

FIG. 3. Same as Fig. 2 but for $E_d = 0.4$ MeV.

the above-mentioned symmetry axis θ_s'' , and these values of θ_2 are shown as circles in Fig. 2. The solid curves in this figure, from top to bottom, represent the following directions relative to the beam direction⁷: (1) plane-wave heavyparticle stripping; (2) ⁸Be_{2.9}(2⁺) recoil direction, c.m.(1); (3) $\theta_2''=0$ (defined in same manner as θ_s'' above); (4) ⁸Be_{2.9}(2⁺) recoil direction, lab; and (5) plane-wave pickup. It is very apparent from Fig. 2 that there is a systematic trend, and that the data agree very well with the curve for plane-wave deuteron pickup, for $E_d = 1.5$ MeV. The same agreement occurs at $E_d = 1.0$ MeV. For $E_d = 0.4$ MeV, as shown in Fig. 3, the points obviously do not fit the pickup curve, but are consistent with the curve for $\theta_2''=0$ which would be indicative of compound-nucleus formation. The errors are estimated to be less that $\pm 6^{\circ}$ in all cases, and in Fig. 3 this is approximately half the difference between the pickup and the $\theta_2''=0$ curves. These results are strongly supported by evidence that this reaction changes from compound-nucleus formation to a direct-interaction mechanism at about 0.7 MeV.^{4,5} This indication of a means of reaction-mechanism identification is being extended to other reactions, especially those with previous evidence of other direct-interaction mechanisms.

*Work supported by the National Science Foundation. ¹Proceedings of the Conference on Correlations of Particles Emitted in Nuclear Reactions, Rev. Mod. Phys. <u>37</u>, 327 (1965); Proceedings of the International Conference on Clustering Phenomena in Nuclei, Bochum, West Germany, 1969 (International Atomic Energy Agency, Vienna, Austria, 1969; Few Body Problems, Light Nuclei and Nuclear Interactions, edited by G. Paić and I. Slaus (Gordon and Breach, New York, 1967).

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Composite Particles in Many-Body Systems

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Presented herein is a second-quantized formulation for a system of interacting nuclei and electrons expressed in terms of the creation and annihilation operators of various species of atoms and ions which can be formed by combining various numbers of the "elementary" particles. Processes such as ionization and recombination appear naturally. Explicit expressions for interatomic forces including exchange effects are generated from a "cluster expansion" reminiscent of the Ursell expansion.

The formulation of the many-body problem of a system of interacting atoms taking into account the composite nature of these particles was accomplished by the work of Girardeau.¹ There are, however, two disadvantages to his method: First, both the bound and continuum states of the

atom are depicted as particles, which precludes the explicit appearance of the ionization and recombination terms in the Hamiltonian; and second, rather stringent conditions are imposed upon the state in order that the symmetry properties of the "elementary" particles under interchange are preserved. The problem has been elegantly resolved by Stolt and Brittin² by proving the existence of partial isometries between the physically permissible states and a subspace of the complete Hilbert space spanned by products of bound- and free-particle wave functions. The second problem was also resolved in a later paper by Girardeau,³ wherein subsidiary conditions were incorporated into the Hamiltonian. The particle-nonconserving terms are still missing, but exchange terms now appear directly in the Hamiltonian. In the present work neither problem appears, but some physical states may have one unbound pair of each type of composite particle. Although these pairs do not present serious mathematical problems, their physical significance is obscure. The present method permits one to directly carry the theory beyond the results achieved by Stolt and Brittin.

Avoiding unnecessary complications, a system of N electrons and N nuclei of spin J is considered. The atom here is the "hydrogen" atom. The complete wave function obeys the usual symmetry property under the interchange of any pair of nuclear coordinates x_1, \dots, x_N and of the electronic coordinates y_1, \dots, y_N , but a basis of products of bound atomic wave functions (or of atomic wave functions and free-particle wave functions) does not have appropriate symmetry.¹ Girardeau observed that it was advantageous to let the Hamiltonian bear the full burden of symmetry and let it operate in the space spanned by the atomic basis.³ He called this the projected Hamiltonian, the eigenstates of which are necessarily the eigenstates of the full Hamiltonian but belong to the subspace with appropriate symmetry. This Letter is an extension of Girardeau's work in two senses: First, a basis composed of bound atoms, free ions, and free electrons rather than bound and continuum atoms will be employed to construct the projected Hamiltonian; and second, a systematic procedure for generating higherorder terms in the projected Hamiltonian based upon a variant of the Ursell expansion is given. One does not completely escape the unbound atom here. A physical state will be seen to contain one (or zero) unbound atoms, because of the need for orthogonality of the basis states.

Consider the projection operator A which projects from the full Hilbert space onto the physical space of appropriate symmetry. Its matrix element is

$$\langle \underline{xy} | A | \underline{x'y'} \rangle = (N!N!)^{-1} \sum_{P} (\pm) \langle \underline{xy} | P \underline{x'y'} \rangle, \qquad (1)$$

where

$$\langle \underline{xy} | \underline{x'y'} \rangle = \delta(x_1, x_1') \cdots \delta(y_N, y_N'), \qquad (2)$$

and where the underscoring denotes the complete set of 2N coordinate vectors and 2N spin variables. The permutation P is the product (permutation of the N electron coordinates) times (permutation of the N nuclear coordinates). The sign factor is the product (signature of the electronic permutation) times [signature of the nuclear permutation (one) if J is odd (even)]. The projected Hamiltonian is given by

$$\langle \underline{xy} | \widetilde{H} | \underline{x'y'} \rangle = \int \langle \underline{xy} | A | \underline{rs} \rangle \langle \underline{rs} | H | \underline{r's'} \rangle \langle \underline{r's'} | A | \underline{x'y'} \rangle d\underline{rds} d\underline{r'ds'},$$
(3)

where the integral sign denotes integration over coordinates and summation over spins. A second A is unnecessary, but for convenience it will be retained.

We introduce now the basis for the subspace of M bound atoms, one unbound atom, N-M-1 ions, and N-M-1 electrons. Only the subspace of N bound atoms does not contain an unbound atom, and the number N-M-1 is then to be interpreted as zero. Let

$$|M\underline{x}\underline{y}\rangle = [M!(N-M-1)!(N-M-1)!]^{-1}\sum_{P}(\pm)\int |\underline{x}'\underline{y}'\rangle \langle \underline{x}'\underline{y}'|\Delta_{M}| P\underline{x}\underline{y}\rangle d\underline{x}'d\underline{y}',$$
(4)

where the projection operator Δ_M is defined as

$$\langle \underline{xy} | \Delta_M | \underline{x'y'} \rangle = I_B(1,1') \cdots I_B(M,M') I_F(M+1,M+1') I(M+2,M+2') \cdots I(N,N'),$$
(5)

and

$$I_{\mathcal{B}}(1,1') \equiv \sum_{\alpha}^{bound} \varphi_{\alpha}(x_1,y_1) \varphi_{\alpha}(x_1',y_1')^*, \qquad (6)$$

$$I_{F}(1,1') \equiv \sum_{\alpha}^{\text{unbound}} \varphi_{\alpha}(x_{1},y_{1})\varphi_{\alpha}(x_{1}',y_{1}')^{*}, \qquad (7)$$

$$I_{B}(1, 1') + I_{F}(1, 1') = I(1, 1') = \delta(x_{1}, x_{1}')\delta(y_{1}, y_{1}'),$$
(8)

in which $\varphi_{\,\alpha}$ are atomic wave functions. The orthogonality and completeness relations are

$$\int \langle \underline{xy} | \Delta_{\underline{M}} | \underline{x'y'} \rangle \langle \underline{x'y'} | \Delta_{\underline{M}'} | \underline{x''y''} \rangle d\underline{x'dy'} = \delta_{\underline{M}\underline{M}'} \langle \underline{xy} | \Delta_{\underline{M}} | \underline{x''y''} \rangle$$
(9)

and

$$\sum_{M=0}^{N} \langle \underline{x}\underline{y} | \Delta_{M} | \underline{x}' \underline{y}' \rangle = \langle \underline{x}\underline{y} | \underline{x}' \underline{y}' \rangle.$$
(10)

The permutation P is the product (permutation of the couples x_1y_1, \dots, x_My_M) times (permutation of the nuclear coordinates x_{M+2}, \dots, x_N) times (permutation of the electron coordinates y_{M+2}, \dots, y_N). The overall sign is the product [signature of the first permutation (one) if 2J+1 is odd (even)] times [signature of the second permutation (one) if 2J is odd (even)] times (signature of the third permutation).

These states are orthogonal in the sense that

$$\langle \underline{M}\underline{x}\underline{y} | \underline{M'}\underline{x'}\underline{y'} \rangle = \delta_{\underline{M}\underline{n'}} | \underline{M}! (N - M - 1)! |^{-1} \sum_{\underline{P}} (\pm) \langle \underline{x}\underline{y} | \Delta_{\underline{M}} | \underline{P}\underline{x'}\underline{y'} \rangle.$$
(11)

We define the operator \tilde{A} by

$$\widetilde{A} = \sum_{\mathbf{M},\mathbf{M}'} \int |\mathbf{M}\underline{x}\underline{y}\rangle \langle \underline{x}\underline{y}| A | \underline{x}'\underline{y}'\rangle \langle \mathbf{M}'\underline{x}'\underline{y}' | d\underline{x}'d\underline{y}'d\underline{x}d\underline{y},$$
(12)

which has the matrix element

$$\langle \underline{x}\underline{y} | \widetilde{A} | \underline{x}' \underline{y}' \rangle = \langle \underline{x}\underline{y} | A | \underline{x}' \underline{y}' \rangle, \tag{13}$$

and the property

$$(\tilde{A})^2 = \tilde{A},\tag{14}$$

so that it is our desired projection operator. The projected Hamiltonian H is given by

$$\widetilde{H} = \widetilde{A} H \widetilde{A} = \sum_{MM'} \int |M\underline{x}\underline{y}\rangle \langle \underline{x}\underline{y}| A H A | \underline{x}'\underline{y}'\rangle \langle M'\underline{x}'\underline{y}' | d\underline{x} d\underline{y} d\underline{x}' d\underline{y}'.$$
(15)

If we use a second quantized form of $|Mxy\rangle$, then

$$|Mxy\rangle = [M!(N-M-1)!(N-M-1)!]^{-1/2} \times \Psi^{\dagger}(z_{1})\cdots \Psi^{\dagger}(z_{N})\Psi^{\dagger}(w)\Psi^{\dagger}(x_{M+2})\Psi^{\dagger}(y_{M+2})\cdots \Psi^{\dagger}(x_{N})\Psi^{\dagger}(y_{N})|0\rangle,$$
(16)

where $\Psi^{\dagger}(x)$ and $\Psi^{\dagger}(y)$ are the usual ion and electron wave function creation operators, and

$$\Psi^{\dagger}(w) = \sum_{\alpha}^{\text{unbound}} a_{\alpha}^{\dagger} \varphi_{\alpha}^{*}(x_{M+1}, y_{M+1}), \qquad (17)$$

$$\Psi^{\dagger}(z_{i}) = \sum_{\alpha}^{\text{bound}} a_{\alpha}^{\dagger} \varphi_{\alpha}^{*}(x_{i}, y_{i}), \qquad (18)$$

which are fermion (boson) operators if 2J+1 is odd (even). The a_{α} obey the usual anticommutation (commutation) rules. In order to avoid sign ambiguities, the normal commutation rules are being used: Boson operators commute with other boson and fermion operators, and fermion operators anticommute with other fermion operators. Upon using the usual second-quantized form for \tilde{H} and \tilde{A} ,

$$\langle \underline{xy} | \widetilde{H} | \underline{x'y'} \rangle = [N!]^{-2} \langle 0 | \Psi(y_r) \cdots \Psi(y_1) \Psi(x_N) \cdots \Psi(x_1) H \Psi^{\dagger}(x_1') \cdots \Psi^{\dagger}(x_N') \Psi^{\dagger}(y_1') \cdots \Psi^{\dagger}(y_N') | 0 \rangle,$$
(19)

$$\langle \underline{xy} \mid \widetilde{A} \mid \underline{x'y'} \rangle = [N!]^{-2} \langle 0 \mid \Psi(y_N) \cdots \Psi(y_1) \Psi(x_N) \cdots \Psi(x_1) \Psi^{\dagger}(x_1') \cdots \Psi^{\dagger}(x_N') \Psi^{\dagger}(y_1') \cdots \Psi^{\dagger}(y_{N'}) \mid 0 \rangle,$$
(20)

and inserting into Eqs. (12) and (15), and using the Ursell expansion, one obtains the following expression:

$$\widetilde{H} = \sum_{\substack{m \\ R'ST'U'}} \sum_{\substack{R'ST'U' \\ r's't'm'}} H(RSTU; R'S'T'U') \prod_{\substack{T's't'm' \\ r's't'm'}} \frac{[A(rstu; r's't'u')]^{m(r\cdots;r'\cdots)}}{m(rstu; r's't'u')!};$$
(21)

with the restrictions

$$\begin{split} &\sum (r'-r+s'-s+t-t')m(rstu; r's't'u') + (R'-R+S'-S+T-T') = 0, \\ &\sum (r'-r+s'-s+u-u')m(rstu; r's't'u') + (R'-R+S'-S+U-U') = 0, \\ &\sum sm(rstu; r's't'u') + S \leq 1, \quad \sum s'm(rstu; r's't'u') + S' \leq 1. \end{split}$$

The cluster term involving R bound-atom creation operators, S (zero or one) unbound-atom creation operators, \dots , U' electron destruction operators is given by

$$H(RSTU; R'S'T'U') = (R \mid S \mid T \mid U \mid R' \mid S' \mid T' \mid U' \mid)^{-1} \int \Psi^{\dagger}(z_{1}) \cdots \Psi^{\dagger}(z_{R}) \Psi_{F}^{\dagger}(w) \Psi^{\dagger}(x_{1}) \cdots \Psi^{\dagger}(x_{T}) \\ \times \Psi^{\dagger}(y_{1}) \cdots \Psi^{\dagger}(y_{U}) \langle y_{U} \cdots y_{1}x_{T} \cdots x_{1}wz_{R} \cdots z_{1} \mid H \mid z_{1}' \cdots z_{R'}'w'x_{1}' \cdots x_{T}'y_{1}' \cdots y_{U'}' \rangle_{C} \\ \times \Psi(z_{U'}') \cdots \Psi(y_{1}') \Psi(x_{T'}') \cdots \Psi(x_{1}') \Psi(w') \Psi(z_{R'}') \cdots \Psi(z_{1}') dz_{1} dz_{1}' \cdots dy_{U} dy_{U'}'$$
(22)

with corresponding expressions for A(rstu; r's't'u'). The operators A(1000; 1000), A(0100; 0100); A(0010; 0001); a(0010; 0001), and A(0001; 0001) do not appear in Eq. (21). The integers m(rstu; r's't'u') are the number of times the corresponding operator appears as a factor. The sum is over all possible sets of the m's. The enclosure by colons denotes normal products. The subscripts C denote "connected" and are defined by the Ursell expansion of which an example is

$$\langle 0 | \Psi(y)\Psi(x)H\Psi^{\dagger}(x')\Psi^{\dagger}(y')|0\rangle = (1 | 1 | 1 | 1 | 1 | 1 | 1^{-1/2}(\langle yx | H | x'y'\rangle_{c} + \langle y | H | y'\rangle_{c}\langle x | x'\rangle_{c} + \langle y | y'\rangle_{c}\langle x | H | x'\rangle_{c})$$

= (1 | 1 | 1 | 1 | 1^{-1/2}\langle z | H | x'y'\rangle_{c} = (1 | 1 | 1 | 1^{-1/2}\langle z | H | z'\rangle_{c}, (23)

$$\langle 0|\Psi(x)\Psi^{\mathsf{T}}(x')|0\rangle = (1\,!\,1\,!)^{-1/2}\langle x|x'\rangle_{C}.$$
(24)

Note that a given matrix element defines several connected matrix elements as in (23). The first line of (23) corresponds to the transition from an ion-electron state to another ion-electron state. The second line describes the transition from an ion-electron state to a bound-atom state, and the third line to a transition from a bound-atom state to another bound-atom state. The normalization factors are written in particularly awkward fashion to show the general rule: a factor of $(n!)^{-1/2}$ for n operators (creation or annihilation) of any particle. Note the sequence of operators and the arguments of the connection matrix elements which must be followed if there is to be no sign error.

Restricting ourselves to terms which do not create or destroy more than two particles, the Hamiltonian becomes the sum $H_0 + H_A + H_1 + H_F$, where H_0 is the usual electron-nuclei Hamiltonian, and H_A is the atomic Hamiltonian of Girardeau³ including both direct and exchange interactions, but the atomic operators are restricted to bound-state operators only.

$$H_{I} = \int \Psi^{\dagger}(z) [H\Psi(y)\Psi(x)] dz + \text{H.c.} + \int \Psi^{\dagger}(z_{1})\Psi^{\dagger}(x_{2})V(z_{1}, x_{2})\Psi(x_{2})\Psi(z_{1}) dx_{2} dz_{1} + \int \Psi^{\dagger}(z_{1})\Psi^{\dagger}(y_{2})V(z_{1}, y_{2})\Psi(y_{2})\Psi(z_{1}) dz_{1} dy_{2} + \int \Psi^{\dagger}(z_{1})\Psi^{\dagger}(x_{2})\frac{1}{2}[-1 + (-1)^{2J}I(x_{1}x_{2})][H\Psi(x_{2})\Psi(z_{1})] dz_{1} dx_{2} + \int \Psi^{\dagger}(z_{1})\Psi^{\dagger}(y_{2})\frac{1}{2}[-1 - I(y_{1}, y_{2})][H\Psi(y_{2})\Psi(z_{1})] dz_{1} dy_{2},$$
(25)

where $V(z_1, x_2)$ and $V(z_1, y_2)$ are the Coulomb interactions between the atom and the ion and between the atom and the electron, respectively, and H is the total unsymmetrized Hamiltonian for the variables concerned. $I(x_1, x_2)$ and $I(y_1, y_2)$ are the exchange operators for the nuclear and electronic coordinates, respectively. The first line describes ionization and recombination process-

es. The remainder describes electron-atom or ion-atom collisions including exchange collisions. H_F is similar to $H_A = H_I$ except for the presence of $\Psi(w)$ and $\Psi^{\dagger}(w)$. Explicit expressions will be given elsewhere. It follows from Eqs. (4) and (10) that the physical state can contain one unbound atom at most.

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It is a trivial matter to extend the formalism to a nucleus of charge Z and an atom of Z electrons. However, one can show then that the lowest-order interaction term represents the complete ionization of the atom into Z electrons and a nucleus, and is suitable only if ionization in unlikely. Consequently, it is necessary to introduce the state of the ions with charges Z - 1, Z $-2, \cdots, Z$. This is readily accomplished by modifying Eq. (5). Now I_B becomes the projection operator onto the states of the Z-electron atom. The product of the identities I(M + 2, M)+2'···I(N, N') itself is decomposed according to Eq. (5): $I_B \cdots I_F I \cdots I$, where I_B and I_F now project onto states of the ion with charge Z - 1. The product $I \cdot \cdot \cdot I$ in the above is again decomposed according to (5) where now the projection operator is that for the states of the ion with the charge Z-2. One continues this process until the nucleus of charge Z and electrons are left or when the

rare-gas core is reached. The physical states will now contain at most one quantum of each of the unbound composites and the Hamiltonian will contain terms corresponding to single ionization, double ionization, etc., of the atom and of the ions. Extension to molecular aggregates and to negative ions is trivial.

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³M. Girardeau, "Formulation of the Many-Body Problem for Composite Particles. III: The Projected Hamiltonian" (to be published).

Gravitational Waves in Closed Universes

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New boundary conditions on the Einstein-Rosen-Bondi gravitational-wave metrics yield closed inhomogeneous universes which solve Einstein's vacuum field equations exactly. Space sections of these universes have either the three-sphere topology S^3 or the wormhole (hypertorus) topology $S^1 \otimes S^2$.

By means of a change of boundary conditions. the Einstein-Rosen-Bondi analysis of cylindrical and plane waves¹ may be used to construct gravitational waves in closed universes. Spacelike sections of these universes have either the threesphere topology S^3 which is familiar from the Friedman universe or the hypertorus topology $S^1 \otimes S^2$ which may be imposed upon the Kantowski-Sachs universe.² Exact solutions to Einstein's field equations are obtained in the absence of matter and nongravitational fields. These solutions provide a new type of cosmological model which is dominated by homogeneity-breaking, coherent gravitational radiation.³ They also provide an important new "theoretical laboratory" for testing and exploring recent formal developments in general relativity.⁴

An Einstein-Rosen-Bondi space-time will be defined to be one which possesses two mutually orthogonal, hypersurface orthogonal, spacelike Killing vector fields. It is well known that any such space-time has a metric which may be put into the form

$$ds^2 = L^2 \left[e^{2a} (d\theta^2 - dt^2) \right]$$

$$+R(B^{-1}e^{2W}d\sigma^{2}+Be^{-2W}d\delta^{2})], \quad (1)$$

where L is a constant length; t, θ , σ , and δ are dimensionless coordinates; and a, W, R, and B are dimensionless functions of θ and t alone.⁵ This form of the metric does not fix the coordinates θ and t completely. In terms of the advanced and retarded coordinates $v \equiv t + \theta$ and $u \equiv t - \theta$, the most general coordinate transformations which preserve the form of the metric are

$$u = F(\tilde{u}), \quad v = G(\tilde{v}), \tag{2}$$

where F and G are arbitrary functions of one variable.⁵ In order to write Einstein's equations for this family of space-times, it is convenient to denote derivatives with respect to v and u by the subscripts + and -, respectively, and to

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