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Tensor Correlations in Nuclear Matter*

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The Jastrow method is extended to the treatment of tensor forces by the incorporation of suitable state dependence into the two-body correlation operator. The one- and two-body parts of the energy expectation value developed in a factor-cluster (Van Kampen) expansion, are evaluated for nuclear matter. Numerical results are presented for three semirealistic hard-core potentials with differing mixtures of central and tensor components. These results point to the necessity for an examination of three-body cluster corrections to the energy expectation value.

I. INTRODUCTION

The Jastrow approach[1,2] to the nuclear many-body problem has a number of features which recommend it as an attractive alternative to the currently more highly developed Brueckner-Bethe-Goldstone scheme.[3,4] Among these are its conceptual simplicity and its variational character, along with the possibility of its systematic improvement within the framework of the method of correlated basis functions.[5] Of considerable interest at the present time is the practicality, in this approach, of explicit and unencumbered evaluation of three- and four-body contributions to the energy expectation value.[4]

To date, the Jastrow method has seen detailed application in the nuclear-matter and other nuclear many-body problems[6,7] only for simple *central* potentials. The conventional Jastrow trial wave function, built with spherically symmetric two-body correlation factors, is not adequate for the treatment of realistic two-nucleon potentials, which contain tensor and spin-orbit components. This inadequacy of the Jastrow approach is developmental rather than intrinsic; its correction will be the aim of this and subsequent studies. Contributions to the energy from tensor and spin-orbit (including "quadratic spin-orbit") components may, of course, be estimated by a second-order perturbation calculation in the correlated basis generated from the Jastrow function according to Ref. 5, and calculations of this nature, using realistic potentials, are in progress. However, the essence of the method of correlated basis functions is the precept to incorporate the most important correlations *at the outset*, i.e., in constructing the basis elements and especially that element (trial wave function) corresponding to the ground state. Thus, in treating nuclear matter with realistic potentials, correlations induced by the tensor force should be incorporated directly into the correlation factor F of the basis function $F\Phi$, where Φ is the ground-state wave function of the Fermi gas. This may be accomplished by building up F from two-body functions not only of the magnitudes of the $\vec{r}_{ij}$, but also of $(\vec{\sigma}_i \cdot \vec{r}_{ij})(\vec{\sigma}_j \cdot \vec{r}_{ij})$, $\vec{\sigma}_i \cdot \vec{\sigma}_j$, and $\vec{\tau}_i \cdot \vec{\tau}_j$.[8] [As before, F must be symmetric with respect to interchange of the coordinates (space, spin, and isospin) of any two nucleons.] The purpose of the present article is to make the first steps toward such a generalization of the Jastrow method. As opposed to a perturbative estimate of tensor effects, this generalization offers some evident advantages, especially in the face of a weighty tensor component (as occurs in the most realistic potentials), for which convergence of the aforementioned perturbation expansion may not be satisfactory.

In Sec. II we carry out a factor-cluster or Van Kampen expansion[9-11] of the expectation value of the Hamiltonian with respect to a general correlated wave function of the type $F\Phi$, where Φ is an independent-particle model function and F introduces dynamical correlations. This expansion establishes a separation of one-body, two-body, three-body,... correlation effects. In Sec. III the correlation operator F, or rather, its two-body part, is specialized to deal with the presence of a tensor component in the two-nucleon potential. We then proceed with the analysis of the two-body contribution to the cluster expansion for the energy. An expression is given for an effective central potential whose Hartree-Fock expectation value leads to the same result for the interaction energy as does the bare potential, treated in the two-body approximation within the present generalized Jastrow scheme. In Sec. IV we outline a very simple procedure for the determination of the generalized two-body correlation factor and present numerical results for three semirealistic nucleon-nucleon interactions containing different even-state central-tensor mixtures. The implications of these results are discussed in Sec. V. In particular, emphasis is placed on the necessity for the inclusion

of three-body (and possibly other higher-order) contributions in the analysis, at least under the guise of some associated restrictions on the variation of the generalized two-body correlation factor. The enumeration and evaluation of three-body contributions to the energy expectation value with tensor correlations will be the concern of a future paper of this series.

II. FACTOR-CLUSTER EXPANSION FOR THE ENERGY EXPECTATION VALUE

We shall now derive a cluster expansion for the expectation value $E=(\Psi, H\Psi)/(\Psi, \Psi)$ of the Hamiltonian

$$H=T+V=\sum_{i=1}^{A} t(i)+\sum_{1\le i<j\le A} v(ij),$$

$$t(i)=-(\hbar^2/2m)\nabla_i^2, \tag{1}$$

with respect to a correlated A-body trial function of the general type

$$\Psi=F\Phi, \tag{2}$$

where F is an appropriate correlation operator and Φ is the normalized ground-state[12] wave function of A independent nucleons.

The central object of analysis is the generalized normalization integral

$$I(\beta)=(\Psi, e^{\beta(H-E_0)}\Psi) \tag{3}$$

corresponding to the quantity $H-E_0$, where E_0 is the ground-state energy of the chosen independent-particle model. The desired energy expectation value may be recovered via

$$E=E_0+\frac{\partial}{\partial\beta}\ln I(\beta)\big|_{\beta=0}. \tag{4}$$

The analysis of $I(\beta)$ begins with the definition of subnormalization integrals, analogs of (3) for subsystems of the A-nucleon system:

$$I_i(\beta)=(i\,|F^\dagger(1)\exp\{\beta[t(1)-\epsilon_i]\}F(1)|\,i),$$

$$I_{ij}(\beta)=(ij|F^\dagger(12)\exp\{\beta[t(1)+t(2)+v(12)-\epsilon_i-\epsilon_j]\}F(12)|\,ij-ji),$$

$$I_{ijk}(\beta)=(ijk|F^\dagger(123)\exp\{\beta[t(1)+t(2)+t(3)+v(12)+v(23)+v(31)-\epsilon_i-\epsilon_j-\epsilon_k]\}$$

$$\times F(123)|\,ijk-ikj+jki-jik+kij-kji), \tag{5}$$

$$\vdots$$

$$I_{i_1\ldots i_A}\equiv I(\beta).$$

Here $i, j, k, \ldots$ are elements of the set $\{i_1\ldots i_A\}$ of A orbitals occupied in Φ. The ϵ_i are the single-particle energies corresponding to these orbitals. The operators $F(1)$, $F(12)$, $F(123), \ldots$ are "appropriate" correlation operators for one-, two-, three-, ... body subsystems. Clearly there is a great deal of freedom in their definition. However in order for the formalism under development to have physical relevance, we do need to require that these F's be symmetric in their particle labels and that they possess the "cluster property"; i.e., $F(1\ldots n)\to F(1\ldots n-1)$ for $r_{1n}, \ldots, r_{n-1,n}\to\infty$, $n=2, \ldots, A$. Further, if a hard core of radius c is present in the two-particle interaction, we demand $F(1\ldots n)=0$ for any $r_{in}\le c$, $i=1, \ldots, n-1$, $n=2, \ldots, A$; analogous short-range behavior is to be imposed for soft cores. It is also desirable that $F(1\ldots n)$, $n=1, \ldots A$, be positive definite in the region of configuration space in which the potential operator for the n-particle subsystem is finite.

Next, a factor-cluster decomposition of the above subnormalization integrals is executed

$$I_i=Y_i,$$

$$I_{ij}=Y_iY_jY_{ij},$$

$$I_{ijk}=Y_iY_jY_kY_{ij}Y_{jk}Y_{ki}Y_{ijk},$$

$$\vdots$$

$$I_{i_1\ldots i_A}=I=\prod_i Y_i\prod_{i<j}Y_{ij}\prod_{i<j<k}Y_{ijk}\ldots Y_{i_1\ldots i_A}. \tag{6}$$

In the last equation the dummy indices range, subject to the indicated restrictions, over the set $\{i_1\ldots i_A\}$. Note that these relations merely serve to *define* the Y's in terms of the I's. Inserting the last of the relations (6) into (4), we arrive at a factor-cluster or Van Kampen-type expansion for the energy expectation value:

$$E=E_0+(\Delta E)_1+(\Delta E)_2+(\Delta E)_3+\cdots+(\Delta E)_A, \tag{7}$$

$$(\Delta E)_1 = \sum_i \frac{\partial}{\partial\beta} \ln Y_i|_{\beta=0},$$

$$(\Delta E)_2 = \sum_{i<j} \frac{\partial}{\partial\beta} \ln Y_{ij}|_{\beta=0},$$

$$(\Delta E)_3 = \sum_{i<j<k} \frac{\partial}{\partial\beta} \ln Y_{ijk}|_{\beta=0},$$

$$\vdots \qquad (8)$$

This expansion may be rendered more explicit by insertion of the solutions of (6) for the Y's in terms of the I's; we find

$$(\Delta E)_1 = \sum_i \frac{\partial I_i}{\partial\beta}\bigg|_{\beta=0},$$

$$(\Delta E)_2 = \sum_{i<j} \left[\frac{1}{I_{ij}} \frac{\partial I_{ij}}{\partial\beta} - \left(\frac{\partial I_i}{\partial\beta} + \frac{\partial I_j}{\partial\beta}\right)\right]\bigg|_{\beta=0},$$

$$(\Delta E)_3 = \sum_{i<j<k} \left[\frac{1}{I_{ijk}} \frac{\partial I_{ijk}}{\partial\beta} - \left(\frac{1}{I_{ij}} \frac{\partial I_{ij}}{\partial\beta} + \frac{1}{I_{jk}} \frac{\partial I_{jk}}{\partial\beta} + \frac{1}{I_{ki}} \frac{\partial I_{ki}}{\partial\beta}\right) + \left(\frac{\partial I_i}{\partial\beta} + \frac{\partial I_j}{\partial\beta} + \frac{\partial I_k}{\partial\beta}\right)\right]\bigg|_{\beta=0},$$

$$\vdots \qquad (9)$$

The general term of (9) is given in Ref. 9.

In the factor-cluster expansion (7) the nth order term $(\Delta E)_n$ involves (irreducibly) exactly n orbitals ("hole lines") and hence is properly called the n-body contribution arising from the assumed dynamical correlations.

Obviously the factor-cluster formalism just developed is very general (perhaps too general), both with regard to the choice of wave function Ψ (it can even be exact) and with regard to the choice of correlation operators $F(1)$, $F(12)$, $F(123), \ldots$. The vast flexibility of cluster-expansion methods has received thorough discussion in Ref. 9. Not only the various Jastrow treatments but also the unitary-operator method[13] may be obtained as special cases of the above formalism.[11] For the simplest Jastrow treatment, one sets

$$F(1) = 1,$$
$$F(12) = f(r_{12}),$$
$$F(123) = f(r_{12}) f(r_{23}) f(r_{31}),$$
$$\vdots$$
$$F(1\ldots A) \equiv F = \prod_{i<j} f(r_{ij}). \qquad (10)$$

If we seek to go beyond this treatment and build subsystem wave functions from two-body functions depending not only on r_{ij} but also more generally on $\vec{r}_{ij}$, $\vec{\sigma}_i$, $\vec{\sigma}_j$, $\vec{\tau}_i$, $\vec{\tau}_j$, and (possibly) the relative momentum $\vec{p}_{ij}$, we still choose

$$F(1) = 1,$$
$$F(12) = f(12) = f(\vec{r}_{ij}, \vec{\sigma}_i, \vec{\sigma}_j, \vec{\tau}_i, \vec{\tau}_j, \vec{p}_{ij}), \qquad (11)$$

but the most judicious choice of $F(123)$, $F(1234)$, ... is rendered ambiguous by noncommutivity of $f(ij)$ and $f(jk)$.[14] This uncertainty assuredly besets the present attempt to extend the Jastrow method to deal with realistic potentials. However, we shall not be forced to confront it until the next paper of this series, where three-body effects of tensor potentials will be examined.

Henceforth we confine our discussion to a uniform extended system like nuclear matter. Thus we take

$$t(1)|i) = \epsilon_i|i),$$
$$T\Phi = E_0\Phi, \qquad (12)$$

so that $I_i = Y_i = 1$ and, hence, $\partial I_i/\partial\beta = 0$, $(\Delta E)_1 = 0$. Furthermore, the "normalizing denominators" $I_{ij}|_0$, $I_{ijk}|_0, \ldots$ appearing in $(\Delta E)_2$, $(\Delta E)_3, \ldots$ differ from unity by terms at most $O(1/A)$. Dropping contributions to E which are of order unity or less compared with A, the two-body portion of the energy expectation value is then given simply by (see the remarks in Ref. 11 on this sort of reduction)

$$(\Delta E)_2 = \sum_{i<j} (ij| \{\tfrac{1}{2}F^\dagger(12)[t(1)+t(2), F(12)] + \tfrac{1}{2}[F^\dagger(12), t(1)+t(2)]F(12) + F^\dagger(12)v(12)F(12)\} |ij - ji). \qquad (13)$$

In our work the correlation operator $F(12)$ is assumed to be Hermitian (rather than unitary as in Ref. 13), so that (13) reduces to

$$(\Delta E)_2 = \sum_{i<j} (ij| \{\tfrac{1}{2}[F(12), [t(1)+t(2), F(12)]] + F(12)v(12)F(12)\} |ij - ji). \qquad (14)$$

For a uniform extended system the differences between the factor-cluster expansion just developed and the more familiar Iwamoto-Yamada expansion[15] are rather minor: The latter may be obtained from the former by regrouping contributions according to the number of *independent* orbitals involved. There is no difference as far as the two-body terms are concerned. For a finite system the differences may be more important. From an over-all formal standpoint the factor-cluster formalism appears the more natural.[11]

III. TWO-BODY EFFECTS OF TENSOR CORRELATIONS

Let us proceed with the study of two-body effects of tensor correlations in nuclear matter, based on

the formalism just developed. We consider a hard-core potential with spin- and parity-dependent central and tensor components:

$$\begin{aligned} v(12) &= +\infty, && r \equiv r_{12} \leq c, \\ &= {}^1V_C^+(r)P_1P^+ + {}^1V_C^-(r)P_1P^- \\ &\quad + {}^3V_C^+(r)P_3P^+ + {}^3V_C^-(r)P_3P^- \\ &\quad + V_T^+(r)P^+S_{12} + V_T^-(r)P^-S_{12}, && r > c. \end{aligned} \tag{15}$$

The operators P_1, P_3 are, respectively, projectors on singlet and triplet states of the two interacting nucleons; P^+, P^- are projectors on even and odd states. The tensor operator

$$S_{12} = 3\,\frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \tag{16}$$

may be equivalently expressed as

$$S_{12} = 6Q - 4P_3, \tag{17}$$

where $Q = (\vec{S} \cdot \vec{r})^2/r^2$, with $\vec{S} = \frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)$, is a projection operator in spin-angle space.[16] The mode of action of Q is given by

$$\begin{aligned} &Q\mathcal{Y}^M_{J0J} = 0, \\ &Q\mathcal{Y}^M_{J1J} = \mathcal{Y}^M_{J1J}, \\ &(2J+1)Q\mathcal{Y}^M_{J+11J} = J\mathcal{Y}^M_{J+11J} + [J(J+1)]^{1/2}\mathcal{Y}^M_{J-11J}, \\ &(2J+1)Q\mathcal{Y}^M_{J-11J} = [J(J+1)]^{1/2}\mathcal{Y}^M_{J+11J} + (J+1)\mathcal{Y}^M_{J-11J}. \end{aligned} \tag{18}$$

The $\mathcal{Y}^M_{LSJ}$ are the usual spin-angle functions.

It is well known that for the simple Jastrow choice $F(12) = f(r_{12})$ the tensor component of (15) gives no contribution to the interaction energy (14). (Any contribution linear in the tensor operator S_{12} is canceled in the spin average.) But tensor effects can easily be included by choosing instead the more general two-body correlation operator

$$F(12) = F^+(12)P^+ + F^-(12)P^- \tag{19}$$

with

$$F^\pm(12) = f_1^\pm(r)P_1 + f_2^\pm(r)P_3Q + f_3^\pm(r)P_3(1-Q). \tag{20}$$

The six independent functions $f_i^\pm(r)$ are required to fulfill the usual conditions for a Jastrow two-body correlation factor,

$$\begin{aligned} &f(r) = 0, && r \leq c, \\ &f \to 1, && r \to \infty. \end{aligned} \tag{21}$$

Ansatz (19)-(20) is in accord with all the relevant invariance properties and reduces to the simple Jastrow choice $F(12) = f(r_{12})$ if the functions $f_i^\pm$ are all equal. It should be emphasized that (19)-(20) allows for different correlations in different spin-parity states even in the absence of tensor effects, in which case (20) reduces to

$$F^\pm(12) = f_1^\pm(r)P_1 + f_2^\pm(r)P_3. \tag{22}$$

The double commutator in (14) may be evaluated in a straightforward manner with the help of the following relations,

$$\begin{aligned} &P_1Q = P_1P_3 = Q(1-Q)P_3 = 0, \\ &[f,[\nabla^2,f]] = -2(\nabla f)^2, \\ &[f,[\nabla^2,Q]] = 0, \\ &[Q,[Q,L^2]] = 2Q - 4P_3 - 2\vec{L}\cdot\vec{S}, \end{aligned} \tag{23}$$

where $\vec{S}$ is the total spin operator and $\vec{L}$ the relative orbital angular momentum operator of the two interacting nucleons. Further reduction of the two-body contribution to the interaction energy is effected upon carrying out the spin sums—all terms proportional to the tensor operator S_{12} or spin-orbit operator $\vec{L}\cdot\vec{S}$ are eliminated. The final result may be conveniently expressed in terms of an effective central potential v_{eff},

$$\langle \Delta E \rangle_2 = \sum_{i<j} (ij|v_{\text{eff}}|ij - ji), \tag{24}$$

with

$$\begin{aligned} v_{\text{eff}} &= P^+[({}^1V_C^+P_1 + {}^3V_C^+P_3)(f_1^+)^2 + (\hbar^2/m)(\nabla f_1^+)^2] \\ &\quad + P^+P_3\{\tfrac{2}{3}({}^3V_C^+ + 2V_T^+)[(f_2^+)^2 - (f_1^+)^2] + \tfrac{2}{3}(\hbar^2/m)[(\nabla f_2^+)^2 - (\nabla f_1^+)^2] \\ &\qquad + \tfrac{1}{3}(4V_T^+ - {}^3V_C^+)[(f_1^+)^2 - (f_3^+)^2] + \tfrac{1}{3}(\hbar^2/m)[(\nabla f_3^+)^2 - (\nabla f_1^+)^2] \\ &\qquad + \tfrac{4}{3}(\hbar^2/m)(1/r^2)(f_2^+ - f_3^+)^2\} \\ &\qquad + \text{same expression for odd states } (+ \to -). \end{aligned} \tag{25}$$

Equation (25) should provide the best possible separation of different correlation effects. Consider the even- or odd-state part of (25): The first line represents the "over-all" correlation effect for the parity in question in that this is the only surviving contribution for $f_1 = f_2 = f_3$. The choice $f_2 = f_3 \neq f_1$ produces a difference in correlations in singlet and triplet states of the given par-

ity without relaxing spherical symmetry of $F(12)$; in this case the second and third lines of the relevant portion of v_{eff} are also nonvanishing. Tensor effects (in particular, terms involving V_T) appear only if we relax spherical symmetry of $F(12)$ by allowing $f_2 \neq f_3$; in this case the second and third lines are modified and the fourth line comes into play.

It need hardly be mentioned that analogous extensions of the Jastrow scheme to treat interactions which contain spin-orbit and quadratic spin-orbit components, as well as interactions which differ in each *JLST* partial wave, are possible. Furthermore, the techniques devised in this paper are not restricted in any essential way to the infinite medium; modifications required to treat finite nuclei should be fairly evident.

IV. NUMERICAL RESULTS FOR SEMIREALISTIC POTENTIALS

For numerical study we have selected three semirealistic potentials of the type (15), the Gammel-Christian-Thaler potential[17] (GCT) used in the early nuclear-matter calculation of Brueckner and Gammel[18] and two other potentials studied by Gammel and Thaler[19] which differ from GCT in the triplet-even state only. The functions ${}^1V_C^{\pm}$, ${}^3V_C^{\pm}$, $V_T^{\pm}$ are all of Yukawa shape,

$$V(r) = A\, e^{-\mu r}/\mu r\,. \tag{26}$$

The state-independent hard-core radius is $c = 0.5$ F for all three potentials. Table I lists the common singlet-even-, triplet-odd-, and singlet-odd-state (extracore) parameters. Table II displays the triplet-even-state parameters of GCT and the other two potentials, code named 5100 and 5200 after the notation of Table 19.3 of Ref. 19. (Note that the GCT triplet-even parameters are close to those labeled 5400 in Ref. 19.)

One of our aims is to see how the energy per particle (given by the method proposed herein) changes as the mixture of central and tensor components is altered, consistent (insofar as is practical) with the two-nucleon data. Thus the three potentials to be studied were chosen with the idea of spanning the physical range of the "central-to-tensor ratio" in the triplet-even state. The ratio of central-to-tensor strength of GCT in the triplet-even state is large; that of 5200, moderate; and that of 5100, small. Notice, however, that a large triplet-even tensor (central) strength is accompanied by a small tensor (central) range, and vice versa.

The potentials GCT, 5200, and 5100 yield satisfactory fits of the low-energy properties of the two-nucleon system: the singlet and triplet scattering lengths and effective ranges and the deuteron binding energy, quadrupole moment, and D-state percentage. They do not yield satisfactory fits of the high-energy data. To obtain acceptable fits to all the known phase shifts, as well as the low-energy data, the form (15) must be supplemented by spin-orbit and quadratic spin-orbit components (as in the Hamada-Johnston potential[20]); indeed, it appears that one may even have to allow for a different potential of the form (15) plus spin-orbit component, *in each JLST wave* (as in the Reid potentials[21]). We do not use such realistic potentials as the Hamada-Johnston and Reid potentials, because their additional complexity would obviously obscure the interpretation of results obtained using the correlation factor (19)-(20) (particularly in regard to dependence on the "central-to-tensor ratio"), not to mention the fact that their proper treatment would require a generalization of the ansatz (19)-(20).

At this stage we shall not exploit the full six-dimensional freedom of (19)-(20). A detailed examination of (25) indicates that the most important features of the correlations induced by the assumed potentials should be adequately represented by the following restricted set of f functions:

$$\begin{aligned} &f_1^+ = f_2^+ = f_1^- = f_3^- \equiv f\,, \\ &f_3^+ = g^+ f\,, \\ &f_2^- = g^- f\,, \end{aligned} \tag{27}$$

with

$$\begin{aligned} &f = 1 - e^{-\lambda(r-c)}\,, \quad r \geq c\,,\ \lambda > 0\,, \\ &g^{\pm} = 1 - \alpha^{\pm}(r-c)^2 e^{-\lambda^{\pm}(r-c)}\,, \quad \alpha^{\pm}, \lambda^{\pm} > 0\,. \end{aligned} \tag{28}$$

Our supporting arguments will be based on the ex-

TABLE I. Common parameters of the three potentials denoted GCT, 5200, and 5100. (The indices C and T refer to central and tensor components, respectively.)

State	A_C (MeV)	μ_C (F^{-1})	A_T (MeV)	μ_T (F^{-1})
Singlet even	−905.6	1.7	···	···
Triplet odd	−150	1.5	57.5	1.12
Singlet odd	113	1.0	···	···

TABLE II. Triplet-even-state parameters of the three potentials studied. (The indices C and T refer to central and tensor components, respectively.)

Potential	A_C (MeV)	μ_C (F^{-1})	A_T (MeV)	μ_T (F^{-1})
GCT	−6395	2.936	−45	0.734 21
5200	−1587.7	2.3576	−238.38	1.1788
5100	−121.94	1.4112	−498.73	1.4112

tremum property of the energy expectation value, supposed to apply for our approximation to it. Consider, for example, the term

$$\tfrac{2}{3}({}^3V_C^+ + 2V_T^+)[(f_2^+)^2 - (f_1^+)^2], \tag{29}$$

present in the effective potential in triplet-even states. Since both ${}^3V_C^+$ and V_T^+ are negative, we need to take $(f_1^+)^2 < (f_2^+)^2$ in order to make the corresponding contribution to the energy as negative as possible; i.e., f_2^+ should be of short range compared to f_1^+. But f_1^+, being determined mainly by the spin-averaged central potential, must in itself be of quite short range. An appreciable difference in f_1^+ and f_2^+ then implies a large difference in the slopes $(\nabla f_1^+)^2$ and $(\nabla f_2^+)^2$ and, hence, a large (and effectively compensating, or over-compensating) positive contribution to the energy from the kinetic term

$$\tfrac{2}{3}(\hbar^2/m)[(\nabla f_2^+)^2 - (\nabla f_1^+)^2]. \tag{30}$$

Thus it would seem that little is to be gained by allowing $f_2^+ \neq f_1^+$. A parallel argument motivates the choice $f_3^- = f_1^-$. Turning to the term

$$\tfrac{1}{3}(4V_T^+ - {}^3V_C^+)[(f_1^+)^2 - (f_3^+)^2], \tag{31}$$

also present in the effective interaction in triplet-even states, we find that $4V_T^+ - {}^3V_C^+$ is negative except possibly at short range (as for GCT). Thus the contribution to the energy from (31) can be lowered by choosing $(f_3^+)^2 < (f_1^+)^2$ at longer range. Here it is important to note that a long-range suppression of f_3^+ relative to f_1^+, as accomplished by the choice (27)-(28), need not imply a large contribution from the kinetic term

$$\tfrac{1}{3}(\hbar^2/m)[(\nabla f_3^+)^2 - (\nabla f_1^+)^2]. \tag{32}$$

A similar argument motivates the choice of form for f_2^-.

In brief, our choice (27)-(28) is well tailored (at least) to the long-range correlation effects of the tensor component. The modifications in short-range correlation produced by the tensor component are relatively unimportant, to the degree that (in even- and odd-parity states) this component is of long range compared to the spin-averaged central component. It is to be stressed that the present calculation is exploratory in nature, the intention being to expose the prominent features of the suggested approach and especially the difficulties which must be overcome to make it work.

TABLE III. Correlation-function parameters determined by a simple minimization procedure.

Potential	λ (F^{-1})	λ^+ (F^{-1})	α^+ (F^{-2})	λ^- (F^{-1})	α^- (F^{-2})
GCT	5.8	1.1	0.7	1.6	0.4
5200	4.8	2.1	4.1	1.6	0.4
5100	4.1	2.4	6.4	1.6	0.4

The five parameters λ, $\lambda^\pm$, and $\alpha^\pm$ in (28) are determined for a given potential and density by the following procedure:

(a) The energy per particle in the two-body approximation,

$$\mathcal{E}^{(2)} = [E_0 + (\Delta E)_2]/A, \tag{33}$$

is minimized with respect to λ, with g^+ and g^- set equal to unity. Thus the "over-all" correlation factor f is determined by the spin-, isospin-averaged central potential alone.

(b) Using the value of λ found in step (a), $\mathcal{E}^{(2)}$ is minimized with respect to the parameters λ^+ and α^+ in g^+, with g^- still set equal to unity.

(c) Using the values of λ, λ^+, and α^+ found in steps (a) and (b), $\mathcal{E}^{(2)}$ is minimized with respect to the parameters λ^- and α^- in g^-.

For all three potentials, the parameters so determined are nearly independent of density within the range of Fermi wave numbers $k_F = 1.4$–1.8 F^{-1}. The sets of values adopted for the five parameters (ignoring any slight density dependence) are given in Table III (the actual values shown are appropriate to $k_F = 1.4$ F^{-1}). The corresponding correlation functions f, f_3^+, and f_2^- are plotted for potentials GCT, 5200, and 5100, respectively, in Figs. 1–3. As expected, the "over-all" correlation function f is of very short range, this range increasing as we go from GCT to 5200 to 5100, while the triplet-even and triplet-odd correlation functions f_3^+ and f_2^- are (typically) of rather long range, the triplet-even range decreasing as we go from GCT

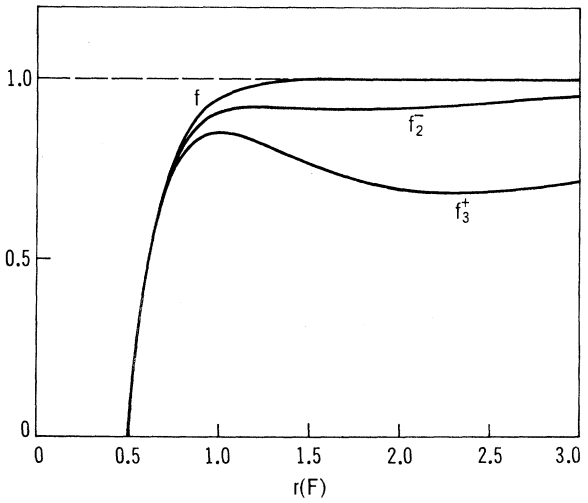

FIG. 1. Correlation functions for the potential denoted GCT, determined at $k_F = 1.4$ F^{-1} by the simple minimization procedure, plotted against radial coordinate r.

to 5200 to 5100.

Figures 4–6 display the energy per particle $\mathcal{E}^{(2)}$ versus Fermi wave number k_F for the three potentials, calculated with the correlation functions specified by Table III. For the GCT potential, results of a reaction-matrix calculation of Brueckner and Gammel[18] (tensor effects present) and a unitary-model-operator calculation of Ristig and Kistler[22] (tensor effects absent) are available for comparison. The assumed correlation functions yield reasonable energies per particle in the physical-density region (the empirical binding energy is some 16 MeV per nucleon at a saturation density corresponding to $k_F = 1.36\ \mathrm{F}^{-1}$). However, they fail to produce saturation of the two-body approximation $\mathcal{E}^{(2)}$ to the expectation value $\mathcal{E} = E/A$ of the energy per particle. It is interesting to note that (at the physical density, for example, where our results are sensible) the binding energy decreases as the even-state central-to-tensor ratio is reduced. This behavior is in accord with the usual assertion that the tensor force is suppressed in nuclear matter relative to an "equivalent" central force. It should also be noted that the odd-state tensor component produces only a minor contribution to $\mathcal{E}^{(2)}$.

V. DISCUSSION

The absence of saturation in the two-body calculation just described implies that *for the particular correlation functions used in that calculation* the three-body (and/or other higher-order) cluster contributions to $\mathcal{E} = E/A$ become large compared to $\mathcal{E}$ itself as the density increases beyond the physical value. If we forget for the moment about cluster contributions beyond $(\Delta E)_3$, then for the GCT potential at $k_F = 1.8\ \mathrm{F}^{-1}$, a value of $(\Delta E)_3/A \approx +24$ MeV would be required to bring $\mathcal{E}$ into agreement with the Brueckner-Gammel result. This situation indicates a rather poor (though not hopeless) convergence of the cluster expansion, since one would have $|(\Delta E)_3/(\Delta E)_2| \approx \frac{1}{3}$. At any rate, the presumption that $\mathcal{E}^{(2)}$ supplies an upper bound to the exact energy per particle clearly breaks down under unrestricted variation of the parameters λ, $\lambda^{\pm}$, $\alpha^{\pm}$, at least at high density.

Similar difficulties encountered in ordinary Jastrow calculations for central potentials are dealt with by imposing appropriate restrictions on the variation of f, with the idea of suppressing three-body and higher-order cluster contributions to $\mathcal{E}$ so as to ensure an upper-bound character for $\mathcal{E}^{(2)}$. Two subsidiary conditions which have received considerable attention (see especially Ref. 6) are:

(a) Normalization condition on the "perturbed" two-body wave function $f\phi_{ij}$:

$$(f\phi_{ij}, f\phi_{ij}) = 1\,, \tag{34}$$

where ϕ_{ij} is the unit-normalized two-body wave function for the noninteracting pair in Fermi-sea orbitals i,j. This condition may be imposed for an "average" pair, or it may be averaged over states of the Fermi sea. One motivation behind its adoption is the desire for as close a correspondence as possible with the unitary-model-operator method.[23] Also, this constraint may be shown to have the effect of stimulating rapid convergence of a certain class of higher-order cluster contributions (called direct ring contributions because

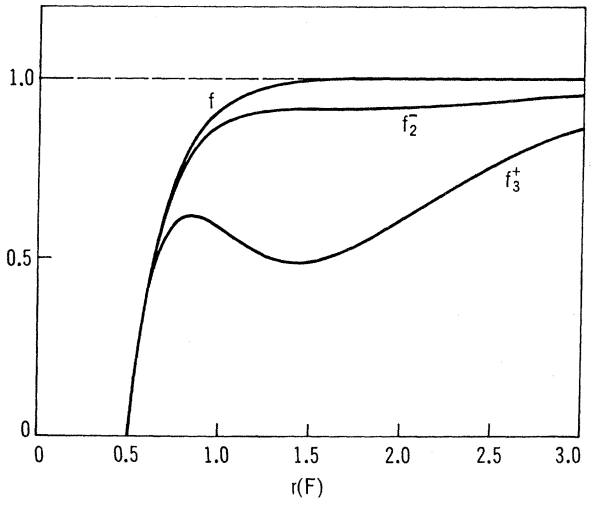

FIG. 2. Correlation functions for the potential denoted 5200, determined at $k_F = 1.4\ \mathrm{F}^{-1}$ by the simple minimization procedure, plotted against radial coordinate r.

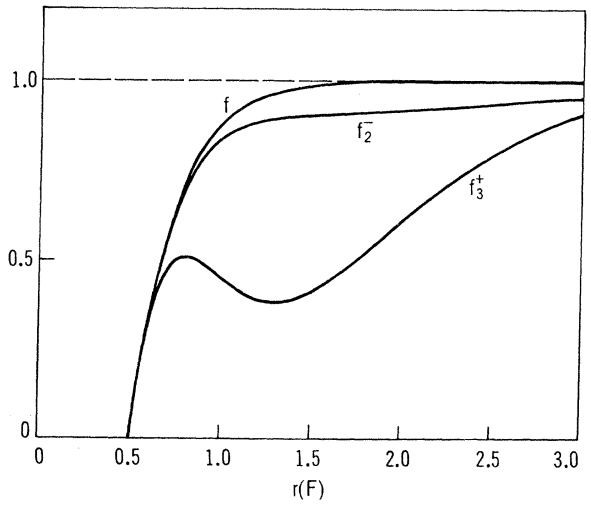

FIG. 3. Correlation functions for the potential denoted 5100, determined at $k_F = 1.4\ \mathrm{F}^{-1}$ by the simple minimization procedure, plotted against radial coordinate r.

of their kinship to the direct ring contributions of the Brueckner-Goldstone expansion).[24]

(b) Pauli condition on the two-body wave function $f\phi_{ij}$:

$$(\phi_{ij} - f\phi_{ij}, \phi_{kl}) = 0, \tag{35}$$

with i, j, k, l all Fermi-sea orbitals. In other words, the defect function $\phi_{ij} - f\phi_{ij}$ should have no components in the Fermi sea. This condition, with $ij = kl$, again may be imposed for an "average" pair, or it may be averaged over the Fermi sea.

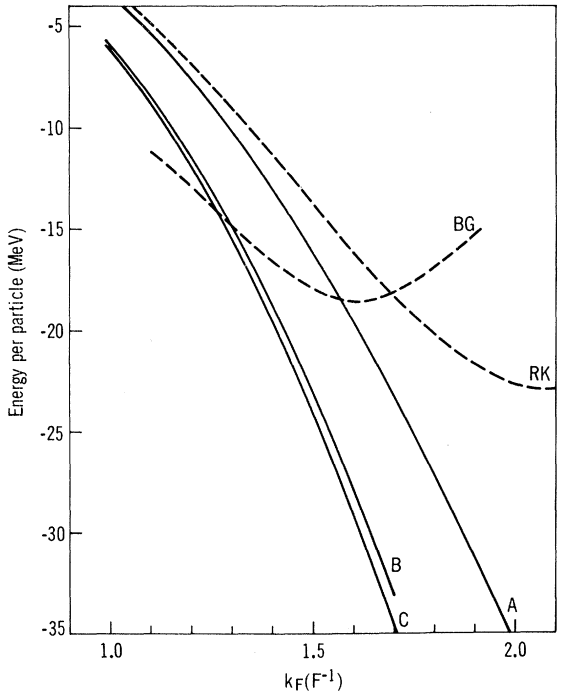

FIG. 4. Calculated energy per particle of nuclear matter for the potential denoted GCT, plotted against the Fermi wave number k_F. Curve A: Minimum value of $\mathcal{E}^{(2)}$ from step (a) of the simple minimization procedure (ordinary Jastrow result, for the "over-all," state-independent correlation factor). Curve B: Minimum value of $\mathcal{E}^{(2)}$ from step (b) of the simple minimization procedure (result of the Jastrow method generalized to treat even-state correlation effects due to the tensor component and spin dependence of central component). Curve C: Minimum value of $\mathcal{E}^{(2)}$ from step (c) of the simple minimization procedure (result of the Jastrow method generalized to treat both even- and odd-state correlation effects due to the tensor component and spin dependence of central component). Curve BG: Energy per particle calculated with the Brueckner method (tensor and spin-dependent correlations present; compare with curve C). Curve RK: Energy per particle calculated with the unitary-model-operator method (tensor and spin-dependent correlations absent; compare with curve A). (In cases A–C, correlation parameters appropriate to $k_F = 1.4$ F^{-1} were used. Only slight modifications would be produced by minimization at each k_F.)

It is motivated by the desire for as close a correspondence as possible with the Brueckner method.[6] Correspondingly, this constraint may be shown to have the effect of suppressing certain higher-order cluster contributions (called Pauli corrections because of their kinship to the Pauli corrections of the Moszkowski-Scott approach[25]).[26]

It is interesting that simultaneous imposition of constraints (a) and (b) leads [because of the fact that $f^2 - 1 = (f-1)^2 + 2(f-1)$] to the *vanishing* of the Jastrow analog of the "smallness parameter" κ of Brueckner-Bethe-Goldstone or compact-cluster-expansion theory.[4,6]

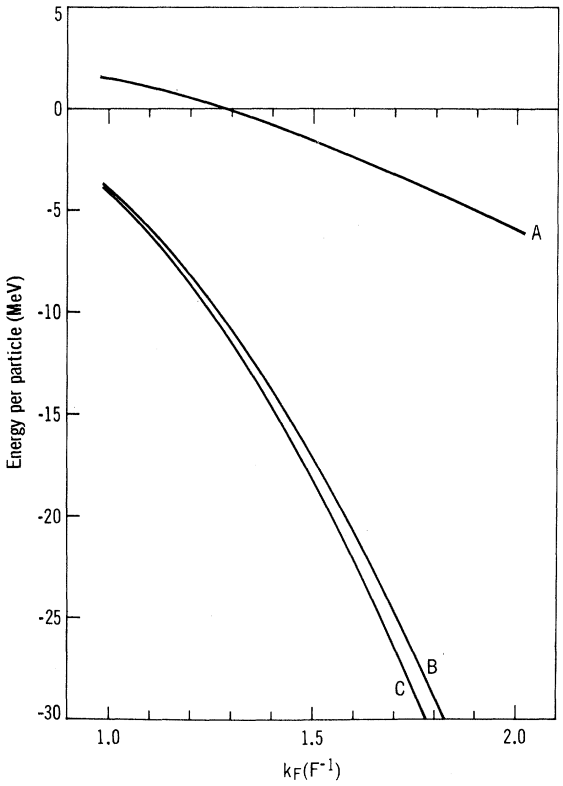

FIG. 5. Calculated energy per particle of nuclear matter for the potential denoted 5200, plotted against the Fermi wave number k_F. Curve A: Minimum value of $\mathcal{E}^{(2)}$ from step (a) of the simple minimization procedure (ordinary Jastrow result, for the "over-all," state-independent correlation factor). Curve B: Minimum value of $\mathcal{E}^{(2)}$ from step (b) of the simple minimization procedure (result of the Jastrow method generalized to treat even-state correlation effects due to the tensor component and spin dependence of central component). Curve C: Minimum value of $\mathcal{E}^{(2)}$ from step (c) of the simple minimization procedure (result of the Jastrow method generalized to treat both even- and odd-state correlation effects due to the tensor component and spin dependence of central component). (In cases A–C, correlation parameters appropriate to $k_F = 1.4$ F^{-1} were used. Only slight modifications would be produced by minimization at each k_F.)

One or more restrictions of this kind may well provide a remedy to the poor high-density behavior of the generalized Jastrow treatment revealed in the results of Sec. IV. Such conditions will, indeed, force a density dependence on the parameters λ, $\lambda^{\pm}$, $\alpha^{\pm}$ which aids saturation. However, it is our conviction that one must always test the efficacy of subsidiary conditions with respect to improvement of cluster convergence by detailed examination of the assessible higher-order corrections, especially the three-body contribution—as was done for the ordinary Jastrow method by Chakkalakal[6] [for restriction (b), and to some extent, restriction (a)]. (It is not enough just to impose some intuitively motivated subsidiary condition, calculate $\mathcal{E}^{(2)}$, and trust to luck.) Work in this direction is in progress; the results will be the subject of the next paper in this series. Underlying our work on the three-body correction is the following important question: In view of the fact that the optimally determined tensor correlations will typically be of rather long range, will one be faced with *intrinsically* poor convergence of the cluster expansion in any attempt at an accurate evaluation of the energy per particle by the extended Jastrow method? (By optimally determined, we mean determined by a hypothetical variation of $\mathcal{E}$ as a whole with respect to the f functions.) The implications of a positive answer would be ominous, not only for our approach, but for other cluster-expansion approaches as well, including the Brueckner-Bethe-Goldstone method.

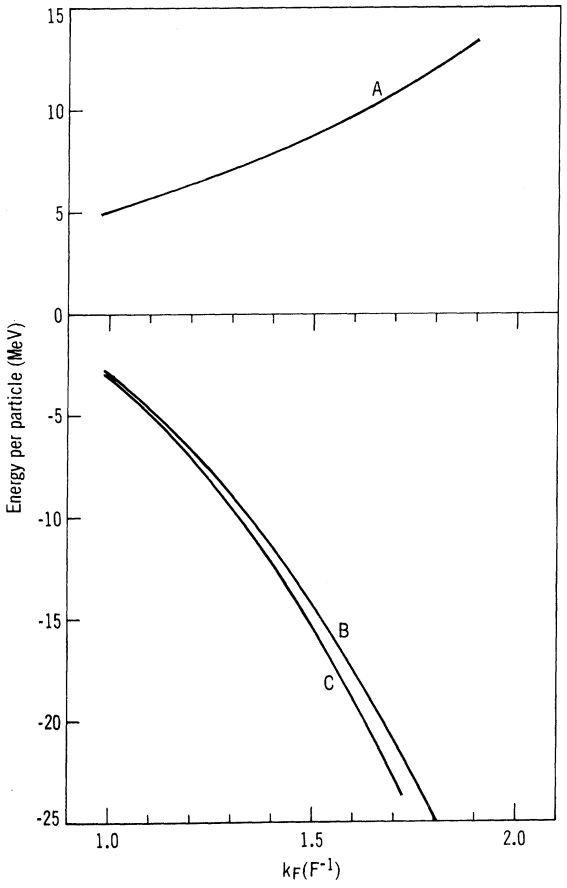

FIG. 6. Calculated energy per particle of nuclear matter for the potential denoted 5100, plotted against the Fermi wave number k_F. Curve A: Minimum value of $\mathcal{E}^{(2)}$ from step (a) of the simple minimization procedure (ordinary Jastrow result, for the "over-all," state-independent correlation factor). Curve B: Minimum value of $\mathcal{E}^{(2)}$ from step (b) of the simple minimization procedure (result of the Jastrow method generalized to treat even-state correlation effects due to the tensor component and spin dependence of central component). Curve C: Minimum value of $\mathcal{E}^{(2)}$ from step (c) of the simple minimization procedure (result of the Jastrow method generalized to treat both even- and odd-state correlation effects due to the tensor component and spin dependence of central component). (In cases A–C, correlation parameters appropriate to $k_F = 1.4$ F^{-1} were used. Only slight modifications would be produced by minimization at each k_F.)

A number of fairly obvious improvements can be made in the choice of f functions of Sec. IV and (more immediately) in the procedure used there for determining correlation-function parameters. In particular, the treatment of short-range correlations can surely be improved: For example, one may allow f_2^+ to deviate from f. Or one may augment steps (a)–(c) of Sec. IV with:

(d) Using the values of $\lambda^{\pm}$, $\alpha^{\pm}$ found in steps (b) and (c), λ is redetermined by minimization of $\mathcal{E}^{(2)}$ with respect to this parameter.

Thereby, the tensor component and the spin and parity dependence of the central component of the potential are permitted to influence the "over-all" correlation function. Such improvements may be of special importance for potential 5100, which has a strong even-state tensor component of the same range as the triplet-even central component and a strongly spin-dependent even-state central component, and could be of some importance for GCT as well, since this potential also has a strongly spin-dependent even-state central component. Thus our results for the dependence of $\mathcal{E}^{(2)}$ on the "central-to-tensor ratio" may be subject to alteration (even near the physical density, where the higher cluster corrections to the results of Sec. IV are probably not yet large). Indeed, it may turn out that the appreciable tensor-suppression effect indicated by the present calculation is attributable in significant measure to greater suitability of our choice of correlation functions for potentials with weak, long-range tensor components than for potentials with strong, short-range tensor components. However, we

shall defer any refinement of our recipe for the short-range correlations until a proper treatment of the more dangerous long-range correlations, i.e., a treatment of these correlations derived from an understanding of the higher-order cluster corrections, is at hand. (In the framework of the present calculation, such refinements would only make matters a bit worse with regard to saturation.)

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