Spin-orbit correlation energy in neutron matter

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We study the relevance of the energy correlation produced by the two-body spin-orbit coupling present in realistic nucleon-nucleon interaction potentials. To this purpose, the neutron matter Equation of State (EoS) is calculated with the realistic two-body Argonne $v'_{8}$ potential. The shift occurring in the EoS when spin-orbit terms are removed is taken as an estimate of the spin-orbit correlation energy. Results obtained within the Bethe-Brueckner-Goldstone expansion, extended up to three hole-line diagrams, are compared with other many-body calculations recently presented in the literature. In particular, excellent agreement is found with the Green’s function Monte-Carlo method. This agreement indicates the present theoretical accuracy in the calculation of the neutron matter EoS.

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I. INTRODUCTION

The properties of nuclear matter at high density play a crucial role in the modeling of neutron stars (NS’s) interior. The observed NS masses are in the range of $\approx (1 - 2)M_\odot$ (where $M_\odot$ is the mass of the sun, $M_\odot = 1.99 \times 10^{33}$ g), and the radii are of the order of 10 km. The matter inside NS’s, below the outer crust, possesses densities ranging from a fraction to a few times the normal nuclear matter density $\rho_0 (\approx 0.17$ fm$^{-3}$). The equation of state (EoS) at such densities is one of the main ingredients to determine the structure parameters of NS’s. Due to beta-stability conditions, NS matter is much closer to neutron matter than to symmetric nuclear matter. Since no phenomenological data can be used to constrain the neutron matter EoS, one has to rely on microscopic many-body calculations based on realistic nucleon-nucleon (NN) interactions. Predictions of the neutron matter EoS based on purely phenomenological Skyrme forces can dramatically differ among each other, even at relatively low density (for a recent compilation see e.g. [2]). For these reasons, an accurate determination of the neutron matter EoS in the density range typical of NS’s, based on many-body theory and realistic NN forces, appears of great relevance. Unfortunately, despite the enormous progress in the many-body theory of nuclear matter in general and neutron matter in particular, discrepancies among different calculations are still persisting. Among the variety of methods that have been developed in the many-body theory of nucleon systems, one can mention the variational method [3], in his various degrees of sophistication (including Monte-Carlo procedures), the Green’s function Monte-Carlo method (GFMC) [4], which represents a numerical algorithm converging in principle to the “exact” solution, and the Bethe-Brueckner-Goldstone (BBG) expansion [5]. It has been pointed out [6] that the spin-orbit interaction and correlations are particularly relevant in neutron and nuclear matter and require accurate many-body and numerical treatments. Indeed, a large fraction of the observed discrepancies seems to reside in the proper treatment of the spin-orbit interaction terms.

In this paper we focus on the many-body effects due to the spin-orbit terms of the NN interaction within the BBG expansion. To this purpose, and for the sake of comparison with the results obtained with other methods, we perform calculations for neutron matter with $v'_{8}$ and $v'_{6}$ NN realistic two-body interactions, including and, respectively, not including the spin-orbit terms. These interactions are simplified versions of the $Av_{18}$ potential, but they can be still considered realistic enough to provide meaningful results. In particular, they both contain tensor interaction operators. This paper is organized as follows. In Sec. II we briefly introduce the BBG expansion method and discuss the corresponding neutron matter EoS in the relevant density range. In Sec. III we make a detailed comparison with the results of other many-body methods, in particular the GFMC and the Auxiliary Field diffusion Monte-Carlo method (AFDMC). Sec. IV is devoted to the conclusions.

II. NEUTRON MATTER EoS AND THE BBG EXPANSION

The main difficulty in the many-body theory of nuclear matter is the treatment of the strong repulsive core, which dominates the short range behavior of the NN interaction. Simple perturbation theory cannot of course be applied, and one way of overcoming this difficulty is to
introduce the two-body scattering G-matrix, which has a much smoother behavior even for a large repulsive core. It is possible to rearrange the perturbation expansion in terms of the reaction G-matrix, in place of the original bare NN interaction, and this procedure is systematically exploited in the BBG expansion \[3\].

The expansion of the ground state energy at a given density, i.e. the EoS at zero temperature, can be ordered according to the number of independent hole-lines appearing in the diagrams representing the different terms of the expansion. This grouping of diagrams generates the so-called hole-line expansion \[4\]. The diagrams with a given number \(n\) of hole-lines are expected to describe the main contribution to the \(n\)-particle correlations in the system. At the two hole-line level one gets the Brueckner-Hartree-Fock (BHF) approximation. The BHF approximation includes the self-consistent procedure of determining the single particle auxiliary potential, which is an essential ingredient of the method. Once the auxiliary self-consistent potential is introduced, the expansion is implemented by introducing the set of diagrams which include “potential insertions” \[5\]. To be specific, the introduction of the auxiliary potential can be formally performed by splitting the Hamiltonian in a modified way from the usual one

\[ H = T + V = T + U + (V - U) = H'_0 + V' , \]

where \(T\) is the kinetic energy and \(V\) the nucleon-nucleon interaction. Then one considers \(V' = V - U\) as the new interaction potential and \(H'_0\) as the new single particle Hamiltonian. The modified single particle energy \(e(k)\) is given by

\[ e(k) = \frac{\hbar^2 k^2}{2m} + U(k) \]

while \(U\) must be chosen in such a way that the new interaction \(V'\) is, in some sense, “reduced” with respect to the original one \(V\), so that the expansion in \(V'\) should be faster converging. The introduction of the auxiliary potential turns out to be essential, otherwise the hole-expansion would be badly diverging. The total energy \(E\) can then be written as

\[ E = \sum_k e(k) + B \]

where \(B\) is the interaction energy due to \(V'\). The first potential insertion diagram cancels out the potential part of the single particle energy of Eq. (2), in the expression for the total energy \(E\). This is actually true for any definition of the auxiliary potential \(U\). At the two hole-line level of approximation, one therefore gets

\[ E = \sum_{k<k_F} \frac{\hbar^2 k^2}{2m} + \tilde{B} \]

The result that only the unperturbed kinetic energy appears in the expression for \(E\) and that all correlations are included in the potential energy part \(\tilde{B}\) holds true to all orders and it is a peculiarity of the BBG expansion. Of course, the modification of the momentum distribution, and therefore of the kinetic energy, is included in the interaction energy part, but it is treated on the same footing as the other correlation effects. This presents a noticeable advantage: in fact, the modification of the kinetic energy itself is quite large and, of course, positive and it should be therefore compensated by an extremely accurate calculation of the (negative) correlation energy, if the two quantities are calculated independently.

Up to three-hole lines, the diagrams for \(\tilde{B}\) can be schematically represented as in Fig. 1. Diagrams (a) and (b) in the first line represent the usual BHF approximation, while the remaining lines include the three hole-line diagrams. The box in the third line represents the three-body scattering matrix \(T^{(3)}\), which can be introduced following a procedure similar to what is done for the Brueckner G-matrix and satisfies the Bethe-Faddeev integral equations \[6\]. Diagram (f) generates, to lowest order in the G-matrix, diagrams (c) and (e), which are usually calculated separately, since they require an accurate numerical procedure (and they cancel each other to a large extent). Diagram (d) is a potential insertion diagram, the only one at the three hole-line level, and it

![FIG. 1: Schematic representation of two hole- and three hole-line diagrams. Both direct and exchange diagrams are included. The wavy line indicates a Brueckner G-matrix, the dotted line an U-insertion. For other details, see text.](image-url)
is non-zero only if the single particle potential is non-zero at momenta larger then the Fermi momentum $k_F$ (e.g. in the so-called “continuous choice” \[2, 3\]).

In a previous paper \[10\] we have shown that the BBG expansion for neutron matter displays a relatively rapid rate of convergence, and that calculating the total energy up to the three hole-line diagrams is enough to get an accurate EoS, even for densities a few times larger than the saturation density. These calculations were done for the Argonne $v_{14}$ and $v_{18}$ potentials, which contain a large set of interaction operators, including the spin-orbit ones. In order to simplify the analysis and the comparison with other methods, we have performed the same type of calculations for the $v_6'$ NN potential \[11\], which is a simplified version of the $v_{18}$ interaction, but still realistic enough to keep the calculations meaningful. To better focus on the effects of the spin-orbit interaction, we have also considered the $v_6''$ potential, which is obtained from $v_6'$ by dropping the spin-orbit terms. The difference of the EoS obtained with these two interactions can, therefore, be taken as an estimate of the contribution and relevance of the spin-orbit NN interaction in neutron matter.

The EoS of neutron matter obtained within the BBG expansion for the two considered NN interactions is shown in Fig. 2 All calculations have been performed in the continuous choice for the single particle potential $U(k)$. As shown in Ref. \[10\], the results are independent, to a high degree of accuracy, of the choice of $U(k)$. At the BHF level the difference between the EoS for the $v_6'$ NN interaction (dash-dotted line) and the EoS for the $v_6''$ NN interaction (dotted line) looks sizable, even at relatively low density. This discrepancy increases with density, reaching about 14 MeV at $\rho = 0.4$ fm$^{-3}$. When three-body correlations are included (dashed and full lines), the gap between the two EoS is reduced, the strength of this reduction being about 40% at the highest considered density.

Notice that the contribution of three hole-lines diagrams is positive for $v_6'$ and negative for $v_6''$, therefore this difference turns out to be quite sensitive to three-body correlations (as defined within the BBG expansion).

It is important to stress that the contribution of three-body correlations is only a few percent with respect to the two-body one (BHF), even at the highest density. Indeed, in the considered density region the interaction energy $B$ of Eq. \(1\) is negative and large and compensates a large fraction of the positive kinetic energy contribution. This substantial cancellation between kinetic energy and interaction energy has the effect of amplifying the (small) differences of the correlation energy obtained in the different EoS calculations for a given NN interaction, as discussed in the next Section.

### III. RESULTS AND DISCUSSION

BBG results for the EoS of neutron matter using the $v_6'$ and $v_6''$ interactions are compared in Fig. 2 and, respectively, in Tables \[1\] and \[11\] with other calculations based on different many-body methods.

Green’s function Monte-Carlo results were obtained in Ref. \[12\] within an unconstrained path (UC) approach, by considering 14 neutrons inside a periodic box and setting the interaction potential discontinuously to zero at distances larger than one-half the box size. The GFMC should give, in principle, the exact ground state energy of the system. For comparison to infinite neutron matter a “box correction” must then be applied. For the $v_6'$ interaction the latter was estimated in Ref. \[12\] using variational chain summation (VCS) techniques and turned out to be mostly due to the truncation of the potential. The resulting box corrected UC-GFMC EoS is listed in the fourth column of Table \[1\] and indicated in Fig. 2 by full circles. Up to the highest density considered in \[12\], the agreement with the BBG results looks remarkable, given the uncertainty contained in the box correction procedure.

The authors of Ref. \[12\] also calculated the neutron matter EoS within the variational chain summation approach, both for 14 neutrons in a periodic box and directly for an uniform gas of neutrons. Their results for the infinite system with the $v_6'$ NN interaction are listed in the last column of Table \[1\] and plotted as stars in Fig. 2. They show fairly good agreement with the other methods, except, maybe, for the last two points at higher density, which seem to display a slightly different slope with respect to UC-GFMC and BBG \[12\].

Switching the spin-orbit interaction terms off and considering the $v_6'$ NN potential, we can again compare the
BBG results with UC-GFMC and variational calculations, which are also available [12]. Unfortunately in this case the box correction to the GMFC has not been provided; however it looks reasonable to use the same corrections as in the $v'_{6}$ case. Once these corrections are applied to the UC-GMF of Ref. [12] for the $v'_{6}$ NN interaction, we obtain the neutron matter EoS listed in Table II and indicated by the open circles in Fig. 2. Again, fairly good agreement with the BBG calculations is observed up to the highest density, $\rho = 0.24$ fm$^{-3}$, considered in [12].

The overall trend seems to indicate that this agreement continues also at higher $\rho$ values.

It is interesting to notice that the inclusion of three-body correlations in the BBG expansion plays a relevant role in improving the agreement with the UC-GMFC results, which is, in any case, already satisfactory at the BHF level. This happens both for the $v'_{6}$ potential, for which, as already mentioned, the contribution of three hole-line diagrams is positive, and for the $v'_{8}$ case, where, instead, the correction is negative.

The variational VCS results, plotted as crosses in Fig. 2, have been obtained also from Ref. [12], again correcting periodic box $v'_{6}$ results with the box correction values given for the $v'_{6}$ interaction. Also in this case the agreement can be considered satisfactory, and again the trend with density seems to be slightly different with respect to UC-GFMC and BBG.

Another Monte-Carlo scheme has been recently developed [6] for neutron matter, the Auxiliary Field Diffusion Monte-Carlo (AFDMC) method.

The recent results of Ref. [6] for $v'_{6}$ are reported in Fig. 2 as open squares. These calculations were performed for 14 neutrons in a cubic box, but using a continuous potential instead of the truncation of Ref. [12] and they therefore should automatically incorporate the largest part of finite size effects. As shown in Table II these results are close to the calculated UC-GFMC EoS, as well as to the BBG EoS in the whole considered density range.

Unfortunately, the same method applied to neutron matter with the $v'_{8}$ NN interaction gives an EoS (full squares in Fig. 2 and third column in Table I) which differs from all other calculations. These findings indicate the difficulty of an accurate calculation of the spin-orbit contribution to neutron matter binding. The AFDMC method has been improved in Ref. [13] to properly deal with the spin-orbit interaction and correlation, by a suitable modification (backflow) of the trial wave function. With this modification the splitting between the two EoS, for the $v'_{6}$ and $v'_{8}$ NN potentials, increases, but it is still too small with respect to the UC-GFMC and BBG results.

### IV. CONCLUSIONS

We have presented calculations of neutron matter EoS for two different NN interactions, the Argonne $v'_{6}$ and $v'_{8}$. The comparison of the results obtained with the two interactions is expected to give an estimate of the correlation coming from spin-orbit interaction terms. We have found close agreement between the EoS calculated within the BBG expansion, extended up to three hole-line contributions, and the UC-GFMC calculations of Ref. [12], for density up to 0.24 fm$^{-3}$. The discrepancy between the correlation energy in the two schemes does not exceed 2%. Such an agreement suggests that the many-body problem for neutron matter with two-body NN interactions is well under control, at least for the considered density range. The splitting between the EoS calculated with the $v'_{6}$ and $v'_{8}$ potentials indicates that the spin-orbit correlation energy in neutron matter can be as large as 4-5 Mev/A and increases with density. The AFDMC methods seems to have some problems when dealing with the spin-orbit correlation.

In all considered calculations only two-body NN forces have been considered. It is well known that three-body forces are needed in nuclear matter. It appears then relevant to perform a similar study including three-body forces. The latter are not so well known, and the ex-

### TABLE I: Neutron matter energy per particle (in MeV), for the Argonne $v'_{6}$ NN interaction. BBG energies are calculated up to the three-hole line level. AFDMC results are taken from Ref. [6] and are calculated for 14 neutrons in a periodic box. UC-GFMC and VCS results are taken from Ref. [12]. VCS results are calculated for a Uniform Gas, while UC-GFMC results include box correction terms.

| $\rho$ (fm$^{-3}$) | BBG   | AFDMC | UC-GFMC | VCS
|-------------------|-------|-------|---------|-------
| 0.04              | 6.469 | –     | 6.0     | 6.7   |
| 0.08              | 8.250 | –     | 8.4     | 9.2   |
| 0.12              | 10.031| 12.32 | –       | –     |
| 0.16              | 11.826| 14.98 | 12.1    | 12.1  |
| 0.20              | 13.705| 17.65 | –       | –     |
| 0.24              | 15.846| –     | 16.9    | 14.8  |
| 0.32              | 21.953| 27.3  | –       | –     |
| 0.40              | 29.044| 35.3  | –       | –     |

### TABLE II: Same as Table I but for the Argonne $v'_{6}$ NN interaction. UC-GFMC and VCS energies are obtained from the periodic box results of Ref. [12], by applying the same box correction (reported in the last column) as for the $v'_{6}$ case.

| $\rho$ (fm$^{-3}$) | BBG   | AFDMC | UC-GFMC | VCS (box corr.)
|-------------------|-------|-------|---------|------------------|
| 0.04              | 6.380 | –     | 6.45    | 7.3 (-0.3)       |
| 0.08              | 9.668 | –     | 9.54    | 10.8 (-1.1)      |
| 0.12              | 12.292| 12.41 | –       | –                |
| 0.16              | 15.092| 15.12 | 14.81   | 16.1 (-5.1)      |
| 0.20              | 18.011| 17.86 | –       | –                |
| 0.24              | 21.262| –     | 20.65   | 22.1 (-11.5)     |
| 0.32              | 28.743| 27.84 | –       | –                |
| 0.40              | 37.552| 36.0  | –       | –                |
extrapolation from finite nuclei, where three-body forces are fitted, to nuclear matter seems not so obvious. In any case, the comparison of the results obtained with different schemes, when three-body forces are included, could be a stringent test for the accuracy of the calculations, in particular for the spin-orbit contribution to correlation energy. This is left to future work, but the agreement obtained up to now between BBG and GFMC appears satisfactory and promising.

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[14] The different density dependence of the UC-GFMC and VCS results when the spin-orbit interaction is included in the NN potential was observed, already in the periodic box results, in Ref. 12, where the possible origin of this behavior was supposed to be due either to an overestimation of spin-orbit contributions in the VCS method or to the employment of a too short imaginary time in the UC-GFMC calculation. The slightly better agreement between UC-GFMC and the trend of the BBG curves shown in Fig. 2 seems to favor the first hypothesis.