Spin-orbit induced backflow in neutron matter with auxiliary field diffusion Monte Carlo

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The energy per particle of zero-temperature neutron matter is investigated, with particular emphasis on the role of the $L \cdot S$ interaction. An analysis of the importance of explicit spin–orbit correlations in the description of the system is carried out by the auxiliary field diffusion Monte Carlo method. The improved nodal structure of the guiding function, constructed by explicitly considering these correlations, lowers the energy. The proposed spin–backflow orbitals can conveniently be used also in Green’s Function Monte Carlo calculations of light nuclei.

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I. INTRODUCTION

In recent investigations of the ground state and the magnetic properties of neutron matter with modern nuclear interactions of the Urbana-Argonne type [1, 2] good agreement was observed between results obtained with the Auxiliary Field Diffusion Monte Carlo (AFDMC) [3], a calculation by Morales, Jr. et al. [4], performed with the Variational Chain Summation (VCS) method [7, 8], and Brueckner Hartree Fock estimates [9, 10].

However, in spite of the overall agreement of the equation of state and the spin susceptibility, marked differences exist between the AFDMC and the VCS calculations, concerning the contribution to the energy due to the spin–orbit component of the two–body interaction. VCS calculations, performed with the Argonne $v_{18}$ [11] and the Urbana-IX three–body potential (AU18 Hamiltonian), find large and negative contributions from the cluster terms $C_{LS}$ with either spin-orbit correlations in the trial function and/or the spin–orbit potential. For instance, in correspondence with optimal trial functions, $C_{LS}$ amounts to -5.8 MeV at a density $\rho = \rho_0 = 0.16$ fm$^{-3}$ and -12.1 MeV at twice the same density. The AFDMC calculations of Ref. [1], performed with the simplified, but still realistic, version of the Argonne two–body potential, $v_{LS}^8$ [4], plus the Urbana IX three–body interaction (AU8' Hamiltonian) get energy differences $\Delta E_{LS}$ between the AU8' Hamiltonians with and without the spin–orbit potential which are small and positive. At $\rho = \rho_0$, $\Delta E_{LS} = 0.2$ MeV and at $\rho = 2\rho_0$, $\Delta E_{LS} = 1.12$ MeV.

Such a discrepancy cannot be ascribed to differences between the two potentials $v_{18}$ and $v_{LS}^8$. It is well known that they provide very close results for the energy per particle [2]. In addition, this discrepancy is confirmed by other FHNC/SOC calculations [1], performed by using the approximations of Ref. [11] and the AU8' Hamiltonian. They give $\Delta E_{LS} = -3.7$ MeV at $\rho_0$ and $\Delta E_{LS} = -10.1$ MeV at $2\rho_0$, with $C_{LS}$ being $-3.9$ MeV and $-10.7$ MeV respectively.

A possible source for this disagreement might be the use of a less than satisfactory guiding function in the AFDMC method [12]. The nodes of the plane wave Slater determinant might be too poor, particularly when the interaction includes a spin–orbit potential, like in AU8'. The results of the FHNC/SOC calculations of Ref. [1] with the AU8' Hamiltonian and a trial function of the type $F_6$ (not containing spin–orbit correlations), give values for $\Delta E_{LS}$ quite close to the AFDMC ones, which may confirm this hypothesis.

To clarify this issue we modify the guiding functions in our quantum Monte Carlo calculations to contain explicit spin–orbit correlations. This is efficiently done by considering orbitals of the spin–backflow form in the Slater determinant, as explained below.

The structure of this paper is as follows. In Sec. II we show the guiding function used. The computational details are given in Sec. III. The results are shown and discussed in Sec. IV. The conclusions and perspectives of the present work can be found in Sec. V.

II. SPIN-ORBIT INDUCED BACKFLOW

The $L \cdot S$ correlation in FHNC/SOC and VCS calculations takes the form

\[ \Delta E_{LS} = \rho \left[ \rho \Delta E_{LS} \right] \]
\[ F_b(1,2) = \frac{1}{4\pi} f_b(r_{12}) \left[ r_{12} \times (\nabla_1 - \nabla_2) \right] \cdot (\sigma_1 + \sigma_2) \]  
where \( r_{12} = |r_{12}| \) and \( \sigma_j \) are the Pauli matrices for the \( j \)th particle.

It is found that, at the two-body level of the FHNC/SOC theory, \( \tilde{F}_b \) leads to an energy which is only \( \sim 10\% \) different from that obtained with \( F_b \).

The important feature of the \( L \cdot S \) correlation of Eq. (2) for AFDMC calculations is that, similarly to the case of standard backflow, it can be implemented in quantum Monte Carlo simulations by substituting the plane wave orbitals of the Slater function with the following spin–backflow ansatz ones

\[
\phi_k(j) = \exp \left( i k \cdot r_j + \frac{\beta}{2} \sum_{k \neq j} f_b(r_{jk})(r_{jk} \times k) \cdot \sigma_j \right),
\]

where \( \beta \) is a spin–orbit strength parameter. For \( \beta = 1 \) there is a direct correspondence of \( \phi_k(j) \) with \( \tilde{F}_b \). This spin–backflow ansatz can also be used in the GFMC simulations of small nuclear systems [14, 15, 12], to include \( L \cdot S \) correlations.

We present and discuss, in the following, the results obtained in AFDMC simulations of neutron matter energy with the \( AU8' \) Hamiltonian and the nodal surface of the spin–backflow Slater function. We will show that these nodes serve to lower the AFDMC energy per particle of neutron matter by a sizable amount, which however is too small to solve the CVS and AFDMC discrepancy, particularly at higher densities.

III. CALCULATION DETAILS

We describe the neutron system by the non relativistic Hamiltonian

\[
H = T + V_2 + V_3 = \frac{\hbar^2}{2m} \sum_{j=1,N} \nabla_j^2 + \sum_{j<k} v_{jk} + \sum_{j<k<l} V_{jkl},
\]

where \( m \) is assumed to be the average of the neutron and proton masses and \( \hbar^2/m = 41.47108 \text{ MeV fm}^2 \); the two-body and three-body potentials, \( v_{ij} \) and \( V_{jkl} \), are the Argonne \( v'_{18} \) and the the Urbana IX potentials [3]. The three-body contributions to the energy are large, particularly at high densities, and cannot be neglected even in a survey calculation like ours.

In neutron matter this interaction can be written in terms of four components:

\[
v_{ij} = \sum_{p=1}^4 v_p(r_{ij})O^p(ij),
\]

\[
O^p(ij) = 1, \sigma_i \cdot \sigma_j, S_{ij}, L \cdot S,
\]

where \( S_{ij} \) and \( L \cdot S \) are the usual tensor and spin–orbit operators. The functions \( v_p(r_{ij}) \) can be found on Ref. [4] and also on Ref. [11].

The Urbana-IX three-body interaction is given by the sum

\[
V_{jkl} = V_{jkl}^{SI} + V_{jkl}^{SD},
\]

where \( V_{jkl}^{SI} \) is a spin independent three–body short range part, and the spin–dependent part, \( V_{jkl}^{SD} \), in neutron matter, reduces to a sum of terms containing only two–body spin operators, with a form and strength that depends on the positions of three particles. Their explicit expressions can be found in Ref. [11].

We have also considered an interaction obtained from \( AU8' \) by dropping the spin–orbit term, and, as in Ref. [11], it is denoted as \( AU6' \). The AFDMC method used in these calculations has been previously described in detail [11]. It allows Monte Carlo simulations to be performed on a relatively large nuclear system at the required accuracy, thanks to the
introduction of auxiliary fields, which uncouple the spin–
dependent interaction between particles by means of a
Hubbard–Stratonovich transformation. While the prop-
agation of the particle coordinates is done as in diffu-
sion Monte Carlo, that of the spin variables, after having
sampled the auxiliary fields, results in a rotation of each
particle’s spinor.

The guiding function used in this work is given by a
Jastrow product correlating an $N \times N$ Slater determinant

$$\langle R, S | \Psi_{JSB} \rangle = \prod_{j<k} f(r_{jk}) \Phi_B(R, S),$$

(8)

where $R$ and $S$ denote the set of particle coordinates and
of spinors respectively. The space and spin orbitals in
$\Psi_E(R, S)$ are given in Eq. 3, and they operate on the
spin states in the following way

$$\phi_k(i) | \uparrow \rangle = e^{ik \cdot r_i} \times \left[ \left( \cosh(A_k(i)) + \tilde{A}^x_k(i) \sinh(A_k(i)) \right) | \uparrow \rangle \right. \right.$$

$$\left. \left. \left. \times \left( \sinh(A_k(i)) - i\tilde{A}^y_k(i) \right) \sinh(A_k(i)) | \downarrow \rangle \right) \right],$$

(9)

where

$$A_k(i) = \frac{\beta}{2} \sum_{j \neq i} f_b(r_{ij}) r_{ij} \times k$$

(10)

and $\tilde{A}_k^\alpha(i), \{\alpha = x, y, z\}$ are the components of an unit
vector in the direction of $A_k(i)$. A similar expression
can be obtained for the action over the spin down single
particle state. We denote this function by JSB as op-
posed to JS which stands for a function without explicit
backflow correlations, i. e., with simple plane waves in the
spatial part of the orbitals in the Slater determinant
($f_b(r) = 0$). The AFDMC method described in Ref. 11
needs only slight modifications to deal with $\langle R, S | \Psi_{JSB} \rangle$ as
guiding function. They refer mainly to calculating the
kinetic energy part of the local energy, and the gradient
of the guiding function in the drift of the walker.

The Jastrow and spin–orbit correlation functions $f(r)$
and $f_b(r)$ have been taken as the first and fourth com-
ponents respectively of the FHNC/SOC correlation op-
erator that minimizes the energy per particle of neutron
matter at the desired density 11.

IV. RESULTS

We have made our calculations within the full simula-
tion box, and we have taken into account the 26 neighbor-
ing boxes in the tabulation of the correlations $f(r)$ and
$f_b(r)$, and of the various components $v_a(r)$ of the two–
body potential, as described in Ref. 11. Our results are
therefore already tail corrected for a Hamiltonian with
two–body force only. Tail corrections for the three-body
potential were not included. However previous analyses
11 have shown that they are small for systems with 66
neutrons.

AFDMC simulations for the $AU8'$ Hamiltonian with
the JSB guiding function have been also carried out for
66 neutrons. As in the case of the 14 neutron system, we
have found a minimum of the energy at $\beta = 0$ in the figure. If we switch off the spin–orbit potential by considering the $AU6'$
interaction, the minimum is found at $\beta = 0$, confirming that the spin–backflow nodes are energetically advantageous
only in the presence of the spin–orbit component of $v_{8'}$.

The dependence of the JSB energy on the density
is roughly independent on $\rho$ for both the $AU8'$ and the $AU6'$ interactions. In spite of sizable differences between the energies per particle of the 14 neutron and the 66 neutron systems, the gain in
energy ($E(JSB) - E(JS) / N$) is roughly independent on the number of particles in the box. The large differences
between $E(14)$ and $E(66)$ are mainly due to the effect of
three–body interaction. It has been shown 11 that the
finite size effects on E(66) are rather small.

The dependence of the JSB energy on the density is
reported in Table II for the 14 neutron system. There is a weak dependence of $\Delta E_{LS}$ on the density, in
contrast with VCS results.

In order to make comparison with recent quantum
Monte Carlo calculations performed for 14 neutrons in-
teracting via the $v_{8'}$ two–body potential by Carlson et al.
15, we report in Table II the corresponding AFDMC
results. The table displays the energy difference $\Delta E_{LS}$
between the energy obtained with $v_{8'}$ and $v_{0}$ two–body
potential.

The calculations of Ref. 15, to which the results re-
ported in Table II refer, have been performed with the $v_{8'}$ potential cut off at the edge of the box. There-
TABLE II: AFDMC energies per particle in MeV for the $AU_6'$ and $AU_8'$ interactions obtained for a system of 14 neutrons in a periodical box with the guiding functions, $\Psi$, JS and JSB (with $\beta = 1$), as a function of the density $\rho$. Error bars for the last digit are shown in parentheses.

| $\rho$   | $AU_6'$ | $JS$  | $JSB$ |
|----------|---------|-------|-------|
| $\rho_0$ | 19.73(5)| 19.76(6)| 18.76(5)|
| $2\rho_0$| 48.27(9)| 48.4(1) | 46.8(1)|

TABLE III: Spin–orbit contribution to the energy per particle in MeV of neutron matter at density $\rho_0$. The constrained (CP) and unconstrained (UC) GFMC results, as well as the VCS ones are taken from Ref. [15]. The AFDMC results obtained with the JS guiding function are taken from Ref. [1]. Error bars for the last digit are shown in parentheses.

| method         | $\Delta E_{LS}$ |
|----------------|-----------------|
| GFMC–CP        | -1.26(4)        |
| GFMC–UC        | -2.9(3)         |
| AFDMC–JS       | -0.14(6)        |
| AFDMC–JSB      | -1.2(1)         |
| VCS            | -3.8            |

Therefore, the values of $\Delta E_{LS}$ extracted from there might not be completely comparable with ours, since ours are already tail corrected and have been obtained without introducing any discontinuity in the potential. AFDMC seems to agree reasonably well with GFMC in the constrained path approximation (GFMC–CP). The VCS estimate seems to be too large.

V. CONCLUSIONS

In this paper we have proposed a new kind of space–spin orbitals with a spin–backflow form, which is particularly useful for taking into account the spin–orbit interaction of nuclear systems in quantum Monte Carlo simulations. An efficient parameterization of the spin–backflow is obtained from the spin–orbit correlation of FHNC/SOC theory. These spin-backflow orbitals can be conveniently used also in other quantum Monte Carlo calculations, for instance the Green’s Function Monte Carlo simulations of small nucleon systems. The nodal surface provided by this new guiding function is able to decrease the energy about 5 per cent. This amount is not sufficient to solve the spin–orbit discrepancy between the variational chain summation and the AFDMC results, however the AFDMC results are in good agreement with constrained GFMC simulations.

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