.889	3.352	-6.825
(1,0)	8.873	-49.836	0	0	-8.873	49.836
(1,1)	6.424	-2.224	12.605	-4.362	6.181	-2.138

4. Neutron matter and polarized neutron matter

In Table III, we show the HF and BHF results at $\rho = 0.16$ fm^{-3} for non-polarized and totally polarized neutron matter. The differences between the HF and BHF results are larger in NM than in PNM, indicating that the effects of NN correlations are smaller in PNM. We also report the interaction energy in the HF ($\langle V\rangle_{\rm HF}$) and taking into account the NN correlations ($\langle V\rangle$), both for NM and PNM. The differences between these two results are larger for NM than for PNM. Finally, the difference of the kinetic energies of the correlated systems with respect to the corresponding FFS are larger for NM than for PNM, showing that the modification of $n(k)$ and, therefore, the role of NN correlations is larger for NM than for PNM. The spin symmetry energy, and its decomposition in kinetic and interaction energies, is also reported in the table. To get a further insight into the role of the interaction energy and its spin dependence, we report in Table IV the spin-channel decomposition of the interaction energy and their contributions to the spin symmetry energy. The main contribution is that of the spin $S = 0$ channel, absent in PNM. On the other hand, the contribution of the $S = 1$ channel is very similar in both NM and PNM.

TABLE III

Kinetic, $\langle T \rangle$, and potential, $\langle V \rangle$, contributions to the total energy per particle of neutron matter and totally polarized neutron matter at $\rho = 0.16$ fm^{-3}. Also shown are the results in the HF approximation and the kinetic energy of the underlying free Fermi sea ($\langle T \rangle_{\rm FS}$). Results are given in MeV.

	$E_{\rm NM}$	$E_{\rm PNM}$	$S_{\rm sym}$
$\langle E \rangle_{\rm HF}$	45.938	73.740	27.802
$\langle E \rangle_{\rm BHF}$	16.777	59.668	42.891
$\langle T \rangle_{\rm FS}$	35.069	55.669	20.600
$\langle V \rangle_{\rm HF}$	10.869	18.071	7.202
$\langle T \rangle$	47.827	64.452	16.625
$\langle V \rangle$	−31.050	−4.784	26.226

TABLE IV

Spin-channel decomposition of the potential energy of neutron matter and spin-polarized neutron matter at $\rho = 0.16$ fm^{-3}. The HF results are also shown. Their contributions to the spin-symmetry energy is reported in the last two columns. All results are given in MeV.

	$V_{\rm NM}^{\rm HF}$	$V_{\rm NM}$	$V_{\rm PNM}^{\rm HF}$	$V_{\rm PNM}$	$S_{\rm sym}^{\rm HF}$	$S_{\rm sym}$
$S = 0$	1.297	−26.875	0	0	−1.297	26.875
$S = 1$	9.572	−4.784	18.071	−4.175	8.499	−0.609

At this density, $E_{\rm NM}$ is smaller than $E_{\rm PNM}$ indicating that the system prefers to be non-polarized. Actually, this is true for all densities, and no indication of a ferromagnetic transition has been detected [30].

Finally, we can conclude that at a given density, SNM is more correlated than NM which, in turn, is more correlated than PNM. The Pauli exclusion principle appears as the responsible for this behavior. The difference in kinetic energies of these systems and the corresponding kinetic energy of the underlying FFS, corroborates these rather intuitive statements.

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