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

L. Brualla,[1,*] S. Fantoni,[1,†] A. Sarsa,[1,‡] K. E. Schmidt,[1,§] and S. A. Vitiello[2,‖]

[1]*International School for Advanced Studies, SISSA, Trieste, Italy*
and INFM DEMOCRITOS National Simulation Center, Via Beirut, I-34014 Trieste, Italy
[2]*Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, Unicamp, Campinas-SP, Brazil*
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The energy per particle of zero-temperature neutron matter is investigated, with particular emphasis on the role of the $\boldsymbol{L} \cdot \boldsymbol{S}$ 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 also be conveniently used in the Green's function Monte Carlo calculations of light nuclei.

I. INTRODUCTION

In recent investigations [1,2] of the ground state and the magnetic properties of neutron matter with modern nuclear interactions of the Urbana-Argonne type [3,4], good agreement was observed between results obtained with the auxiliary field diffusion Monte Carlo (AFDMC) [5], a calculation by Ref. [6], 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} [3] 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, $v_{8'}$ [4], plus the Urbana IX three-body interaction ($AU8'$ Hamiltonian), yield energy differences ΔE_{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 $v_{8'}$. It is well known that they provide very close results for the energy per particle [4].

In addition, this discrepancy is confirmed by other Fermi-hypernetted chain/single operator chain (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 ρ_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.[1] The nodes of the plane wave Slater determinant might be too poor, particularly when the interaction includes a spin-orbit potential, like in the $AU8'$ case. 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 ΔE_{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 $\boldsymbol{L} \cdot \boldsymbol{S}$ correlation in FHNC/SOC and VCS calculations takes the form

$$F_b(1,2) = \frac{1}{4i} f_b(r_{12})[\boldsymbol{r}_{12} \times (\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)] \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2), \quad (1)$$

*Email address: lbrualla@sissa.it

†Email address: fantoni@sissa.it

‡Present address: Departamento de Física Moderna, Universidad de Granada, E-18071 Granada, Spain. Email address: sarsa@ugr.es

§Permanent address: Department of Physics and Astronomy, Arizona State University, Tempe, AZ 85287. Email address: kevin.schmidt@asu.edu

‖Email address: vitiello@unicamp.br

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[1]In the AFDMC method a path constraint is used to deal with the fermion sign or phase problem. In all the calculations reported here the real part of the guiding function (evaluated at the walker position and spin) is constrained to be positive, in analogy with the fixed node approximation for central potentials. For convenience, we refer to the effect of the constraint as the nodal structure of the guiding function.

where $r_{12} = |\boldsymbol{r}_{12}|$ and $\boldsymbol{\sigma}_j$ are the Pauli matrices for the jth particle.

By inspection of the cluster terms of $\langle AU8' \rangle$ at the two-body order, one observes that the largest of the spin-orbit terms are those usually denoted as bbc and cbb in the FHNC/SOC theory [12]. In the calculations of Ref. [1] these terms are responsible for $\sim 80\%$ of the total contribution from all the $C_{LS}^{(2)}$ terms in the density range $(3/4)\rho_0 \leq \rho \leq (5/2)\rho_0$. One can easily prove that exactly the same expressions of the cbb and bbc terms are obtained by the following simplified $\boldsymbol{L} \cdot \boldsymbol{S}$ correlation:

$$\widetilde{F}_b(1,2) = \frac{1}{4i} f_b(r_{12})[\boldsymbol{r}_{12} \cdot (\boldsymbol{\nabla}_1 \times \boldsymbol{\sigma}_1 - \boldsymbol{\nabla}_2 \times \boldsymbol{\sigma}_2)]. \quad (2)$$

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

The important feature of the $\boldsymbol{L} \cdot \boldsymbol{S}$ correlation of Eq. (2) for AFDMC calculations is that, similar to the case of standard backflow [13], it can be implemented in quantum Monte Carlo simulations by substituting the plane wave orbitals of the Slater function with the following spin-backflow ones:

$$\exp(i\boldsymbol{k} \cdot \boldsymbol{r}_j) \rightarrow \phi_{\boldsymbol{k}}(j) = \exp\left(i\boldsymbol{k} \cdot \boldsymbol{r}_j \right.$$
$$\left. + \frac{\beta}{2} \sum_{k \neq j} f_b(r_{jk})(\boldsymbol{r}_{jk} \times \boldsymbol{k}) \cdot \boldsymbol{\sigma}_j \right), \quad (3)$$

where β is the spin-orbit strength parameter. For $\beta = 1$, there is a direct correspondence of $\phi_{\boldsymbol{k}}(j)$ with $\widetilde{F}_b$. This spin-backflow ansatz can also be used in the GFMC simulations of small nuclear systems [4,14,15], to include $\boldsymbol{L} \cdot \boldsymbol{S}$ 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 the neutron matter by a sizable amount, which, however, is too small to solve the VCS and AFDMC discrepancy, particularly at higher densities.

III. CALCULATION DETAILS

We describe the neutron system by the nonrelativistic Hamiltonian

$$H = T + V_2 + V_3 = -\frac{\hbar^2}{2m} \sum_{j=1,N} \nabla_j^2 + \sum_{j<k} v_{jk} + \sum_{j<k<l} V_{jkl}, \quad (4)$$

where m is assumed to be the average of the neutron and proton masses and $\hbar^2/m = 41.471\,08$ MeV fm^2; the two-body and three-body potentials v_{ij} and V_{jkl} are the Argonne v_8' and the the Urbana-IX potentials [4]. The three-body con-
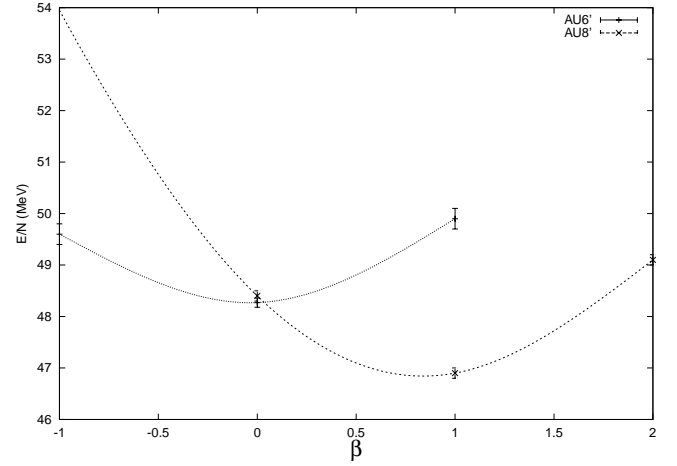

FIG. 1. Neutron matter energy per particle in MeV as a function of the strength β of the spin-orbit correlation function f_b at $\rho = 2\rho_0$ for 14 neutrons. The solid line stands for the $AU6'$ interaction, and the dotted line for the $AU8'$ potential.

tributions 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:

$$v_{ij} = \sum_{p=1}^{4} v_p(r_{ij}) O^p(ij), \quad (5)$$

$$O^p(ij) = 1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}, \boldsymbol{L} \cdot \boldsymbol{S}, \quad (6)$$

where S_{ij} and $\boldsymbol{L} \cdot \boldsymbol{S}$ are the usual tensor and spin-orbit operators. The functions $v_p(r_{ij})$ can be found in Ref. [4] and also in Ref. [1].

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

$$V_{jkl} = V_{jkl}^{SI} + V_{jkl}^{SD}, \quad (7)$$

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 a strength which depend on the positions of the three particles. Their explicit expressions can be found in Ref. [1].

We have also considered an interaction obtained from the $AU8'$ by dropping the spin-orbit term, and as in Ref. [1], it is denoted as $AU6'$.

The AFDMC [5] method used in these calculations has been previously described in detail [1]. 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 that uncouple the spin-dependent interaction between particles by means of a Hubbard-Stratonovich transformation. While the propagation of the particle coordinates is done as in diffusion Monte Carlo, that of the spin variables, after having sampled the auxiliary fields, results in a rotation of each particle's spinor.

TABLE I. AFDMC energies per particle in MeV for the $AU6'$ and $AU8'$ interactions obtained for a system of 14 or 66 neutrons in a periodical box with the guiding functions Ψ, JS, and JSB (with $\beta=1$) at $2\rho_0$. Error bars for the last digit are shown in parentheses.

Ψ	$N=14$	$N=66$
JS($AU6'$)	48.27(9)	53.11(9)
JS($AU8'$)	48.4(1)	54.4(6)
JSB($AU8'$)	46.8(1)	52.9(2)

TABLE II. AFDMC energies per particle in MeV for the $AU6'$ and $AU8'$ interactions obtained for a system of 14 neutrons in a periodical box with the guiding functions Ψ, JS, and JSB (with $\beta=1$) as a function of the density ρ. Error bars for the last digit are shown in parentheses.

ρ	JS($AU6'$)	JS($AU8'$)	JSB($AU8'$)
ρ_0	19.73(5)	19.76(6)	18.76(5)
$2\rho_0$	48.27(9)	48.4(1)	46.8(1)

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

$$\langle R,S|\Psi_{JSB}\rangle = \prod_{j<k} f(r_{jk})\Phi_B(R,S), \qquad (8)$$

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

$$\phi_{\bf k}(i)|\uparrow\rangle = e^{i{\bf k}\cdot{\bf r}_i}[(\cosh[A_{\bf k}(i)] + \hat{A}^z_{\bf k}(i)\sinh[A_{\bf k}(i)])|\uparrow\rangle$$

$$+ (\hat{A}^x_{\bf k}(i) + i\hat{A}^y_{\bf k}(i))\sinh[A_{\bf k}(i)]|\downarrow\rangle], \qquad (9)$$

where

$$A_{\bf k}(i) = \frac{\beta}{2} \sum_{j\neq i} f_b(r_{ij}){\bf r}_{ij}\times{\bf k} \qquad (10)$$

and $\hat{A}^\alpha_{\bf k}(i)$, ($\alpha=x,y,z$) are the components of an unit vector in the direction of $A_{\bf k}(i)$. A similar expression can be obtained for the action over the spin down single-particle state. We denote this function by JSB, as opposed 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. [1] needs only slight modifications to deal with $\langle R,S|\Psi_{JSB}\rangle$ as a 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 components, respectively, of the FHNC/SOC correlation operator that minimizes the energy per particle of neutron matter at the desired density [11].

IV. RESULTS

We have made our calculations within the full simulation box, and we have taken into account the 26 neighboring boxes in the tabulation of the correlations $f(r)$ and $f_b(r)$, and of the various components $v_p(r)$ of the two-body potential, as described in Ref. [1]. 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 [1] have shown that they are small for systems with 66 neutrons.

Figure 1 shows the AFDMC energies per particle of 14 neutrons in a periodic simulation cell at $\rho=2\rho_0$ for the $AU6'$ and $AU8'$ interactions, as a function of the strength parameter β. One can see that for the $AU8'$ interaction the energy minimum is around $\beta=1$, consistent with the conjecture that $f_b(r)$ moves the nodes in the optimal way when the spin-orbit potential is included in the Hamiltonian. We have obtained a lowering of the energy of 1.6 MeV with respect to the case of the JS nodal surface, which corresponds to $\beta=0$ 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 $v_{8'}$.

AFDMC simulations for the $AU8'$ Hamiltonian with the JSB guiding function have also been carried out for 66 neutrons. As in the case of the 14-neutron system, we have found a minimum of the energy at $\beta\sim1$. The result obtained is compared in Table I with those at $\beta=0$ 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 of the number of particles in the box. The large differences between $E(14)$ and $E(66)$ are mainly due to the effect of the three-body interaction. It has been shown [1] 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 very weak dependence of ΔE_{LS} on the density, in contrast with VCS results.

In order to make a comparison with recent quantum

TABLE III. Spin-orbit contribution to the energy per particle in MeV of neutron matter at density ρ_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	ΔE_{LS}
GFMC-CP	$-1.26(4)$
GFMC-UC	$-2.9(3)$
AFDMC-JS	$-0.14(6)$
AFDMC-JSB	$-1.2(1)$
VCS	-3.8

Monte Carlo calculations performed for 14 neutrons interacting via the v_8' two-body potential by Ref. [15], we report in Table III the corresponding AFDMC results. The table displays the energy difference ΔE_{LS} between the energy obtained with v_8' and v_6' two-body potential.

The calculations of Ref. [15], to which the results reported in Table III refer, have been performed with the $v_{8'}$ potential cutoff at the edge of the box. Therefore, the values of ΔE_{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 the 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 parametrization of the spin backflow is obtained from the spin-orbit correlation of FHNC/SOC theory. These spin-backflow orbitals can also be conveniently used 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 by about 5%. 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.

[1] A. Sarsa, S. Fantoni, K.E. Schmidt, and F. Pederiva, nucl-th/0303035.

[2] S. Fantoni, A. Sarsa, and K.E. Schmidt, Phys. Rev. Lett. **87**, 181101 (2001).

[3] R.B. Wiringa, V.G.J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).

[4] B.S. Pudliner, V.R. Pandharipande, J. Carlson, S.C. Pieper, and R.B. Wiringa, Phys. Rev. C **56**, 1720 (1997).

[5] K.E. Schmidt and S. Fantoni, Phys. Lett. B **446**, 93 (1999).

[6] J. Morales, Jr., V.R. Pandharipande, and D.G. Ravenhall, Phys. Rev. C **66**, 054308 (2002).

[7] A. Akmal and V.R. Pandharipande, Phys. Rev. C **56**, 2261 (1997).

[8] A. Akmal, V.R. Pandharipande, and D.G. Ravenhall, Phys. Rev. C **58**, 1804 (1998).

[9] M. Baldo, G. Giansiracusa, U. Lombardo, and H.Q. Song, Phys. Lett. B **473**, 1 (2000).

[10] I. Vidaña, A. Polls, and A. Ramos, Phys. Rev. C **65**, 035804 (2002).

[11] R.B. Wiringa, V. Fiks, and A. Fabrocini, Phys. Rev. C **38**, 1010 (1988).

[12] V.R. Pandharipande and R.B. Wiringa, Rev. Mod. Phys. **51**, 821 (1979).

[13] K.E. Schmidt, M.A. Lee, M.H. Kalos, and G.V. Chester, Phys. Rev. Lett. **47**, 807 (1981).

[14] S.C. Pieper, K. Varga, and R.B. Wiringa, Phys. Rev. C **66**, 044310 (2002).

[15] J. Carlson, J. Morales, Jr., V.R. Pandharipande, and D.G. Ravenhall, nucl-th/0303041.