and

$$S_{j,l}^{\mathrm{HF}}(\epsilon(k)) = 1 - 2\pi i\, T_{j,l}(\epsilon(k)), \tag{A15}$$

where

$$T_{j,l} = \int dr\, dr'\, r^2 r'^2 \left(\frac{2mk}{\pi\hbar^2}\right)^{1/2} j_l(k, r) \mathcal{V}_{l,j}^{\mathrm{HF}}(r, r') R_{l,j}{}^{\dagger}(k, r') . \tag{A16}$$

Here the total Hartree-Fock Hamiltonian is assumed to have a form

$$\mathcal{V}_{l,j}^{\mathrm{HF}}(\vec{\mathrm{r}}, \vec{\mathrm{r}}') = \sum_{j,\mu,l} \mathcal{Y}_{j,\mu,l}(\hat{r}) \mathcal{Y}_{j,\mu,l}{}^{\dagger}(\hat{r}') \mathcal{V}_{j,l}^{\mathrm{HF}}(r, r') . \tag{A17}$$

Further Clebsch-Gordan algebra useful in simplifying (A13) may be done; however, we shall not pursue this avenue.

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Brueckner Reaction Matrix and Separable Potentials

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The binding energy of He^4 and O^{16} was calculated using reaction matrix elements of Tabakin's potential. A separable form of the potential has been used to reduce the basic equation to a simple linear algebraic system. The Pauli operator Q defined in terms of harmonic-oscillator intermediate states permits an easy and accurate calculation. Our numerical results for the binding energies include the first- and second-order contributions. A very resonable agreement between the experimental and theoretical values has been obtained, since the occupied-state energies are made nearly self-consistent and a cancellation of other important higher-order contributions has been achieved by a shift of the entire harmonic-oscillator spectra.

I. INTRODUCTION

A uniform description of the free nucleon-nucleon scattering and nuclear-structure data belongs apparently to the most important and very popular problems in present-day nuclear theory. It is now well known that the Brueckner reaction matrix t should be introduced in the nuclear-structure calculations rather than the free N-N interaction v. The idea is to treat the interaction inside the particle pairs ("two-body cluster") to all orders before letting any of the particles from the pair interact with the remaining particles. New progress is understanding the nature of Brueckner's perturbation expansion was provided recently in articles by Rajaraman and Bethe[1] and Brandow,[2] where earlier references can also be found.

The t matrix can be defined by the operator equation

$$t = v - v\frac{Q}{e}t, \tag{1}$$

where the Pauli operator Q prevents scattering into the occupied states, and the energy denominator e stands for the difference between intermediate and starting energies: $e = H_{12} - E_s$.

The reference-spectrum method[3] has proved to be the most useful approximation in solving Eq. (1). One introduces a simple expression Q^R/e^R (where $Q^R = 1$ is a frequent choice) and defines the reference matrix t^R by

$$t^R = v - v\frac{Q^R}{e^R}t^R. \tag{2}$$

By iterating the exact relation

$$t = t^R - t^R\left(\frac{Q}{e} - \frac{Q^R}{e^R}\right)t, \tag{3}$$

a perturbation expansion for the t matrix in powers of t^R originates. The method is practicable if the first two terms of the expansion provide a sufficiently accurate result.

At present, two types of free-nucleon interactions are available, which are derived from the experimental scattering data:

(1) The realistic potentials with infinite repulsive cores such as the Yale, Hamada-Johnston, and Reid potentials enjoy a great popularity mainly because of their correct (from the point of view of the mesonic theory) asymptotic behavior and extremely good fit to the scattering data.

(2) The nonlocal potentials which describe dynamically the N-N repulsion at short separation distances constitute another widely accepted class of realistic nucleon-nucleon interactions. Tabakin's[4] separable potential, being fitted with a very reasonable accuracy to the scattering phase shifts up to 320 MeV, is, so far, probably the best of the given class.

It has been pointed out as a result of numerous calculations,[5,6] that Tabakin's and other realistic potentials are to a great extent equivalent from the point of view of nuclear-structure investigations. A comparison of the relative-motion matrix elements of Tabakin's potential with those extracted directly from the experimental phase shifts by Elliott *et al.*[7] show a striking similarity as well.

The recent nuclear t-matrix studies by Kuo and Brown[8] and Wong[9] have been performed with the Hamada-Johnston potential. It is felt, however, that the original ambitious program of investigating such a complicated potential in the Brueckner theory could be diminished considerably by the computing difficulties. In particular, a rather crude treatment of the Pauli operator Q ($Q^R = 1$) in Refs. 8 and 9 should be mentioned here. Becker, MacKellar, and Morris[10] observed, when comparing Wong's[9] results with their own calculation, that the use of the rather accurate Eden-Emery[11] approximation Q^{EE} for Q^R in the reference-matrix calculation has a greater effect than the use of the same Q^{EE} in calculating correction terms to t^R obtained with $Q^R = 1$. Moreover, a slow convergence of the t-matrix expansion in powers of t^R has been found by Bhargava and Sprung[12] in a nuclear-matter calculation with $Q^R = 1$. A similar situation would be expected in finite nuclei.

In the present approach, we would like to introduce the Pauli operator Q in the most accurate way, stating clearly all the approximations with the aim of calculating the corresponding correction terms according to Eq. (3) later. Because of the mentioned equivalence of the realistic potentials, we have chosen the Tabakin potential for calculating the t matrix elements in the He^4 and O^{16} nuclei. Using the separability of the Tabakin interaction, Eq. (1) reduces to a system of linear algebraic equations, instead of much more complicated integrodifferential or differential equations which arise in the case of local potentials with static repulsion.

Of course, Tabakin's potential can be formally used in the nuclear-structure calculation even in its bare form. From the physical consideration it is clear, however, that at least corrections for the multiple-scattering processes must be included in this case. The problem has been investigated up to the second order in Hartree-Fock bases by Bassichis and Strayer.[13] They used a truncated but very large configuration space, and the calculation can, in this respect, be considered complete for light nuclei. Their results are twofold: (i) Total second-order correction to the binding energy is comparable or even larger than the first-order term (Hartree-Fock energy), and (ii) the most important contributions to the second-order term originate from the intermediate states lying as high as $6\hbar\omega$ and $8\hbar\omega$.

Consequently, there is no good reason to expect small third- and higher-order terms, and the calculation of the reaction matrix, which represents a sum of all higher-order processes, seems to be inevitable.

The problems of the single-particle (s.p) basis states in the Brueckner theory are briefly reviewed in Sec. II. Our choice of the harmonic-oscillator s.p. basis is supported mainly by the possibility of an accurate representation for Pauli projection operator Q, which is introduced in Sec. III. In Sec. IV, the basic equations are derived. The accuracy of our numerical procedures is discussed in Sec. V, and the final results for the binding energy in He^4 and O^{16} together with the most important conclusions are given in Sec. VI.

II. BASIS STATES

Brueckner's approximation to the ground-state binding energy in the first order [Fig. 1(a)] is given by

$$E^{(1)} = \sum_{\vec{h}}^{\text{occ}} \langle \vec{h} | T | \vec{h} \rangle + \frac{1}{2} \sum_{\vec{h}_1 \vec{h}_2}^{\text{occ}} \langle \vec{h}_1 \vec{h}_2 | t(E_{12}) | \vec{h}_1 \vec{h}_2 \rangle , \tag{4}$$

where T symbolizes the kinetic-energy operator, the s.p. states are labeled by a set of quantum numbers $\vec{n}_i \equiv (n_i, l_i, j_i, m_i, \tau_i)$, and the summation is over the occupied states. All our two-body matrix elements are antisymmetrized. The reliability of the lowest approximation [Eq. (4)] depends on the choice of the s.p. basis used in calculating the t matrix.

Definition of the Hamiltonian for a system of A particles

$$H = -\frac{\hbar^2}{2} \sum_{i=1}^{A} \frac{\nabla_i^2}{M_i} + \frac{1}{2} \sum_{i \neq j}^{A} v(i,j) = \sum_{i=1}^{A} T_i + V , \tag{5}$$

may be rewritten in the usual way as

$$H = H_0 + (V - \sum_{i=1}^{A} U_i) , \tag{6}$$

with

$$H_0 = \sum_{i=1}^{A} H_0(i) = \sum_{i=1}^{A} (T_i + U_i) , \tag{7}$$

where U_i is an external potential.

For further calculation, it is essential to perform transformation from the individual-particle basis into the relative and the center-of-mass (r.c.m.) coordinate systems. It can be done in a simple way for two cases only.

(1) Free state spectrum (plane waves)

$$e^{i(\vec{k}_1 \cdot \vec{r}_1 + \vec{k}_2 \cdot \vec{r}_2)} = e^{i(\vec{k} \cdot \vec{r} + \vec{K} \cdot \vec{R})} , \tag{8}$$

with

$$\vec{k} = (\vec{k}_1 - \vec{k}_2)/\sqrt{2} , \quad \vec{r} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2} ,$$
$$\vec{K} = (\vec{k}_1 + \vec{k}_2)/\sqrt{2} , \quad \vec{R} = (\vec{r}_1 + \vec{r}_2)/\sqrt{2} , \tag{9}$$

appears naturally in the nuclear matter t matrix. It has also been frequently used for the intermediate states in finite nuclei. To do it consistently, the procedure must include an orthogonalization of the continuum states to the low-lying localized states as well as new continuum states among themselves.[9, 10] As far as we know, such a program has never yet been performed. Another drawback of the plane-wave basis in the finite-nuclei t-matrix calculation is a rather difficult and less transparent treatment of the Pauli exclusion principle (see also Sec. III).

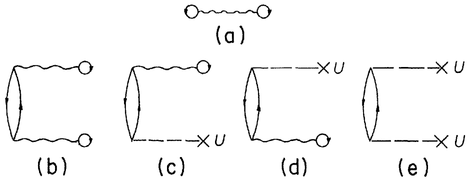

FIG. 1. First- and second-order Brueckner-Goldstone diagrams.

(2) The harmonic-oscillator (h.o.) basis has become rather popular in the most recent t-matrix studies, in both nuclear matter[14] and finite nuclei.[10, 15, 16] It is also the choice adopted in the present paper. An L-S vector-coupled pair function of h.o. orbitals can be transformed into the r.c.m. system, Eq. (9) by

$$| n_1 l_1, n_2 l_2; LSM_L M_S \rangle = \sum_{nl\mathfrak{N}\mathfrak{L}} (nl, \mathfrak{N}\mathfrak{L}; L | n_1 l_1, n_2 l_2; L \rangle | nl, \mathfrak{N}\mathfrak{L}; LSM_L M_S) , \tag{10}$$

where n, l, $\mathfrak{N}$, $\mathfrak{L}$ stand for principal and orbital quantum numbers of the relative and the c.m. motion, respectively. Transformation coefficients $(nl, \mathfrak{N}\mathfrak{L}; L | n_1 l_1, n_2 l_2; L\rangle$ were tabulated by Brody and Moshinsky.[17] Round brackets symbolize r.c.m. states, angular brackets the individual particle states.

In accordance with Refs. 10, 15, and 16, we follow systematically the procedure suggested by Eden and Emery[11] and modify the energy spectrum of the h.o. Hamiltonian in such a way that all properties of s.p. wave functions, including that of Eq. (10), are preserved. The modification consists in assuming for the s.p. Hamiltonian of ith particle the form

$$H_0(i) = T_i + U_i^{\text{h.o.}} - \sum_{\vec{h}}^{\text{occ}} \eta_h | \vec{h} \rangle \langle \vec{h} | - C , \tag{11}$$

where $T_i + U_i^{\text{h.o.}} = H_i^{\text{h.o.}}$ is the usual h.o. Hamiltonian, h stands for n and l quantum numbers of the s.p. state $\vec{h}$ below the Fermi sea, and the state vector $|\vec{h}\rangle$ is the same for both $H_i^{\text{h.o.}}$ and $H_0(i)$. According to the above choice, all the states of the h.o. spectrum are shifted by a constant amount C. An additional state-dependent shift η_h applies to the occupied states only.

Many higher-order contributions to the binding energy may be included already in the first order, if the parameters C and η_h are appropriately chosen, S.p. states below and above the Fermi sea should be considered separately as discussed below.

(i) The most preferable choice for the occupied s.p. states consists of calculating the Hartree-Fock energies with a s.p. potential satisfying Brueckner self-consistency. Then the terms with bubble and potential insertions in hole lines [Figs. 2(a), 2(b)] cancel each other; in particular, all second-order processes, Figs. 1(b)–1(e), give zero total contribution.

Energy shifts in the hole states defined by the self-consistent condition

$$\begin{aligned}\langle\vec{\mathrm{h}}|U|\vec{\mathrm{h}}\rangle&=\langle\vec{\mathrm{h}}|U^{\mathrm{h.o.}}|\vec{\mathrm{h}}\rangle-\eta_h-C\\&=\sum_{\vec{\mathrm{h}}'}^{\mathrm{occ}}\langle\vec{\mathrm{h}}\vec{\mathrm{h}}'|t(E_{hh'})|\vec{\mathrm{h}}\vec{\mathrm{h}}'\rangle\end{aligned}\tag{12}$$

together with the t-matrix definition, Eq. (1), cause cancellation of diagonal insertions into hole lines only. Complete self-consistency including off-diagonal insertion would require refraining from using the h.o. wave functions. In particular, all the second-order diagrams, Figs. 1(b)–1(e), must and will be calculated in our approach. Since the right-hand side of Eq. (12) depends on the individual j_h quantum numbers, the spin-orbit splitting has been removed in calculating η_h.

(ii) Such a choice is not suitable when treating insertions in particle lines, since the bubble-insertion diagrams of Fig. 2(c) is a part of the three-body cluster term, which absorbs several apparently large contributions. Their sum is usually expected to be small, following an analogy with infinite nuclear matter.[1]

The theoretically interesting result of Köhler,[18] that the potential insertions in particle lines are included to all orders by defining

$$t(E_S)=v-v\frac{Q}{QTQ-E_S}t(E_S)\,,\tag{13}$$

instead of the usual expression

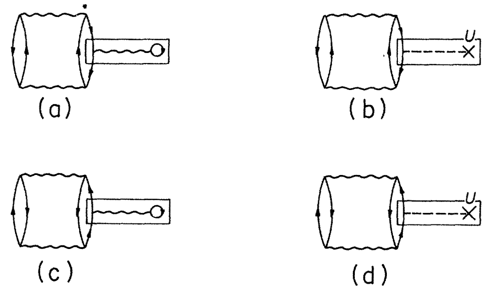

FIG. 2. Third-order Brueckner-Goldstone diagrams used for modification of harmonic-oscillator spectra.

$$t(E_S)=v-v\frac{Q}{H_1^{\mathrm{ind}}+H_2^{\mathrm{ind}}-E_S}t(E_S)\,,\tag{14}$$

is unfortunately not easy to apply in calculation, because Eq. (13) cannot be properly solved without many additional approximations. Therefore, we attempt here rather to minimize the contributions of diagrams with the potential inserted into the particle line by an appropriate choice of the constant C. The most important graph of this type seems to be the one given in Fig. 2(d). The corresponding contribution to the binding energy can be written as[16]

$$\begin{aligned}\overline{\Delta E}^{(3)}=\frac{1}{4}&\sum_{\vec{\mathrm{h}}_1\vec{\mathrm{h}}_2}^{\mathrm{occ}}\sum_{\vec{\mathrm{a}}\vec{\mathrm{b}}\vec{\mathrm{c}}\vec{\mathrm{d}}}^{\mathrm{unocc}}\langle\vec{\mathrm{h}}_1\vec{\mathrm{h}}_2|t(E_S)|\vec{\mathrm{a}}\vec{\mathrm{b}}\rangle\\&\times\frac{1}{E_{ab}-E_s}\{\langle\vec{\mathrm{a}}|U|\vec{\mathrm{c}}\rangle\delta_{\vec{\mathrm{b}}\vec{\mathrm{d}}}+\langle\vec{\mathrm{b}}|U|\vec{\mathrm{d}}\rangle\delta_{\vec{\mathrm{a}}\vec{\mathrm{c}}}\}\\&\times\frac{1}{E_{cd}-E_s}\langle\vec{\mathrm{c}}\vec{\mathrm{d}}|t(E_s)|\vec{\mathrm{h}}_1\vec{\mathrm{h}}_2\rangle\,,\end{aligned}\tag{15}$$

where

$$E_s=E_{h_1}^{\mathrm{h.o.}}+E_{h_2}^{\mathrm{h.o.}}-2C-\eta_{h_1}-\eta_{h_2}\,.$$

The contribution of the simplest diagram which contains only excitations of order $2\hbar\omega$ is exactly zero with

$$C=(2n_p+l_p+\tfrac{3}{2})\hbar\omega/2\,,\tag{16}$$

where n_p and l_p stand for the quantum numbers of the lowest unoccupied state, i.e., one which enters only into the considered diagram ($0p$ for He^4, $1s0d$ for O^{16}).

Our choice for the constant C can be compared with the one adopted by Becker, MacKellar, and Morris.[10] The last-named authors put an additional condition, $\eta_{0s}=2\eta_{0p}$, in their O^{16} calculation. Then both η_{0s} and C can be calculated from the Brueckner-Hartree-Fock Eqs. (12) and (14). It implies almost twice as large a value for C as that given by Eq. (16), and the resulting energy gap between the occupied and unoccupied s.p. states seems to be underestimated.

III. PAULI PROJECTION OPERATOR

The exclusion principle represented by the Pauli projection operator

$$Q=\sum_{\vec{\mathrm{p}}\vec{\mathrm{r}}}^{\mathrm{unocc}}|\vec{\mathrm{p}}\vec{\mathrm{r}}\rangle\langle\vec{\mathrm{p}}\vec{\mathrm{r}}|\,,\tag{17}$$

introduces tremendous complications into reaction-matrix calculations for finite nuclei. Both $Q^R=1$ and the angle-average approximation borrowed from the nuclear matter calculations have been frequently chosen in earlier investigations[8,9] performed with plane-wave intermediate states.

The most advantageous property of a h.o. basis is probably the possibility of a simple and accurate approximation for the operator Q, which carries the main bulk of the exclusion effects and permits an easy evaluation of the corresponding correction terms. Moreover, the expression we derive below can be considerably simplified, and still retain good accuracy. The latter approximation was suggested by Eden and Emery[11]; a comparison of the results corresponding to Q^{EE} with our more accurate treatment is presented in Sec. V. A Pauli operator defined in terms of oscillator states has also been used together with a free-particle plane-wave spectrum.[9]

In the h.o. basis, Eq. (10), and with modified energy spectra implied by the Hamiltonian, Eq. (11), we have for the propagator

$$\frac{Q}{e^R} = \sum_{pr}^{\text{unocc}} \sum_{LSM_LM_S} \frac{|n_pl_p, n_rl_r; LSM_LM_S\rangle\langle n_pl_p, n_rl_r; LSM_LM_S|}{E_{pr} - E_s}$$

$$= \sum_{pr}^{\text{unocc}} \sum_{1,2} \sum_{LSM_LM_S} (n_1l_1, \mathfrak{N}_1\mathcal{L}_1; L|n_pl_p, n_rl_r; L\rangle\langle n_pl_p, n_rl_r; L|n_2l_2, \mathfrak{N}_2\mathcal{L}_2; L)$$

$$\times \frac{|n_1l_1, \mathfrak{N}_1\mathcal{L}_1; LSM_LM_S)(n_2l_2, \mathfrak{N}_2\mathcal{L}_2; LSM_LM_S|}{E. - E}, \tag{18}$$

where $\sum_{pr}$ goes over n_p, l_p, n_r, and l_r, $\sum_i$ goes over n_i, l_i, $\mathfrak{N}_i$, and $\mathcal{L}_i$ with $i = 1, 2$. The energy E_{pr} of the intermediate state depends in our model Eq. (11), on the shell number $\rho_{pr} = 2n_p + l_p + 2n_r + l_r$. Omitting throughout the additive constant $3\hbar\omega$, we have

$$E_{pr} = (2n_p + l_p + 2n_r + l_r)\hbar\omega - 2C = (2n_1 + l_1 + 2\mathfrak{N}_1 + \mathcal{L}_1)\hbar\omega - 2C\,. \tag{19}$$

Transformation to a relative J representation where $\vec{l}_i + \vec{S} = \vec{J}_i$, $i = 1, 2$ gives

$$\frac{Q}{e^R} = \sum_{\substack{1,2\\ \mathfrak{M}_1\mathfrak{M}_2}} \sum_{\substack{J_1M_1J_2M_2\\ S}} \frac{|n_1l_1SJ_1M_1, \mathfrak{N}_1\mathcal{L}_1\mathfrak{M}_1)(n_2l_2SJ_2M_2, \mathfrak{N}_2\mathcal{L}_2\mathfrak{M}_2|}{(2n_1 + l_1 + 2\mathfrak{N}_1 + \mathcal{L}_1)\hbar\omega - 2C - E_s}$$

$$\times (n_1l_1SJ_1M_1, \mathfrak{N}_1\mathcal{L}_1\mathfrak{M}_1|\hat{Q}|n_2l_2SJ_2M_2, \mathfrak{N}_2\mathcal{L}_2\mathfrak{M}_2)\,, \tag{20}$$

where the matrix elements of $\hat{Q}$ include the summation of the Clebsch-Gordan coefficients

$$(1|\hat{Q}|2) = \sum_{pr}^{\text{unocc}} \sum_{L} (n_1l_1, \mathfrak{N}_1\mathcal{L}_1; L|n_pl_p, n_rl_r; L\rangle\langle n_pl_p, n_rl_r; L|n_2l_2, \mathfrak{N}_2\mathcal{L}_2; L)$$

$$\times\Big\{\sum_{m_1m_2M_LM_S} (l_1\mathcal{L}_1m_1\mathfrak{M}_1|LM_L)(l_1Sm_1M_S|J_1M_1)(l_2\mathcal{L}_2m_2\mathfrak{M}_2|LM_L)(l_2Sm_2M_S|J_2M_2)\Big\}\,. \tag{21}$$

The exact expression in Eq. (20) of the Q/e^R propagator is nondiagonal in all the quantum numbers of both the relative and c.m. motions including the relative-motion total momentum J. Two approximations adopted in the present investigation are:

(i) We keep only terms diagonal in the c.m.-motion quantum numbers, i.e., $\mathfrak{N}_1 = \mathfrak{N}_2 = \mathfrak{N}$, $\mathcal{L}_1 = \mathcal{L}_2 = \mathcal{L}$, and $\mathfrak{M}_1 = \mathfrak{M}_2 = \mathfrak{M}$ in the model operator Q^R.

(ii) Since the matrix elements of Q^R still depend on the projections $\mathfrak{M}$, we use their average value Calculation of the average applies only to expression in braces of Eq. (21) with the result

$$\frac{1}{2\mathcal{L}+1}\sum_{\mathfrak{M}}\Big\{\quad\Big\} = \frac{2L+1}{(2l_1+1)(2\mathcal{L}+1)}\,\delta_{l_1l_2}\,\delta_{J_1J_2}\,\delta_{M_1M_2}. \tag{22}$$

It follows from the assumption (i), Eq. (22), and from the properties of the Brody-Moshinsky transformation brackets that also $n_1 = n_2 = n$. Then the final expression for the operator Q^R/e^R is

$$\frac{Q^R}{e^R} = \sum_{\substack{nl\mathfrak{N}\mathcal{L}\mathfrak{M}\\ SJM}} \frac{|nlSJM, \mathfrak{N}\mathcal{L}\mathfrak{M})(nlSJM, \mathfrak{N}\mathcal{L}\mathfrak{M}|}{(2n + l + 2\mathfrak{N} + \mathcal{L})\hbar\omega - 2C - E_s}\, A_{nl}^{\mathfrak{N}\mathcal{L}}\,, \tag{23}$$

where

$$A_{nl}^{\mathfrak{N}\mathfrak{L}} = \sum_{\substack{n_p l_p n_r l_r \\ L}} \frac{2L+1}{(2l+1)(2\mathfrak{L}+1)} (nl, \mathfrak{N}\mathfrak{L}; L \,|\, n_p l_p, n_r l_r; L)^2 . \tag{24}$$

IV. REACTION MATRIX IN AN OSCILLATOR BASIS

Equation (14) can be rewritten with the operator Q^R/e^R given by Eq. (23) in a matrix representation by

$$\begin{aligned}(nlSJM, \mathfrak{N}\mathfrak{L}\mathfrak{M} \,|\, t^R(E_s) \,|\, n'l'S'J'M', \mathfrak{N}'\mathfrak{L}'\mathfrak{M}') &= (nlSJ \,|\, v \,|\, n'l'SJ)\, \delta(SJM\mathfrak{N}\mathfrak{L}\mathfrak{M}; S'J'M'\mathfrak{N}'\mathfrak{L}'\mathfrak{M}') \\ &\quad - \sum_{n_1 l_1} A_{n_1 l_1}^{\mathfrak{N}\mathfrak{L}} \frac{(nlSJ \,|\, v \,|\, n_1 l_1 SJ)(n_1 l_1 SJM, \mathfrak{N}\mathfrak{L}\mathfrak{M} \,|\, t^R(E_s) \,|\, n'l'S'J'M', \mathfrak{N}'\mathfrak{L}'\mathfrak{M}')}{(2n_1 + l_1 + 2\mathfrak{N} + \mathfrak{L})\hbar\omega - 2C - E_s} ,\end{aligned} \tag{25}$$

where

$$\begin{aligned}\delta(i_1 \cdots i_n; j_1 \cdots j_n) &= 1 \quad \text{if } i_k = j_k, k = 1, \ldots, n \\ &= 0 \quad \text{otherwise.}\end{aligned}$$

With $\delta(SJM\mathfrak{N}\mathfrak{L}\mathfrak{M}; S'J'M'\mathfrak{N}'\mathfrak{L}'\mathfrak{M}') = 0$, the inhomogeneous equations (25) degenerate into a homogeneous system which has zero as its only solution; we conclude, therefore, that the (nonzero) t^R matrix elements are diagonal in quantum numbers SJM and $\mathfrak{N}\mathfrak{L}\mathfrak{M}$, and obey the equation

$$(nlSJ \,|\, t^R(E_s) - v \,|\, n'l'SJ) = -\sum_{n_1 l_1} A_{n_1 l_1}^{\mathfrak{N}\mathfrak{L}} \frac{(nlSJ \,|\, v \,|\, n_1 l_1 SJ)(n_1 l_1 SJ \,|\, t^R(E_s) \,|\, n'l'SJ)}{(2n_1 + l_1 + 2\mathfrak{N} + \mathfrak{L})\hbar\omega - 2C - E_s} . \tag{26}$$

The t^R-matrix diagonal in the SJT quantum numbers originates from the interaction diagonal in them; on the other hand, the diagonality in the c.m. motion has been assumed by us explicitly, and the accuracy of such a model must be investigated.

The method of solution of Eq. (26) is based on the separability of Tabakin's potential. Matrix elements in relative coordinates are of the form

$$(nl\,SJ \,|\, v^{\text{Tabakin}} \,|\, n'l'SJ) = \sum_{i=1}^{2} \xi_i G_{nlSJ}^{(i)} G_{n'l'SJ}^{(i)} , \tag{27}$$

where the two terms in the sum on the right-hand side represent the repulsive and attractive parts of interaction according to whether $\xi = \pm 1$. Detailed formulas for the corresponding radial intergrals $G_{nlSJ}^{(i)}$ can be found in Ref. 5.

Introducing a 2×2 matrix

$$W_{ij} = \sum_{n_1 l_1} \xi_j \frac{G_{n_1 l_1 SJ}^{(i)} G_{n_1 l_1 SJ}^{(j)} A_{n_1 l_1}^{\mathfrak{N}\mathfrak{L}}}{(2n_1 + l_1 + 2\mathfrak{N} + \mathfrak{L})\hbar\omega - 2C - E_s} , \tag{28}$$

we can write a linear algebraic system

$$x^{(i)} + \sum_{j=1}^{2} W_{ij} x^{(j)} = \sum_{j=1}^{2} W_{ij} G_{n'l'SJ}^{(j)} , \tag{29}$$

for the coefficients $x^{(i)} \equiv x_{n'l'SJ\mathfrak{N}\mathfrak{L}}^{(i)}$, $i = 1, 2$ which enter the final formula for calculating our t^R matrix elements

$$(nlSJ \,|^{\mathfrak{N}\mathfrak{L}}\, t^R(E_s) \,|\, n'l'SJ) = \sum_{i=1}^{2} \xi_i G_{nlSJ}^{(i)} (G_{n'l'SJ}^{(i)} - x_{n'l'SJ\mathfrak{N}\mathfrak{L}}^{(i)}) . \tag{30}$$

A concluding remark concerns the starting energy $E_s = (2n' + l' + 2\mathfrak{N} + \mathfrak{L})\hbar\omega - 2C - \eta_{h_1} - \eta_{h_2}$, since the trace of the individual-particle quantum numbers h_1 and h_2 has been formally lost in the Talmi-Moshinsky transformation to the r.c.m. system. This is not the case, however, for the lightest nuclei such as He^4 and O^{16}, which we consider here. With $\rho = 2n' + l' + 2\mathfrak{N} + \mathfrak{L}$, we have

ρ	$\eta_{h_1} + \eta_{h_2}$
0	$2\eta_{0s}$
1	$\eta_{0s} + \eta_{0p}$
2	$2\eta_{0p}$.

In more complicated nuclei, an additional approximation must be introduced at this point; e.g., an assumption that $2\eta_{0p} = \eta_{0s} + \eta_{1d0s}$ would be sufficient and probably appropriate for the Ca^{40} nucleus.

V. NUMERICAL PROCEDURE

The radial integrals $G_{nlSJ}^{(i)}$ of Tabakin's potential bave been calculated by the 15-point Gauss-

Laguerre quadrature formula. We use here modified parameters of the ${}^1P_1$-channel potential suggested by Baranger and Clement in Ref. 5.

The time-consuming calculation of the $A_{nl}^{\mathcal{N}\mathcal{L}}$ coefficients can be considerably shortened by employing the completeness of the Moshinsky-Brody brackets, since a sum complementary to that of Eq. (24) involves fewer terms and simpler transformation brackets.

In Fig. 3, some of the coefficients $A_{nl}^{\mathcal{N}\mathcal{L}}$ are plotted against the shell number for $l=0,1,2$ channels. It is clear from the figure that only a few coefficients need actually be calculated. The substitution $A_{nl}^{\mathcal{N}\mathcal{L}}=1$ becomes well justified rapidly with increasing shell number. Nevertheless, the different rates of convergence for various l channels should be emphasized.

As already noted, our approximation $A_{nl}^{\mathcal{N}\mathcal{L}}$ for the Pauli exclusion principle can be further simplified according to the suggestion by Eden and Emery.[11] They put

$$A_{nl}^{\mathcal{N}\mathcal{L}}=0 \quad \text{if } 2n+l+2\mathcal{N}+\mathcal{L}<\rho_{\min} \qquad (31)$$
$$=1, \quad \text{otherwise.}$$

The model can be visualized in Fig. 4, where circles and squares correspond to the states allowed and forbidden by the Pauli principle, respectively, and the shadowed areas indicate the states left out by the Eden-Emery method, with a different $\rho_{\min}$.

The binding energy of the O^{16} nucleus in the lowest order, together with some of the most important t matrix elements calculated in the model [Eq. (31)] should be compared with the "exact" results [$A_{nl}^{\mathcal{N}\mathcal{L}}$ from Eq. (24)] rather than with the experimental values, since a model interaction

$$G_{nlSJ}^{(i)}(\text{MODEL})=G_{nlSJ}^{(i)}(\text{TABAKIN}) \quad \text{if } 2n+l\leq 12 \qquad (32)$$
$$=0, \quad \text{otherwise,}$$

has been used in this case. Although the Eden-Emery-approximated matrix elements exhibit considerable deviations, both to smaller and larger values, from the exact results (column 6 of Table I), an integral effect represented by the binding energy is nicely approximated in the Eden-Emery method with $\rho_{\min}=5$. The model assumption, Eq. (32), clearly cannot be used apart from the de-

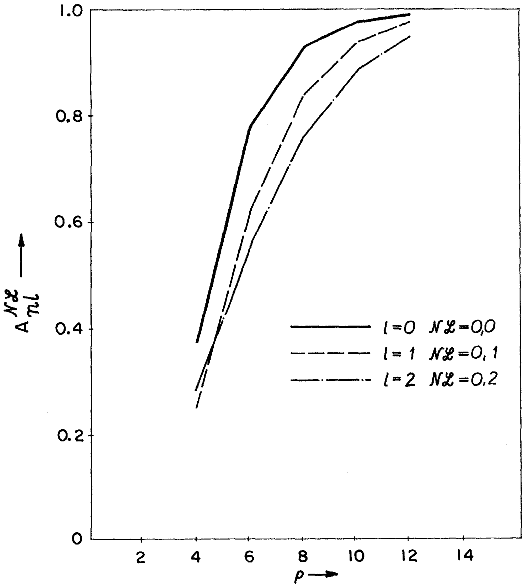

FIG. 3. Dependence of Pauli coefficients $A_{nl}^{\mathcal{N}\mathcal{L}}$ [Eq. (24)] on the shell number $\rho=2n+l+2\mathcal{N}+\mathcal{L}$ in O^{16}.

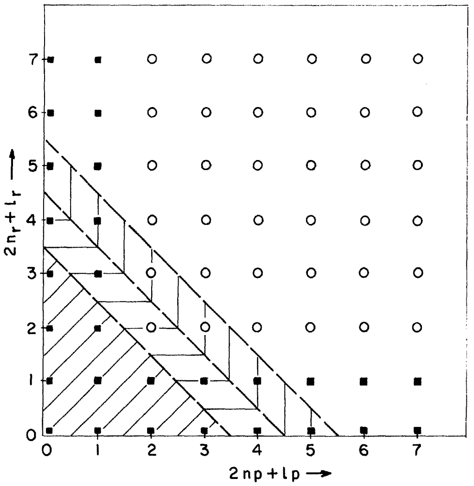

FIG. 4. The Eden-Emery approximation for the pair states in the O^{16} nucleus. The states allowed and excluded by the Pauli principle are indicated by circles and squares, respectively. The operator Q^{EE} permits scattering into states above one of the dashed diagonal lines.

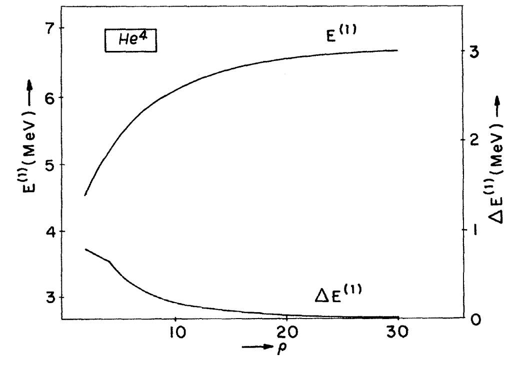

FIG. 5. First-order contribution to the He^4 binding energy plotted against number of intermediate states included in the sum of Eq. (28) and subsequent increments $\Delta E^{(1)}(\rho)=E^{(1)}(\rho)-E^{(1)}(\rho-2)$. The h.o. spring constant $b=1.3$ F. The right-hand-side scale applies to $\Delta E^{(1)}$.

scribed test of the Eden-Emery approximation, and all the results below correspond to the usual Tabakin interaction.

We show in Figs. 5 and 6 the dependence of $E^{(1)}$, the binding energy of He^4 and O^{16} nuclei in the lowest order, on the number of high-lying intermediate states included in the summation, Eq. (28). Non-negligible contributions come even from rather highly excited states. The calculation could be easily extended beyond the $30\hbar\omega$ limit (all $A_{nl}^{\mathfrak{N}\mathfrak{L}} \approx 1$ in this region). It would be very hard, however, to justify such a procedure, since the phase shifts are known and have meaning only below about 300 MeV. The matrix elements of specific potentials, such as that of Tabakin, should already be quite unreliable for large values of n_p, n_r which correspond to $30\hbar\omega$ (roughly 500 MeV in s-d-shell nuclei) excitation. The contributions from the "dangerous" high-lying states constitute, however, only a few percent of the total result, and we can consider the binding energies calculated with $\rho_{\max} = 30$ as a reasonable compromise between the extreme requirements of terminating the summation in Eq. (28) at about 300 MeV and extending it up to the point where a clear asymptotic value of the binding energy has been reached. The same problem arises, of course, in all t-matrix calculations; only it may be hidden by a more complicated formalism.

The subsequent increments of $E^{(1)}$ are also plotted in Figs. 5 and 6. It can be seen that the most important excited states which contribute to the O^{16} binding energy are those with $(4-8)\hbar\omega$ excitation energy in qualitative accordance with earlier findings by Bassichis and Strayer.[13] The last-named authors consider, however, only the second-order diagrams.

TABLE I. Diagonal singlet and triplet S-state reaction matrix elements ($n = 0$), and binding energies of O^{16} calculated in the Eden-Emery approximation for the Pauli projection operator Q^{EE} and with the accurate Q^R operator defined in Sec. III. A simplified Tabakin interaction [Eq. (32)] has been used in the calculation.

		t^{EE}			
	$\mathfrak{N}\mathfrak{L}$	$\rho_{\min}=4$	$\rho_{\min}=5$	$\rho_{\min}=6$	t^R
$^1S_0$	0 0	−9.8397	−9.5083	−9.5083	−9.5952
	0 1	−9.8105	−9.8105	−9.4775	−9.5850
	0 2	−11.1041	−9.8105	−9.8105	−9.8569
	1 0	−11.1041	−9.8105	−9.8105	−10.3389
$^3S_1$	0 0	−14.2517	−12.8252	−12.8252	−13.1373
	0 1	−14.0195	−14.0195	−12.6179	−12.9975
	0 2	−18.8855	−14.0195	−14.0195	−13.9191
	1 0	−18.8855	−14.0195	−14.0195	−15.1796
$E^{(1)}$		−13.0916	−8.2345	−6.9365	−7.7084

As a result of the above numerical experiments, summarized in Figs. 3–6 and Table I, the following prescription has been adopted: We calculate $A_{nl}^{\mathfrak{N}\mathfrak{L}}$ coefficients from the formula in Eq. (24) for $2n + l + 2\mathfrak{N} + \mathfrak{L} \leq 12$ and put $A_{nl}^{\mathfrak{N}\mathfrak{L}} = 1$ for larger values of the shell number. Contributions from all excited states through $30\hbar\omega$ are included in our t matrix.

VI. RESULTS AND DISCUSSION

The binding energies of He^4 and O^{16} have been calculated with reaction matrix elements corresponding to the model described in Secs. II–V. The results are presented in Fig. 7. The solid curves are for the total binding energies $E = E^{(1)} + E^{(2)}$, where $E^{(1)}$ corresponds to our Eq. (4) corrected for c.m. ($\Delta E_{\text{c.m.}} = -\frac{3}{4}\hbar\omega$) and Coulomb effects.

The second-order corrections [Figs. 1(b)–1(e)] are calculated with intermediate states from the

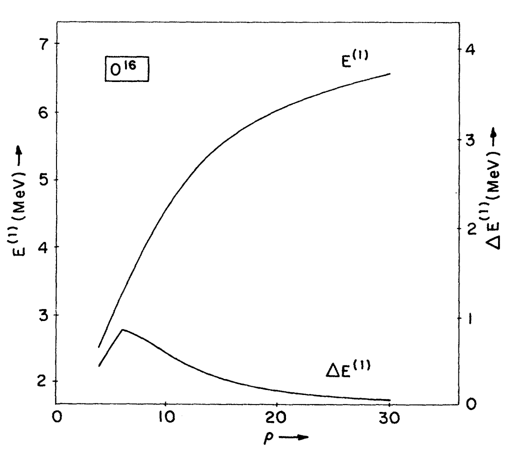

FIG. 6. The same as Fig. 5, but for the O^{16} nucleus. The spring constant of the h.o. wave function is $b = 1.4$ F.

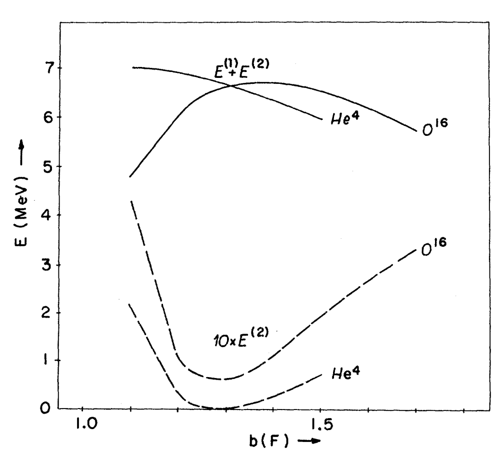

FIG. 7. Dependence of total binding energies and second-order contributions for He^4 and O^{16} on the oscillator length unit. $b = (\hbar/m\omega)^{1/2}$.

TABLE II. Energetics of He^4 in MeV calculated from t^R using the Tabakin interaction. The columns correspond to different choices of the constant C which controls the gap between occupied and unoccupied states. Self-consistency was imposed on η_{0s}, $b = 1.3$ F.

C^{a}	0.5	0.75	1.25	1.5	2	2.5
$n\ l\ j$						
$0\ 0\ \frac{1}{2}$	−21.940	−22.243	−22.992	−23.468	−24.735	−26.722
η_s	46.476	40.671	29.192	23.517	12.430	2.006
$E^{(2)}$	−0.001	−0.0003	−0.0001	−0.001	−0.008	−0.038
E	−6.196	−6.347	−6.722	−6.961	−7.601	−8.624

[a] In units of $\hbar\omega$.

lowest unoccupied major shell only. The dashed curves in Fig. 7, which show $E^{(2)}$ terms, exhibit remarkable minima for $b = 1.3$ F. Such a minimum in the Brueckner-Hartree-Fock-violating term should be interpreted as an additional improvement of the self-consistency. Our conditions, Eqs. (12) and (14), ensure the cancellation of potential and bubble insertions in diagonal matrix elements only. A minimum in the calculated $E^{(2)}$ curve then means that a certain nondiagonal insertion has been canceled as well. Therefore, the most reasonable choice for the value of the parameter b is to take it at the minimum of $E^{(2)}$.

We have stressed already that the proper definition of the parameters η_h and C in Eq. (11) modifying the s.p. basis is crucial for the rapid convergence of the Brueckner expansion. The self-consistent prescription [Eq. (12)] is well justified; much work, however, remains before the problem of appropriate modification of particle spectra can be completely settled. In Tables II and III we show how the binding energy of He^4 and O^{16} depends on the choice of the parameter C, which modifies the particle-hole gap in our calculation. It can be seen that much better agreement between calculated and experimental data would be obtained with C values different from those of Eq. (16). For example, the procedure adopted by Becker, MacKellar, and Morris[10] gives in O^{16} roughly the same value for three different realistic potentials – ($C \approx -66$ MeV $\approx -(\frac{13}{4}\hbar\omega)$), which should be compared with our estimate in Eq. (16) of $C = -(\frac{7}{4})\hbar\omega$. The binding energy of O^{16} for $C = -(\frac{13}{4})\hbar\omega$ and Tabakin's potential would be about −8.4 MeV, in surprisingly good agreement with Becker's, MacKellar's, and Morris's[10] results −7.3, −7.5, and −7.8 MeV for Yale, Reid, and Hamada-Johnston potentials, respectively. The choice of the constant C should, nevertheless, be made independently in order to minimize the higher-order contributions to the binding energy, rather than be made from the numerical fit to the experimental value. Inclusion of the third-order processes [Fig. 2(d)] with more than $2\hbar\omega$ excitation in the intermediate states is indeed highly desirable in the place of our crude guess [see Eq. (16)].

To our knowledge, the previous results of binding-energy calculations with true realistic potentials are in most cases in rather strong disagreement (B.E. ≈−3 to −4 MeV) with the experimental values B.E.(He^4) = −7.07 MeV and B.E.(O^{16}) = −7.975 MeV, unless additional tailor-made assumptions

TABLE III. Energetics of O^{16} in MeV calculated with Tabakin's potential for different choices of the constant C, and the self-consistency condition [Eq. (12)] imposed on η_{0s} and η_{0p}, compared with corresponding results of Becker, MacKellar, and Morris (see Ref. 10) obtained with the Hamada-Johnston potential and the additional condition $\eta_{0s} = 2\eta_{0p}$.

	Tabakin				Hamada-Johnston[b]
C^{a}	1.75	2.5	3.0	3.5	3.25
$n\ l\ j$					
$0\ 0\ \frac{1}{2}$	−64.87	−65.91	−66.77	−67.80	−60.29
$0\ 1\ \frac{3}{2}$	−32.93	−34.12	−35.17	−36.56	−34.96
$0\ 1\ \frac{1}{2}$	−18.41	−19.76	−20.95	−22.52	−25.54
η_s	59.54	44.85	35.12	25.44	24.05
η_p	43.94	29.48	20.01	10.66	12.02
$E^{(2)}$	−0.113	−0.168	−0.229	−0.332	−0.46
E	−6.727	−7.378	−7.956	−8.733	−7.80

[a] In units of $\hbar\omega$.

[b] Ref. 10, $b = 1.414$ F.

are introduced. The better agreement obtained by the present approach is probably due to the more appropriate treatment of the Pauli exclusion principle, and consistent modification of s.p. spectra. The most important additional effects responsible for our slightly underestimated results are: (i) the three-body cluster term, (ii) the second-order diagrams [Figs. 2(b)–2(e)] with excitation over several major shells, and (iii) a better choice for the parameter C, as already discussed.

In our treatment of the c.m. motion, only the term $-\frac{3}{4}\hbar\omega$ corresponding to the unperturbed ground-state wave function has been taken into account. A more consistent description of the c.m. effects in the He^4 nucleus has been suggested recently by Blank[19] in the framework of the Lipkin model with an external h.o. potential field acting on the c.m. degrees of freedom. His preliminary results obtained with the Hamada-Johnston potential show that c.m. motion probably influences the expansions for the rms radius and charge distribution only.

The present approach is based on the assumption that the three-body forces produce negligible effects on the nuclear states. Tabakin's potential was used for the evaluation of the two-body reaction matrix elements in terms of modified h.o. states for He^4 and O^{16}. Two approximations in the treatment of the Pauli projection operator Q are: (1) We keep only terms diagonal in the c.m. quantum numbers $\mathcal{N}$, $\mathcal{L}$, $\mathcal{M}$, and (2) the $\mathcal{M}$-dependent matrix elements of Q are replaced by their average values. The validity of the last two assumptions should be carefully investigated, despite very reasonable numerical results obtained for He^4 and O^{16} binding energies.

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