Spin-Orbit Correlations in Nuclear Matter.

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The study of the properties of nuclear matter within the variational or correlated wave function theory is at present of great interest (1). Vigorous efforts have been particularly addressed to a reliable numerical evaluation of the ground-state energy employing realistic nucleon-nucleon potentials (2-4). The correlated-basis functions (CBF) approach may provide an efficient method for an accurate treatment of that problem (5,6). A straightforward « compromise program » has been described in detail in ref. (7) which takes appropriate account of the crucial noncentral correlations due to the $^3S-{}^3D$ tensor force. However, the numerical applications (5-8) have been hitherto confined to potentials of the form

$$v_6(12) = \sum_{s=1}^{6} v^{(s)}(r_{12}) o_s(12) ,$$

where $o_s = 1$, $\sigma_1 \cdot \sigma_2$, $\tau_1 \cdot \tau_2$, $\sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2$, S_{12}, $S_{12} \tau_1 \cdot \tau_2$, respectively.

In this letter we extend the CBF procedure described in ref. (6-8) to deal with potentials of the more general v_8-class,

$$v_8(12) = \sum_{s=1}^{8} v^{(s)}(r_{12}) o_s(12) \tag{1}$$

which include the spin-orbit components $o_7(12) = \boldsymbol{L} \cdot \boldsymbol{S}$, $o_8(12) = \boldsymbol{L} \cdot \boldsymbol{S} \tau_1 \cdot \tau_2$. We begin with a brief summary of the formalism needed. The trial ground-state wave function is of the form $\Psi_0 = F \Phi_0$, Φ_0 being the normalized ground-state wave function of a

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system of A noninteracting fermions. The correlation operator $F(1 \ldots A)$ is considered to be symmetric with respect to the particle labels and obeys the cluster property ([8,9]). The energy expectation value $E_0 = \langle \Psi_0|H|\Psi_0\rangle / \langle \Psi_0|\Psi_0\rangle$ is then developed into the series ([7])

$$E_0 = E_F + (\Delta E)_2 + (\Delta E)_3 + \ldots , \tag{2}$$

where E_F is the ground-state energy of A noninteracting nucleons. The two- and three-body contributions to the factor cluster expnasion (2) are

$$(\Delta E)_2 = \sum_{i<j} \langle ij|\omega_2(12)|ij - ji\rangle \tag{3}$$

and

$$(\Delta E)_3 = \sum_{i<j<k} \langle ijk|w_3(123)|ijk - ikj + jki - jik + kij - kji\rangle - \\ - \sum_{ijk} \langle ik|F_2^2(12) - 1|ik - ki\rangle \langle ij|w_2(12)|ij - ji\rangle .$$

The labels i, j, k indicate normalized plane-wave orbitals occupied in the Fermi sea. The effective potentials $w_2(12)$ and $w_3(123)$ appearing in eqs. (3) are defined by

$$w_2(12) = \tfrac{1}{2}[F_2(12), [t(1) + t(2), F_2(12)]] + F_2(12)v(12)F_2(12) \tag{4}$$

and

$$w_3(123) = \tfrac{1}{2}[F_3(123), [t(3), F_3(123)]] + F_3(123)v(12)F_3(123) - w_2(12) + \text{cycl} .$$

Equations (3) and (4) involve the correlation operators $F_2(12)$ and $F_3(123)$ for the two- and three-body subsystems. In accordance with the prescription of ref. ([6-8]) we adopt the expressions

$$F_2(12) = f(r_{12}) + [f_T(r_{12}) - f(r_{12})] P_\tau^1(12) P^3(12) [1 - Q(12)] \tag{5}$$

and

$$F_3(123) = f(r_{12}) f(r_{23}) f(r_{13}) + \{f(r_{13}) f(r_{23}) [f_T(r_{12}) - f(r_{12})] P_\tau^1(12) P^3(12) [1 - Q(12)] + \text{cycl.}\} .$$

In keeping with the notation of earlier work we use the spin triplet (singlet) projector P^3 (P^1), the isospin triplet (singlet) projector P_τ^3 (P_τ^1) and the tensor projector $Q(12) = r_{12}^{-2}(\boldsymbol{S}\cdot\boldsymbol{r}_{12})^2 = \frac{1}{6}(S_{12} + 4P^3)$. Choice (5) takes proper account of the most important spatial and tensor correlations present in nuclear matter ([7]).

Explicit expressions for the effective potentials (4) of the class v_6 based on ansatz (5) have been given in ref. ([5,7]). Writing the spin-orbit components, $s = 7, 8$, of potential (1) as

$$v^{LS}(12) = V_{LS}^+(r_{12}) P_\tau^1 \boldsymbol{L}\cdot\boldsymbol{S} + V_{LS}^-(r_{12}) P_\tau^3 \boldsymbol{L}\cdot\boldsymbol{S} \tag{6}$$

([9]) J. W. CLARK and M. L. RISTIG: in *The Nuclear Many-Body Problem*, edited by F. CALOGERO and C. CIOFI DEGLI ATTI, Vol. **2** (Bologna, 1973).

the associated two-body effective potential is

$$(7)\qquad w_2^{LS}(12) = -\tfrac{2}{3}[f_T(r_{12}) - f(r_{12})]^2\, V_{LS}^{+}(r_{12})\, P_\tau^1 P^3 + \\ + \tfrac{1}{6}[2f_T(r_{12}) + f(r_{12})][f_T(r_{12}) - f(r_{12})]\, V_{LS}^{+}(r_{12})\, P_\tau^1 S_{12} + \\ + f(r_{12})\, f_T(r_{12})\, V_{LS}^{+}(r_{12})\, P_\tau^1 \boldsymbol{L}\cdot\boldsymbol{S} + f^2(r_{12})\, V_{LS}^{-}(r_{12})\, P_\tau^3 \boldsymbol{L}\cdot\boldsymbol{S}\,.$$

In deriving relation (7) we have exploited the operator identities ([10]) $Q\boldsymbol{L}\cdot\boldsymbol{S}Q = -Q$ and $Q\boldsymbol{L}\cdot\boldsymbol{S} + \boldsymbol{L}\cdot\boldsymbol{S}Q = \boldsymbol{L}\cdot\boldsymbol{S} - 3Q + 2P^3$. We note that the even-state portion of the spin-orbit force contributes to the diagonal matrix elements $\langle ij|w_2^{LS}(12)|ij - ji\rangle$. The odd-state part can only contribute to the exact ground-state energy value through the perturbation corrections to the expectation value. An explicit expression for the effective three-body potential (4) corresponding to the spin-orbit interaction (6) and correlation operators (5) may also be derived by elementary algebraic manipulations. The result is available but rather lengthy and will be given in a more detailed publication.

To improve upon our description of the nuclear matter ground-state we next apply perturbation theory, formulated in terms of a basis of dynamically correlated states arriving at

$$(9)\qquad E_G = E_0 + (\delta E)^{(2)} + \ldots$$

for the exact ground-state energy ([7]). In two-body cluster approximation the second-order perturbation correction $(\delta E)^{(2)}$ is given by ([7,8])

$$(10)\qquad (\delta E)^{(2)} \sim (\delta E)_2^{(2)} = -\sum_{p<q}\sum_{i<j} (\varepsilon_p + \varepsilon_q - \varepsilon_i - \varepsilon_j)^{-1} \cdot \\ \cdot |\langle ij|w_2(12)|pq - qp\rangle + \tfrac{1}{2}(\varepsilon_p + \varepsilon_q - \varepsilon_i - \varepsilon_j)\langle ij|F_2^2(12) - 1|pq - qp\rangle|^2\,.$$

Here, p, $q(i, j)$ denote particle (hole) orbitals and the quantity ε_a represents the single-particle (hole) energies

$$(11)\qquad \varepsilon_a = \frac{\hbar^2 k_a^2}{2m} + \sum_i \langle ia|w_2(12)|ia - ai\rangle\,.$$

For a numerical study of the spin-orbit effects we select the Hamada-Johnston (HJ) potential ([11]) stripped of the *quadratic* $\boldsymbol{L}\cdot\boldsymbol{S}$-component. Further, we employ the « optimal » correlation functions $f(r)$ and $f_T(r)$ which have been determined by a constrained Euler-Lagrange procedure for the HJ potential *sans* spin-orbit components ([7]). To calculate the perturbation correction we follow MacKenzie's procedure ([12]) which has been already employed in earlier works ([6-8]). We use a partial-wave decomposition of the effective two-body potential truncated at the D-state level together with the angle-averaging approximation. A free spectrum has been adopted for single-particle states and an effective mass approximation for hole states.

As a first step we have repeated the calculations of the quantities $(\Delta E)_2$ and $(\delta E)_2^{(2)}$, performed by KÜRTEN *et al.* ([6,7]) for the HJ potential v_6. Our results are collected in

([10]) J. C. OWEN, R. F. BISHOP and J. M. IRVINE: *Nucl. Phys. A*, **277**, 45 (1977).
([11]) T. HAMADA and J. D. JOHNSTON: *Nucl. Phys.*, **34**, 382 (1962).
([12]) J. J. MACKENZIE: *Phys. Rev.*, **179**, 1002 (1969).

table I. The two- and three-body cluster contributions (the latter data are taken from ref. ([6])), and the perturbation correction are gives as functions of the Fermi wave number k_F for various values of the healing distance d. The values of the correction terms $(\delta E)_2^{(2)}$ given in ref. ([6,7]), differ from those listed in table I because of a computational error detected in the previous work. (Kürten's corrected data for the HJ potential v_6 reported in ref. ([8]), agree now with the data of table I within numerical accuracy.)

TABLE I. – *Two- and three-body cluster contributions* $(\Delta E)_2$ *and* $(\Delta E)_3$ *to the expectation value* E_0, *and approximation* (10) *to second-order perturbation correction* $(\delta E)^{(2)}$, *for* HJ *potential* v_6 *and various choices of Fermi wave number* k_F *and healing distance* d (*energies in* MeV *per particle*).

	k_F (fm^{-1})	1.3	1.4	1.5	1.6	1.7	1.8
$d=2.2$ fm	$(\Delta E)_2$	−27.14	−31.88	−36.79	−41.73	−46.77	−50.72
	$(\Delta E)_3$	1.36	2.13	3.36	5.29	8.27	12.77
	$(\delta E)_2^{(2)}$	− 2.34	− 2.87	− 3.61	− 4.63	− 6.20	− 8.81
$d=2.5$ fm	$(\Delta E)_2$	−27.48	−32.46	−37.74	−43.21	−48.87	−54.55
	$(\Delta E)_3$	1.01	1.65	2.72	4.44	7.15	11.26
	$(\delta E)_2^{(2)}$	− 1.62	− 1.86	− 2.15	− 2.57	− 3.21	− 4.31
$d=3.0$ fm	$(\Delta E)_2$	−27.31	−32.29	−37.65	−43.46	−49.17	−55.24
	$(\Delta E)_3$	0.61	1.04	1.80	3.04	5.01	8.04
	$(\delta E)_2^{(2)}$	− 1.33	− 1.41	− 1.49	− 1.58	− 1.76	− 2.15

TABLE II. – *Two- and three-body cluster contributions* $(\Delta E)_2^{LS}$ *and* $(\Delta E)_3^{LS}$ *to the expectation value* E_0, *second-order perturbation correction in two-body cluster approximation* $(\delta E)_2^{(2)LS}$, *and net energy change* $E_G^{LS} = (\Delta E)_2^{LS} + (\Delta E)_3^{LS} + (\delta E)_2^{(2)LS}$ *induced by the spin-orbit component of* HJ *potential* v_8 *for various choices of Fermi wave number* k_F *and healing distance* d. (Energies in MeV per particle.)

	k_F (fm^{-1})	1.3	1.4	1.5	1.6	1.7	1.8
$d=2.2$ fm	$(\Delta E)_2^{LS}$	−0.24	−0.31	−0.38	−0.46	−0.56	−0.69
	$(\Delta E)_3^{LS}$	−0.39	−0.61	−0.92	−1.35	−1.92	−2.75
	$(\delta E)_2^{(2)LS}$	−2.64	−3.27	−3.93	−4.55	−5.01	−5.41
	E_G^{LS}	−3.27	−4.18	−5.23	−6.36	−7.49	−8.85
$d=2.5$ fm	$(\Delta E)_2^{LS}$	−0.21	−0.27	−0.33	−0.41	−0.49	−0.59
	$(\Delta E)_3^{LS}$	−0.35	−0.54	−0.81	−1.18	−1.70	−2.38
	$(\delta E)_2^{(2)LS}$	−2.60	−3.23	−3.91	−4.57	−5.10	−5.64
	E_G^{LS}	−3.16	−4.04	−5.05	−6.15	−7.30	−8.61
$d=3.0$ fm	$(\Delta E)_2^{LS}$	−0.18	−0.23	−0.29	−0.35	−0.43	−0.51
	$(\Delta E)_3^{LS}$	−0.30	−0.47	−0.71	−1.03	−1.47	−2.05
	$(\delta E)_2^{(2)LS}$	−2.58	−3.23	−3.92	−4.59	−5.19	−5.79
	E_G^{LS}	−3.07	−3.93	−4.92	−5.98	−7.08	−8.35

The additional spin-orbit contributions to the various quantities $(\Delta E)_2$, etc. induced by the $\boldsymbol{L}\cdot\boldsymbol{S}$ components (6) of the HJ potential v_s are called $(\Delta E)_2^{LS}$, ... and are listed in table II. The absolute value of the quantity $E_G^{LS} = (\Delta E)_2^{LS} + (\Delta E)_3^{LS} + (\delta E)_2^{(2)LS}$ gives

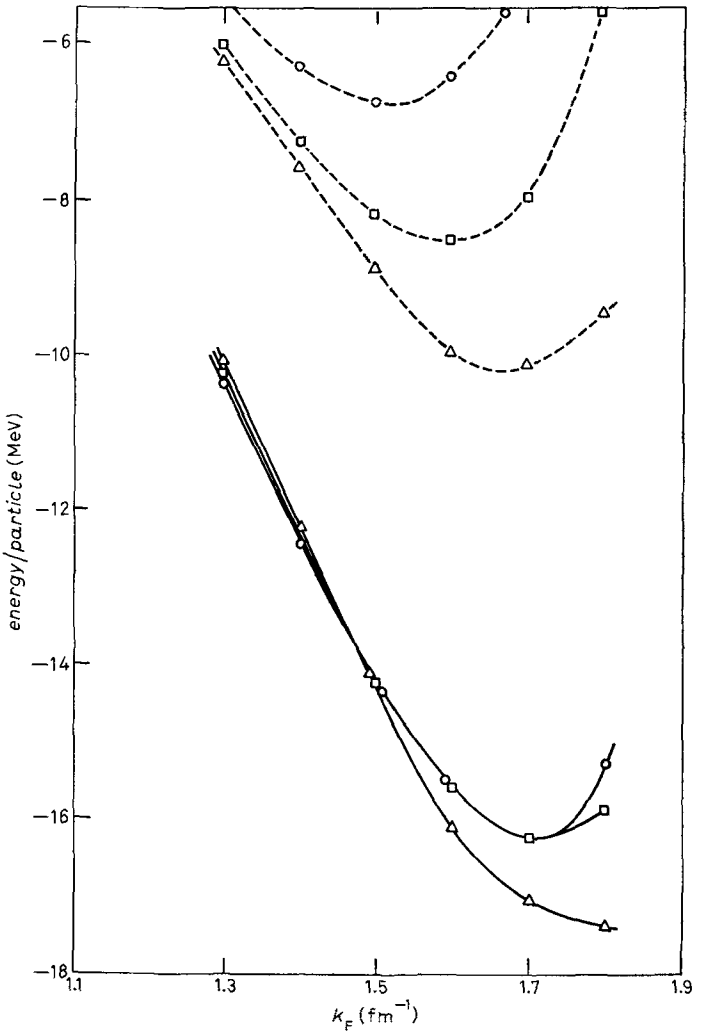

Fig. 1. – Energy per particle as a function of Fermi wave number k_F at various healing distances, for the HJ potential v_s. Dashed curves: three-body cluster approximation to energy expectation value. Solid curves: energy estimate $E_G = E_F + (\Delta E)_3 + (\Delta E)_3 + (\delta E)_2^{(2)}$ including two-body cluster approximation to second-order perturbation correction. o $d = 2.2$ fm, □ $d = 2.5$ fm, △ $d = 3.0$ fm.

the net increase in nuclear binding energy due to the spin-orbit potential (6). We note that the various contributions are insensitive to the choice of the separation distance d. The two- and three-body cluster contributions are rather small; the main gain in energy is essentially coming from the spin-orbit perturbation correction.

Figure 1 depicts our results for the energy expectation value in three-body cluster approximation $E_0 \simeq E_F + (\Delta E)_2 + (\Delta E)_3$ and for the energy estimate $E_G \simeq E_F + (\Delta E)_2 + + (\Delta E)_3 + (\delta E)_2^{(2)}$ based on the v_8-model of the HJ potential. As expected from the earlier studies of the v_6-model we find that, except at the highest densities considered, the values of the quantity E_G are almost independent of the separation distance d in contrast to the expectation value E_0. The estimate E_G indicates saturation at too high a density, $k_F \sim 1.7\ \mathrm{fm}^{-1}$. However, once the repulsive effect due to the quadratic spin-orbit component of the nuclear force has been taken into account, the saturation density might shift to some extent, towards a more realistic density.