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Completely integrable N-body quantum systems in three dimensions: II. N identical spin-$\frac{1}{2}$ fermions

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Abstract. If one begins with N non-interacting fermions, the Pauli principle can be easily incorporated by the use of Slater determinants. This is not the case for N interacting fermions. We consider here exactly soluble 'Coulomb-type' quantum systems in three dimensions of N interacting identical spin-$\frac{1}{2}$-fermions. A systematic procedure for constructing Pauli antisymmetry-adapted wavefunctions is given. The resulting antisymmetric wavefunctions are labelled by conserved 'good' quantum numbers. In particular, for $N=2$, all the physically acceptable states are obtained. For $N=3$, we present a class of antisymmetric states which consists of all the ground states, all the first excited states and the states obtained by the hyperradial excitations of these. For $N=2$ and 3, the ground states of our model systems are found to be $^1S(s^2)$ and $^2P(s^2p)$, respectively, in the quantum numbers of the interacting system.

1. Introduction

The study of exactly soluble non-trivial systems of N interacting particles is of interest not only for purely theoretical considerations but also from the point of view of practical applications to realistic systems. In a previous paper (Barut and Kitagawara 1981, to be referred to as I) we discussed a family of completely integrable, three-dimensional, N-body quantum systems which are described by the Hamiltonian

$$H=\tfrac{1}{2}(\boldsymbol{p}_1^2+\boldsymbol{p}_2^2+\ldots+\boldsymbol{p}_N^2)-\zeta/(\boldsymbol{r}_1^2+\boldsymbol{r}_2^2+\ldots+\boldsymbol{r}_N^2)^{1/2}+V, \tag{1.1}$$

where $\boldsymbol{p}_j=-\mathrm{i}\nabla_j$, $\zeta=$ constant and V is a homogeneous function of degree -2. When the system consists of N distinguishable spinless particles, and $V=0$, we can choose a complete set of commuting operators which are Casimir operators of the dynamical group $O(3N+1,2)$ of this problem, and of its subgroups. The problem is completely solved by the dynamical group $O(3N+1,2)$ and its representations (see I).

However, for an application to a system of N identical fermions, the system must satisfy the Pauli principle, and consequently a new set of commuting operators must be chosen (§ 2). In this paper, we consider a system of N identical spin-$\frac{1}{2}$ fermions which is described by the Hamiltonian (1.1) with $V=0$. After the introduction of hyperspherical coordinates (§ 3), we give in § 6 a systematic procedure to construct the antisymmetry-adapted wavefunctions for any number of spin-$\frac{1}{2}$ fermions. The discussion is based on Kotani *et al* (1963) and Knirk (1974). In § 7 we apply this systematic procedure to the case $N=2$ and obtain all the antisymmetry-adapted states. In § 8, we present a class of antisymmetry-adapted wavefunctions which includes all the ground

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states, all the first excited states and the states obtained by the hyperradial excitations of these. Applications to realistic problems are briefly discussed in § 9.

The Hamiltonian (1.1) is spin independent. The energy spectrum of (1.1) is still soluble if we take in V terms depending on the spin operators, like $V = \boldsymbol{\sigma} \times \boldsymbol{r}/r^3$ (charge–dipole potential). In this paper, however, we consider for simplicity a spin-independent Hamiltonian, and take the main effect of the spin to be the Pauli principle.

2. Statement of the problem

The energy eigenvalues of the system described by the Hamiltonian (1.1) with $V = 0$ are given by I,

$$E_n = -\zeta^2/2n^2, \qquad n = s + \lambda + \tfrac{1}{2}(3N-1) \qquad (s, \lambda = 0, 1, 2, \ldots) \tag{2.1}$$

(ζ real for discrete spectrum, pure imaginary for continuous spectrum). Here n is the 'principal quantum number' of the system. In a special representation given in I, the quantum number n labels the representation of the $O(3N+1)$ subgroup of the dynamical group $O(3N+1, 2)$. The quantum number λ labels that of the $O(3N)$ subgroup of the degeneracy group $O(3N+1)$. It was shown that the set of Casimir operators of the following subgroup chain (2.2) gives a complete set of commuting operators (CSCO) of the system:

$$\begin{array}{l} O(3N+1, 2) \supset O(2N+1)^n \times O(2)^n \\ \qquad\qquad\qquad\quad \cup \\ \qquad\qquad\qquad\quad O(3N)_\lambda \end{array} \tag{2.2a}$$

$$\begin{array}{l} O(3N+1, 2) \supset O(3N)^\lambda \times O(2, 1)^\lambda \\ \qquad\qquad\qquad\qquad\quad \cup \\ \qquad\qquad\qquad\qquad\quad O(2)_n \end{array} \tag{2.2b}$$

$$\begin{array}{l} O(3N)^\lambda \supset O(3N-3)^{\lambda_{N-1}} \times {}^N O(3)^{(l_N, m_N)} \\ \qquad\quad \cup \\ \qquad\quad O(3N-6)^{\lambda_{N-2}} \times {}^{N-1} O(3)^{(l_{N-1}, m_{N-1})} \\ \qquad\quad \cup \\ \qquad\quad \vdots \\ \qquad\quad \cup \\ \qquad\quad O(6)^{\lambda_2} \times {}^3 O(3)^{(l_3, m_3)} \\ \qquad\quad \cup \\ \qquad\quad {}^1 O(3)^{(l_1, m_1)} \times {}^2 O(3)^{(l_2, m_2)}. \end{array} \tag{2.2c}$$

Here we have also indicated the quantum numbers which label these subgroups. These are conserved 'good' quantum numbers for the system of N interacting distinguishable spinless particles whose motions are described by the model Hamiltonian (1.1) with $V = 0$. Thus the stationary states are completely specified by these quantum numbers and the state vectors are denoted by

$$|n\gamma lm\rangle \equiv |n;\, \gamma_N, \gamma_{N-1}, \ldots, \gamma_2;\, l_N, l_{N-1}, \ldots, l_1;\, m_N, m_{N-1}, \ldots m_1\rangle, \tag{2.3}$$

where the quantum numbers $\gamma = \{\gamma_2, \gamma_3, \ldots, \gamma_N\}$ are defined as

$$\lambda_j = \lambda_{j-1} + l_j + 2\gamma_j, \qquad \lambda \equiv \lambda_N, \qquad l_1 \equiv \lambda_1, \qquad j = 2, 3, \ldots, N. \tag{2.4}$$

As we will show in § 9, state vectors $|n\gamma lm\rangle$, or linear combinations of these state vectors, $\Sigma_{\gamma,l,m} C_{\gamma,l,m}|n\gamma lm\rangle$, can be used as zeroth-order state vectors for a new perturbation theory for more realistic N-body problems.

For an application of this model to the system of N identical spin-$\frac{1}{2}$ fermions, the strong restrictions imposed by the Pauli principle have to be taken into account. In this case, for Pauli antisymmetry-adapted states, the quantum numbers $\gamma = \{\gamma_2, \gamma_3, \ldots, \gamma_N\}$, $l = \{l_1, l_2, \ldots, l_N\}$ and $m = \{m_1, m_2, \ldots, m_N\}$ are no longer good. However, as we shall see in § 6, the quantum numbers n and λ still remain good. We shall also see that not all of the solutions of the Schrödinger equation with Hamiltonian (1.1) are allowed by the Pauli principle. In particular, from equation (2.1), the minimum value of E_n is obtained when $s = \lambda = 0$, but the states obtained in this way are not in general the antisymmetry-adapted states.

It is important to know the physically acceptable states and their conserved 'good' quantum numbers for a system of N identical spin-$\frac{1}{2}$ fermions. These states are the ones which should be used as zeroth-order states for a perturbation theory to realistic problems.

3. Description of the Hamiltonian by hyperspherical coordinates

In this section, we rewrite our model Hamiltonian (1.1) in terms of hyperspherical coordinates. We will see that this is the natural coordinate system to describe the state vectors (2.3) in coordinate representation.

In hyperspherical coordinates, we replace the $3N$ independent coordinates $\{x_i, y_i, z_i \,|\, i = 1, 2, \ldots, N\}$ by a set of $(3N-1)$ hyperspherical angles and a hyperspherical radius. Among the $(3N-1)$ hyperspherical angles, we can choose $2N$ angles to be the ordinary three-dimensional spherical polar angles $\{\theta_i, \varphi_i \,|\, i = 1, 2, \ldots, N\}$ of individual particles. By means of the ordinary spherical polar radii $\{r_i \,|\, i = 1, 2, \ldots, N\}$, the remaining $(N-1)$ hyperspherical angles are defined by the following set of equations:

$$\begin{aligned}
r_N &= r \cos \eta_N, \\
r_{N-1} &= r \sin \eta_N \cos \eta_{N-1}, \\
r_{N-2} &= r \sin \eta_N \sin \eta_{N-1} \cos \eta_{N-2}, \\
&\vdots \\
r_2 &= r \sin \eta_N \sin \eta_{N-1} \sin \eta_{N-2} \ldots \sin \eta_3 \cos \eta_2, \\
r_1 &= r \sin \eta_N \sin \eta_{N-1} \sin \eta_{N-2} \ldots \sin \eta_3 \sin \eta_2.
\end{aligned} \tag{3.1}$$

The angles η_j can also be expressed as

$$\sin^2 \eta_j = R_{j-1}^2 / R_j^2, \tag{3.2}$$

where

$$R_k^2 = \sum_{i=1}^{k} r_i^2. \tag{3.3}$$

The hyperspherical radius r is defined by

$$r^2 = R_N^2 = \sum_{i=1}^{N} r_i^2 \tag{3.4}$$

The volume element in the $3N$-dimensional space described by the hyperspherical coordinates is

$$d\tau = r^{3N-1}\, dr\, d\Omega, \tag{3.5}$$

where

$$d\Omega = \prod_{j=2}^{N} (\cos^2 \eta_j \sin^{3j-4} \eta_j\, d\eta_j) \prod_{i=1}^{N} (\sin \theta_i\, d\theta_i\, d\varphi_i). \tag{3.6}$$

Using these coordinates, the Hamiltonian (2.1) with $V = 0$ is written as

$$H = -\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{3N-1}{2}\frac{1}{r}\frac{\partial}{\partial r} + \frac{\Lambda^2(\Omega)}{2r^2} - \frac{\zeta}{r} \tag{3.7}$$

where $\Lambda^2(\Omega)$ is defined by

$$\Lambda^2(\Omega) \equiv \Lambda_N^2,$$

$$\Lambda_j^2 = -\frac{\partial^2}{\partial \eta_j^2} - \frac{(3j-4)\cos^2 \eta_j - 2\sin^2 \eta_j}{\sin \eta_j \cos \eta_j}\frac{\partial}{\partial \eta_j} + \frac{\Lambda_{j-1}^2}{\sin^2 \eta_j} + \frac{\boldsymbol{L}_j^2}{\cos^2 \eta_j},$$

$$\Lambda_1^2 \equiv \boldsymbol{L}_1^2. \tag{3.8}$$

In the above equations, $\boldsymbol{L}_j^2$ is the square of the ordinary angular momentum operator for particle j:

$$\boldsymbol{L}_j^2 = -\frac{1}{\sin \theta_j}\frac{\partial}{\partial \theta_j}\left(\sin \theta_j \frac{\partial}{\partial \theta_j}\right) - \frac{1}{\sin^2 \theta_j}\frac{\partial^2}{\partial \varphi_j^2}. \tag{3.9}$$

The operators Λ^2, Λ_j^2 and $\boldsymbol{L}_j^2$ are, in fact, Casimir invariants of $O(3N)$, $O(3j)$ and ${}^jO(3)$ in the subgroup chain (2.2). Therefore, in order to represent the state vectors $|n\gamma lm\rangle$ in spactial coordinates, the hyperspherical coordinate system is the most natural one.

4. The Schrödinger wavefunction

We can separate the Schrödinger equation, $(H - E)\psi = 0$, into a hyperangular part and a hyperradial part:

$$\Lambda^2(\Omega) S(\Omega) = \varepsilon S(\Omega), \tag{4.1}$$

$$\left(\frac{d^2}{dr^2} - [\varepsilon + \tfrac{3}{4}(3N-1)(N-1)]\frac{1}{r^2} + \frac{2\zeta}{r} + 2E\right) r^{(3N-1)/2}\mathcal{R}(r) = 0, \tag{4.2}$$

where ε is the separation constant and

$$\psi(\boldsymbol{r}) = \mathcal{R}(r)\, S(\Omega). \tag{4.3}$$

The hyperangular part (4.1) is well known from the general theory of harmonic polynomials (Erdely *et al* 1953, Grynberg and Koba 1964). There are two methods by which the eigenfunctions $S(\Omega)$ can be obtained. One is the direct solution of the differential equation in hyperspherical coordinates. The other method involves the construction of the linearly independent homogeneous polynomial solutions of Laplace's equation in $3N$ dimensions. Both methods have their own advantages and

disadvantages. The former gives state vectors which are exactly eigenvectors of CSCO given by the set of Casimir invariants of the subgroup chain shown in (2.2). By this method, it is straightforward to write a wavefunction for any value of N. On the other hand, it is not easy to see the transformation properties of the wavefunctions under the operations of particle exchanges. It is necessary to know these properties in the construction of the antisymmetry-adapted wavefunctions. The other method, however, provides a convenient form of the wavefunction appropriate for the study of its transformation property. The former method is discussed in § 4.1, the latter in § 4.2. For §§ 4.1 and 4.2, we will closely follow the discussion by Knirk (1974). The treatment of the hyperradial part (4.2) is straightforward and the function $\mathcal{R}(r)$ is explicitly given in § 4.3.

4.1. The direct solution of the hyperangular equation

Since the operator $\Lambda^2(\Omega)$ is defined recursively by equation (3.8), the hyperangular part can be solved by analysing the eigenvalue problems of operators $\Lambda_j^2(\Omega_j)$,

$$\Lambda_j^2(\Omega_j)S_j(\Omega_j) = \varepsilon_j S_j(\Omega_j). \tag{4.4}$$

Here Ω_j implies the collection of variables $\Omega_j = \{\eta_2, \eta_3, \ldots, \eta_j; \theta_1, \theta_2, \ldots, \theta_j; \varphi_1, \varphi_2, \ldots, \varphi_j\}$. It is well known that the eigenvalue ε_j can be written in the form

$$\varepsilon_j = \lambda_j(\lambda_j + 3j - 2), \qquad \lambda_j = 0, 1, 2, \ldots, \tag{4.5}$$

Because of the recursive form (3.8) of the operator $\Lambda_j^2(\Omega_j)$, equation (4.4) separates into variables η_j, Ω_{j-1}, θ_j and φ_j by setting

$$S_j(\Omega_j) = G(\lambda_{j-1}, l_j, \gamma_j \,|\, t_j) S_{j-1}(\Omega_{j-1}) Y(l_j, m_j \,|\, \omega_j). \tag{4.6}$$

Here

$$t_j \equiv 1 - 2\sin^2\eta_j, \qquad \omega_j = \{\theta_j, \varphi_j\}, \tag{4.7}$$

$Y(l_j, m_j \,|\, \omega_j)$ is the usual three-dimensional spherical harmonic $Y_{l_j,m_j}(\theta_j, \varphi_j)$ and γ_j is a quantum number associated with the eigenvalue ε_j. The function G in equation (4.6) is the solution of the ordinary differential equation

$$4(1-t_j^2)\frac{\mathrm{d}^2 G}{\mathrm{d}t_j^2} - [6jt_j + (6j-12)]\frac{\mathrm{d}G}{\mathrm{d}t_j} + \left(\varepsilon_j - \frac{2\lambda_{j-1}(\lambda_{j-1}+3j-5)}{1-t_j} - \frac{2l_j(l_j+1)}{1+t_j}\right)G = 0. \tag{4.8}$$

The physically acceptable function G is

$$G(\lambda_{j-1}, l_j, \gamma_j \,|\, t_j) = (1+t_j)^{l_j/2}(1-t_j)^{\lambda_{(j-1)}/2} P_{\gamma_j}^{(\lambda_{j-1}+3j/2-5/2, l_j+1/2)}(t_j), \tag{4.9}$$

where $P_\gamma^{(\alpha,\beta)}(t)$ is the Jacobi polynomial of order γ. The eigenvalue ε_j is given by the form in equation (4.5) with

$$\lambda_j = \lambda_{j-1} + l_j + 2\gamma_j, \qquad \gamma_j = 0, 1, 2, \ldots, \tag{4.10}$$

In equations (4.6) and (4.10), we have the identifications

$$S_1(\Omega_1) = Y(l_1, m_1 \,|\, \omega_1), \qquad \lambda_1 = l_1. \tag{4.11}$$

As we have shown in equations (2.4) and (2.5), we label our state with $\{\gamma_j\}$ rather than $\{\lambda_j\}$. It is now clear that the hyperangular wavefunction can be written as

$$S(\gamma, l, m\,|\,\Omega) = H(\gamma, l\,|\,\eta)A(l, m\,|\,\omega), \tag{4.12}$$

where

$$H(\gamma, l\,|\,\eta) = G(\lambda_{N-1}, l_N, \gamma_N\,|\,1-2\sin^2\eta_N)G(\lambda_{N-2}, l_{N-1}, \gamma_{N-1}\,|\,1-2\sin^2\eta_{N-1})\ldots$$
$$\times G(\lambda_2, l_3, \gamma_3\,|\,1-2\sin^2\eta_3)G(l_1, l_2, \gamma_2\,|\,1-2\sin^2\eta_2) \tag{4.13}$$

and

$$A(l, m\,|\,\omega) = \prod_{i=1}^{N} Y(l_i, m_i\,|\,\omega_i). \tag{4.14}$$

In equation (4.12), $\eta = \{\eta_j\}$ and $\omega = \{\omega_i\}$. The function S is the simultaneous eigenfunction of the operators $\Lambda^2 \equiv \Lambda_N^2, \Lambda_{N-1}^2, \Lambda_{N-2}^2, \ldots, \Lambda_3^2, \Lambda_2^2$ and $\boldsymbol{L}_N^2, \boldsymbol{L}_{N-1}^2, \ldots, \boldsymbol{L}_2^2, \boldsymbol{L}_1^2$; $(L_z)_N, (L_z)_{N-1}, \ldots, (L_z)_2, (L_z)_1$. These operators are in fact Casimir operators of the chain O(3N), O(3$N-3$), O(3$N-6$), ..., O(9), O(6) and ^{N}O(3), $^{N-1}$O(3), ..., ^{2}O(3), ^{1}O(3) which appear in the subgroup chain (2.2). The function S further satisfies

$$\Lambda^2(\Omega)S(\gamma, l, m\,|\,\Omega) = \lambda(\lambda+3N-2)S(\gamma, l, m\,|\,\Omega), \tag{4.15a}$$

$$\Lambda_j^2(\Omega_j)S(\gamma, l, m\,|\,\Omega) = \lambda_j(\lambda_j+3j-2)S(\gamma, l, m\,|\,\Omega), \tag{4.15b}$$

$$\boldsymbol{L}_i^2(\omega_i)S(\gamma, l, m\,|\,\Omega) = l_i(l_i+1)S(\gamma, l, m\,|\,\Omega), \tag{4.15c}$$

$$(L_z)_i(\varphi_i)S(\gamma, l, m\,|\,\Omega) = m_iS(\gamma, l, m\,|\,\Omega). \tag{4.15d}$$

In equation (4.15a),

$$\lambda = \xi + 2\beta, \qquad \xi = \sum_{i=1}^{N} l_i, \qquad \beta = \sum_{j=2}^{N} \gamma_j. \tag{4.16}$$

4.2. The homogeneous polynomial solutions of Laplace's equation in 3N dimensions

It is possible to construct another equivalent set of solutions to equation (4.1) by considering Laplace's equation in 3N dimensions. Let us define a function $U(\boldsymbol{r})$ by

$$U(\boldsymbol{r}) = r^\lambda S_\lambda(\Omega). \tag{4.17}$$

Operating the 3N-dimensional Laplacian on $U(\boldsymbol{r})$, we obtain

$$\left(\sum_{i=1}^{N}\nabla_i^2\right)U(\boldsymbol{r}) = \left(\frac{\partial^2}{\partial r^2}+\frac{3N-1}{r}\frac{\partial}{\partial r}-\frac{\Lambda^2(\Omega)}{r^2}\right)r^\lambda S_\lambda(\Omega)$$
$$= r^{\lambda-2}[\lambda(\lambda+3N-2)-\Lambda^2(\Omega)]S_\lambda(\Omega). \tag{4.18}$$

Hence the relation

$$\Lambda^2(\Omega)S_\lambda(\Omega) = \lambda(\lambda+3N-2)S_\lambda(\Omega) \tag{4.19}$$

is the necessary and sufficient condition for $U(\boldsymbol{r})$ to be a solution of the 3N-dimensional Laplace equation

$$\left(\sum_{i=1}^{N}\nabla_i^2\right)U(\boldsymbol{r}) = 0. \tag{4.20}$$

From the previous discussion in § 4.1 and equation (4.19), it is obvious that the function $S_\lambda(\Omega)$ is, in general, expressed by an arbitrary linear combination of the functions $S(\gamma, l, m\,|\,\Omega)$ as

$$S_\lambda(\Omega) = \sum_{\lambda_2,\lambda_3,\ldots,\lambda_{N-1}} \sum_{l_1,\ldots,l_N} \sum_{m_1,\ldots,m_N} C(\lambda_2, \ldots, \lambda_{N-1}; l_1, \ldots, l_N; m_1, \ldots, m_N) S(\gamma, l, m\,|\,\Omega). \tag{4.21}$$

We now try to find the homogeneous polynomial solutions of the Laplace equation (4.20). Once they are obtained, the functions $S_\lambda(\Omega)$ are determined by (4.18).

We first separate the harmonic polynomial U in ordinary spherical polar angles:

$$U(r) = Q(\beta, l\,|\,r_1, \ldots, r_N) A(l, m\,|\,\omega) \tag{4.22}$$

where $Q(\beta, l\,|\,r_1, \ldots, r_N)$ is a homogeneous polynomial of degree λ in $r_1, r_2, \ldots, r_N$, and $A(l, m\,|\,\omega)$ is defined in equation (4.14). It is shown that the hyperharmonic polynomial Q takes the form

$$Q(\beta, l\,|\,r_1, \ldots, r_N) = \sum_\alpha C_\alpha(\beta, l) \ell_\alpha(\beta, l\,|\,r_1, \ldots, r_N) \tag{4.23}$$

where

$$\ell_\alpha(\beta, l\,|\,r_1, \ldots, r_N) = r_1^{l_1+2\alpha_1} r_2^{l_2+2\alpha_2} \ldots r_N^{l_N+2\alpha_N}. \tag{4.24}$$

Here α denotes a set of N non-negative integers $\alpha = \{\alpha_1, \alpha_2, \ldots, \alpha_N\}$. Since λ is the degree of homogeneity of the polynomial Q, from equations (4.24) and (4.16), it is evident that

$$\beta = \sum_{j=2}^{N} \gamma_j = \sum_{i=1}^{N} \alpha_i. \tag{4.25}$$

Substituting equation (4.23) into equation (4.20), we obtain an equation which determines the set of coefficients $C_\alpha(\beta, l)$,

$$\sum_\alpha C_\alpha(\beta, l) \sum_{i=1}^{N} \alpha_i(2\alpha_i + 2l_i + 1) \frac{\ell_\alpha(\beta, l\,|\,r_1, \ldots, r_N)}{r_i^2} = 0. \tag{4.26}$$

Equating all the coefficients of linearly independent terms in equation (4.26) to zero, we can evaluate C_α. Generally equation (4.26) gives more than one possible set of coefficients C_α. The corresponding linearly independent polynomials Q can be labelled as

$$Q(\beta, l; i\,|\,r_1, \ldots, r_N) \tag{4.27}$$

where

$$i = 1, 2, \ldots, n_\beta, \qquad n_\beta = \binom{\beta + N - 2}{N - 2}.$$

We can now write a set of hyperspherical functions as

$$S(\beta, l, m; i\,|\,\Omega) = r^{-\lambda} Q(\beta, l; i\,|\,r_1, \ldots, r_N) A(l, m\,|\,\omega_1, \ldots, \omega_N). \tag{4.28}$$

As indicated in equation (4.21), the function $S(\beta, l, m; i\,|\,\Omega)$ is an eigenfunction of the operator Λ^2, but it is not an eigenfunction of operators $\Lambda_j^2, j = 1, 2, \ldots, N-1$. Since Q is a polynomial in the variables $r_1, r_2, \ldots, r_N$ which are ordinary spherical polar radii of

individual particles, it allows us immediately to see the transformation properties of the wavefunction under the exchange of particles. Furthermore, using equation (3.1), we can express Q in terms of the hyperspherical coordinates.

4.3. The hyperradial solution

The hyperradial equation (4.2) can be solved in the usual manner (I) and the result is

$$E_n = -\zeta^2/2n^2, \qquad n = s + \lambda + \tfrac{1}{2}(3N-1), \qquad s = 0, 1, 2, \ldots, \tag{4.29}$$

$$\mathcal{R}(n, \lambda \,|\, r) = N_{n,\lambda}\, \mathrm{e}^{-\rho/2}\rho^{\lambda} F(-n + \lambda + \tfrac{1}{2}(3N-1), 2\lambda + 3N - 1; \rho), \tag{4.30}$$

$\rho \equiv (2\zeta/n)r.$

In the above equation, $F(\alpha, \lambda\,; \rho)$ is the confluent hypergeometric function and $N_{n,\lambda}$ is the normalisation constant. The normalisation of the wavefunction $\psi(\boldsymbol{r}) = \mathcal{R}(n, \lambda \,|\, r)S_{\lambda}(\Omega)$ is

$$\int_0^{\infty} \mathrm{d}r\, r^{3N-1} \int \mathrm{d}\Omega\, \psi^*(\boldsymbol{r})\psi(\boldsymbol{r}) = 1, \tag{4.31}$$

where $\mathrm{d}\Omega$ is given in equation (3.6). From this normalisation, $N_{n,\lambda}$ is calculated to be

$$N_{n,\lambda} = \left[\left(\frac{2\zeta}{n}\right)^{3N} \frac{[n + \lambda + \frac{3}{2}(N-1)]!}{(2n)[n - \lambda - \frac{1}{2}(3N-1)]![(2\lambda + 3N - 2)!]^2}\right]^{1/2}. \tag{4.32}$$

5. The total angular momentum representation

The addition of the angular momentum operators of individual particles defines the total angular momentum operator $\boldsymbol{L}$:

$$\boldsymbol{L} = \boldsymbol{L}_1 + \boldsymbol{L}_2 + \ldots + \boldsymbol{L}_N. \tag{5.1}$$

Since the operators $\boldsymbol{L}^2$ and L_z commute with the Hamiltonian, our state function can be constructed as an eigenfunction of these. This representation is necessary when we consider perturbation problems to realistic systems. We couple the angular momenta of individual particles as

$$\begin{aligned} B(l_1, \ldots, l_N; L_2, \ldots, L_{N-1}; L, M_L \,|\, \omega) \\ = \sum_{M_{N-1}, m_N} (L_{N-1}, M_{N-1}, l_N, m_N \,|\, L_{N-1}, l_N, L, M_L) \\ \times \sum_{M_{N-2}, m_{N-1}} (L_{N-2}, M_{N-2}, l_{N-1}, m_{N-1} \,|\, L_{N-2}, l_{N-1}, L_{N-1}, M_{N-1}) \times \ldots \\ \times \sum_{M_2, m_3} (L_2, M_2, l_3, m_3 \,|\, L_2, l_3, L_3, M_3) \sum_{m_1, m_2} (l_1, m_1, l_2, m_2 \,|\, l_1, l_2, L_2, M_2) \\ \times A(l_1, \ldots, l_N; m_1, \ldots, m_N \,|\, \omega), \end{aligned} \tag{5.2}$$

where $(L_{j-1}, M_{j-1}, l_j, m_j \,|\, L_{j-1}, l_j, L_j, M_j)$ are Clebsch–Gordan coefficients. In this way we can realise the total angular momentum L by various possible ways indicated by the different sets of intermediate angular momenta $\{L_2, L_3, \ldots, L_{N-1}\}$. For simplicity of

notation, we shall denote a set $\{L_2, \ldots, L_{N-1}\}$ by a single index k. We denote the number of possible sets of intermediate angular momenta k by $n_L(l)$.

The hyperangular functions in the total angular momentum representation are now written as

$$S^{L,M_L}(\gamma, l; k \,|\, \Omega) = H(\gamma, l \,|\, \eta) B(l; k; L, M_L \,|\, \omega) \tag{5.3a}$$

or

$$S^{L,M_L}(\beta, l; k, i \,|\, \Omega) = r^{-\lambda} Q(\beta, l; i \,|\, r_1, \ldots, r_N) B(l; k; L, M_L \,|\, \omega). \tag{5.3b}$$

6. Construction of the Pauli antisymmetry-adapted wavefunctions

For a system of N identical fermions, the total wavefunction is restricted by the Pauli principle. If one starts from an independent particle model for an N-fermion system as one does customarily, the Pauli principle can easily be taken into account using the Slater determinants. However, it is not an easy problem for our model system, since the motions of particles are strongly coupled to one another. Here we can make use of the Kotani–Yamanouchi formalism (Kotani *et al* 1963) which provides a systematic method of constructing the antisymmetry-adapted wavefunctions for a system of N identical spin-$\frac{1}{2}$ fermions. We will now discuss this formalism.

In the space of spin functions for a system of N spin-$\frac{1}{2}$ fermions, we have 2^N linearly independent spin functions,

$$\theta_1(\sigma_1)\theta_2(\sigma_2) \ldots \theta_N(\sigma_N), \tag{6.1}$$

where each of $\theta_1, \theta_2, \ldots, \theta_N$ can be either α or β such that

$$s_i^2 \theta(\sigma_i) = \tfrac{1}{2}(\tfrac{1}{2}+1)\theta(\sigma_i), \qquad (s_i)_z \alpha(\sigma_i) = \tfrac{1}{2}\alpha(\sigma_i), \qquad (s_i)_z \beta(\sigma_i) = -\tfrac{1}{2}\beta(\sigma_i).$$

The monomial functions (6.1) are eigenfunctions of the total spin operator $\mathscr{S}_z$ with the eigenvalue M_s. They are not, however, eigenfunctions of $\mathscr{S}^2$, where

$$\mathscr{S} = s_1 + s_2 + \ldots + s_N.$$

In order to construct eigenstates of $\mathscr{S}^2$, the monomial functions (6.1) can be coupled according to a genealogical scheme. The vector coupling formulae according to this scheme are written as follows:

$$\begin{aligned}
&\Theta^{S,M_s}_{S_1,S_2,\ldots,S_{N-2},S+1/2}(\sigma_1, \ldots, \sigma_N) \\
&\quad = -\left(\frac{S-M_s+1}{2S+2}\right)^{1/2} \Theta^{S+1/2,M_s-1/2}_{S_1,S_2,\ldots,S_{N-2}}(\sigma_1, \ldots, \sigma_{N-1})\alpha(\sigma_N) \\
&\quad\quad + \left(\frac{S+M_s+1}{2S+2}\right)^{1/2} \Theta^{S+1/2,M_s+1/2}_{S_1,S_2,\ldots,S_{N-2}}(\sigma_1, \ldots, \sigma_{N-1})\beta(\sigma_N),
\end{aligned} \tag{6.2a}$$

$$\begin{aligned}
&\Theta^{S,M_s}_{S_1,S_2,\ldots,S_{N-2},S-1/2}(\sigma_1, \ldots, \sigma_N) \\
&\quad = \left(\frac{S+M_s}{2S}\right)^{1/2} \Theta^{S-1/2,M_s-1/2}_{S_1,S_2,\ldots,S_{N-2}}(\sigma_1, \ldots, \sigma_{N-1})\alpha(\sigma_N) \\
&\quad\quad + \left(\frac{S-M_s}{2S}\right)^{1/2} \Theta^{S-1/2,M_s+1/2}_{S_1,S_2,\ldots,S_{N-2}}(\sigma_1, \ldots, \sigma_{N-1})\beta(\sigma_N),
\end{aligned} \tag{6.2b}$$

where S_1 is always $\frac{1}{2}$; S_2 can be either 1 or 0 etc. For simplicity of notation, we denote a set $\{S_1, S_2, \ldots, S_{N-1}\}$ by a single index κ. The functions Θ_κ^{S,M_s} form a complete set of functions in spin space of N spin-$\frac{1}{2}$-fermions. Therefore, the total wavefunction with specified L, M_L, S and M_s can be expanded as

$$\Psi^{L,M_L;S,M_s}(\boldsymbol{r}, \boldsymbol{\sigma}) = \sum_{\kappa}^{f(S)} \psi_\kappa^{L,M_L;S}(\boldsymbol{r})\Theta_\kappa^{S,M_s}(\boldsymbol{\sigma}), \tag{6.3}$$

where $f(S)$ is the number of different sets κ which give the same total spin S. For the rest of this section, we will omit the indices L, M_L, S and M_s to simplify the notation.

The functions Θ_κ with specified S and M_s provide a basis set for an $f(S)$-dimensional irreducible representation of the symmetric group S_N. Let the permutation of particle coordinates, both space and spin, be denoted by P. Then

$$P\Theta_\kappa = \sum_{\kappa'=1}^{f(S)} \Theta_{\kappa'} V_{\kappa',\kappa}(P). \tag{6.4}$$

The Pauli principle then requires that

$$P\Psi = \varepsilon_P \Psi, \tag{6.5}$$

where ε_P is $+1$ or -1 according to P even or odd. Combining equations (6.3), (6.4) and (6.5), we find the transformation properties of the spatial functions ψ_κ:

$$P\psi_\kappa = \sum_{\kappa'=1}^{f(S)} \psi_{\kappa'} U_{\kappa',\kappa}(P), \tag{6.6}$$

where

$$U(P) = \varepsilon_P V^{\mathrm{T}}(P^{-1}).$$

V^{T} is the transpose matrix of V. The set of matrices $\{U(P)\}$ also gives an irreducible representation of the symmetric group S_N.

In order to construct the antisymmetric wavefunctions, we must thus find the Schrödinger wavefunctions satisfying equation (6.6). The hyperradial function is invariant under operations P; thus we want to find the hyperangular functions which have the special transformation properties shown in equation (6.6). The totality of hyperangular functions supplies a basis for an infinite-dimensional matrix representation of S_N. At this point, it is convenient to classify the hyperangular functions by four invariant labels. They are L, M_L, τ and β. L and M_L are invariant under the permutations because

$$[P, \boldsymbol{L}^2] = [P, L_z] = 0. \tag{6.7}$$

The symbol τ represents the 'l structure' of the function. It is defined by

$$\tau = \{(l^a)^{n_a}(l^b)^{n_b}(l^c)^{n_c}\ldots\} \qquad (n_a + n_b + n_c + \ldots = N) \tag{6.8}$$

where n_a is the number of l_j with $l_j = l^a$, n_b is the number of l_j with $l_j = l^b$, and so on. For a given τ, there are

$$n_\tau = N!/n_a!n_b!n_c!\ldots \tag{6.9}$$

distinct sets of l_j ordering [l_j ordering $[l_1, l_2, \ldots, l_N]$. We will index each set with a single integer j. The quantum number β is defined by equation (4.16):

$$\beta = \tfrac{1}{2}(\lambda - \xi) = \tfrac{1}{2}[\lambda - (n_a l^a + n_b l^b + n_c l^c + \ldots)] \tag{6.10}$$

Since $[P, \Lambda^2] = 0$, λ is invariant. From the invariance of λ and τ, it is evident that β is also an invariant. As shown in equation (4.27), for a given β and fixed L, M_L and τ, there are

$$n_\beta = \binom{\beta + N - 2}{N - 2} \tag{6.11}$$

linearly independent functions. We will index each one with a single integer i. Hence, the convenient labelling of the hyperangular function is given by

$$S_\mu^{L,M_L}(\beta, \tau | \Omega), \qquad \mu = \{i, j, k\}. \tag{6.12}$$

In a subspace specified by L, M_L, β and τ, the subset of functions $S_\mu^{L,M_L}(\beta, \tau|\Omega)$ supplies a finite-dimensional reducible representation of S_N:

$$PS_\mu = \sum_{\mu'=1}^{g(L,\beta,\tau)} S_{\mu'} X_{\mu',\mu}(P). \tag{6.13}$$

In the above expression and in the rest of this section, we omit the indices L, M_L, β and τ. The dimensionality of this representation is denoted by $g(L, \beta, \tau)$ and it can be calculated to be

$$g(L, \beta, \tau) = n_L(\tau) n_\beta n_\tau. \tag{6.14}$$

If the representation $\{X(P)\}$ contains the irreducible representation $\{U(P)\}$, it is possible to take linear combinations of the functions S_μ to construct new functions $\mathcal{S}_\kappa$ which provide a basis set for $\{U(P)\}$:

$$P\mathcal{S}_\kappa = \sum_{\kappa'} \mathcal{S}_{\kappa'} U_{\kappa',\kappa}(P), \tag{6.15}$$

where

$$\mathcal{S}_\kappa = \sum_\mu S_\mu C_{\mu,\kappa}. \tag{6.16}$$

Using this $\mathcal{S}_\kappa$, the spatial function ψ_κ in equation (6.3) is written as

$$\psi_\kappa(\boldsymbol{r}) = \mathcal{R}(n, \lambda | r) \mathcal{S}_\kappa(\Omega). \tag{6.17}$$

Combining equations (6.15), (6.16) and (6.13), we obtain a set of equations for $C_{\mu,\kappa}$:

$$\sum_\mu X_{\mu'\mu}(P) C_{\mu,\kappa} = \sum_{\kappa'} C_{\mu',\kappa'} U_{\kappa',\kappa}(P), \tag{6.18a}$$

or, in matrix notation,

$$\boldsymbol{X}(P)\boldsymbol{C} = \boldsymbol{C}\boldsymbol{U}(P). \tag{6.18b}$$

Solving equation (6.18) for $\boldsymbol{C}$, we can obtain $\mathcal{S}_\kappa$. However, in practice, it is more convenient to make use of projection operators to determine $\mathcal{S}_\kappa$. Equation (6.16) means that a basis function of an irreducible representation $\{U(P)\}$ designated by the total spin S is constructed by a linear combination of the independent functions S_μ:

$$\mathcal{S}_\kappa^{(S)} = \sum_\mu S_\mu C_{\mu,\kappa}^{(S)}. \tag{6.16'}$$

Here the designation of the irreducible representation is made by the superscript (S). Equation (6.16') conversely tells us that an S_μ is expressed as a linear combination of

the functions $\mathscr{S}_\kappa^{(S)}$:

$$S_\mu = \sum_{(S)} \sum_\kappa \mathscr{S}_\kappa^{(S)} a_{(S),\kappa;\mu}. \tag{6.19}$$

There is a projection operator $\mathscr{P}_\kappa^{(S)}$ which picks up a particular $\mathscr{S}_\kappa^{(S)}$ component from a function S_μ:

$$a_{(S),\kappa;\mu}\mathscr{S}_\kappa^{(S)} = \mathscr{P}_\kappa^{(S)} S_\mu. \tag{6.20}$$

Such an operator $\mathscr{P}_\kappa^{(S)}$ is given by (see e.g. Hamermesh 1962)

$$\mathscr{P}_\kappa^{(S)} = \frac{f(S)}{N!} \sum_P U_{\kappa,\kappa}^{(S)}(P)P. \tag{6.21}$$

For a given set of $\{L, \beta, \tau\}$, there are $g(L, \beta, \tau)$ linearly independent functions S_μ. If the representation $\{X(P)\}$ contains the irreducible representation $\{U^{(S)}(P)\}$, $\mathscr{P}_\kappa^{(S)} S_\mu$ are non-zero at least for one of S_μ. The function $\mathscr{S}_\kappa^{(S)}$ is proportional to $\mathscr{P}_\kappa^{(S)} S_\mu$ and $C_{\mu,\kappa}^{(S)}$ can be written as

$$C_{\mu,\kappa}^{(S)} = b_\kappa^{(S)} \frac{f(S)}{N!} \sum_P U_{\kappa,\kappa}^{(S)}(P) X_{\mu,\mu^*}(P), \tag{6.22}$$

where $b_\mu^{(S)}$ is the proportionality constant. The μ^* is a set of quantum numbers i, j, k for which $\mathscr{P}_\kappa^{(S)} S_{\mu^*}$ is non-zero. The correct set of the proportionality constants $b_\kappa^{(S)}$ can be easily determined by substituting equation (6.22) into equation (6.18). Therefore, knowing the transformation properties of S_μ in the form of equation (6.13), the use of equations (6.22) and (6.18) determines $\mathscr{S}_\kappa^{(S)}$. Using these $\mathscr{S}_\kappa^{(S)}$, the correct antisymmetry-adapted wavefunctions are constructed by equations (6.3) and (6.17).

7. Antisymmetry-adapted wavefunctions for $N = 2$

In this section, we use the hyperangular functions of the form given in equation (5.3*a*):

$$S^{L,M_L}(\gamma, l\,|\,\Omega) = H(\gamma, l\,|\,\eta)B(l; L, M_L\,|\,\omega), \tag{7.1}$$

where

$$l = [l^a, l^b], \qquad H(\gamma, l\,|\,\eta) = G(l^a, l^b, \gamma\,|\,1 - 2\sin^2\eta). \tag{7.2}$$

We now consider the function $S_\mu^{L,M_L}(\beta, \tau\,|\,\Omega)$. For $N = 2$, it is evident that $n_b = 1$ and $n_L(\tau) = 1$. When the l-structure is given by $\tau = \{(l^a)^2\}$, $n_\tau = 1$. However, for $\tau = \{(l^a)^1(l^b)^1\}$ with $l^a \neq l^b$, $n_\tau = 2$. Hence we have two different cases. The former gives a one-dimensional representation of the symmetric group S_2, and the latter gives a two-dimensional reducible representation:

$$g(L, \beta, \tau = \{(l^a)^2\}) = 1, \qquad g(L, \beta, \tau = \{(l^a)^1(l^b)^1\}) = 2. \tag{7.3}$$

We denote the permutation operators by

$$I \equiv \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix}, \qquad P_{21} \equiv \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}. \tag{7.4}$$

Under the P_{21} operation, H and B transform as

$$P_{21}B([l^a, l^b]; L, M_L\,|\,\omega_1, \omega_2) = (-)^{-l^a - l^b + L} B([l^b, l^a]; L, M_L\,|\,\omega_1, \omega_2) \tag{7.5}$$

and

$$P_{21}H(\gamma,[l^a,l^b]|\eta)=(-)^{-\gamma}H(\gamma,[l^b,l^a]|\eta). \tag{7.6}$$

Therefore equation (6.13) can be written as

$$\begin{aligned}&IS^{L,M_L}(\gamma,[l^a,l^b]|\Omega)=S^{L,M_L}(\gamma,[l^a,l^b]|\Omega),\\&P_{21}S^{L,M_L}(\gamma,[l^a,l^b]|\Omega)=(-)^{-l^a-l^b-\gamma+L}S^{L,M_L}(\gamma,[l^b,l^a]|\Omega).\end{aligned} \tag{7.7}$$

For $\tau=\{(l^a)^2\}$, equations (6.22) and (7.7) give

$$\begin{aligned}C^{(S)}&=\tfrac{1}{2}b^{(S)}f(S)[U^{(S)}(I)\times 1+U^{(S)}(P_{21})(-1)^{L-\gamma}]\\&=\tfrac{1}{2}b^{(S)}f(S)[1\times 1+(-1)^S(-1)^{L-\gamma}]\\&=\tfrac{1}{2}b^{(S)}f(S)[1+(-1)^{L-\gamma+S}].\end{aligned} \tag{7.8}$$

From equations (6.16′) and (7.8), with proper normalisation, we obtain

$$\mathcal{S}^{L,M_L;(S)}(\beta=\gamma,\tau=\{(l^a)^2\}|\Omega)=\tfrac{1}{2}[1+(-1)^{L-\gamma+S}]S^{L,M_L}(\gamma,[l^a,l^a]|\Omega). \tag{7.9}$$

For $\tau=\{(l^a)^1(l^b)^1\}$ with $l^a\neq l^b$, $C_\mu^{(S)}$ are written as

$$\begin{aligned}&C^{(S)}_{[l^a,l^b]}=(\tfrac{1}{2})b^{(S)}f(S)[U^{(S)}(I)\times 1+U^{(S)}(P_{21})\times 0]=(\tfrac{1}{2})b^{(S)}(S),\\&C^{(S)}_{[l^b,l^a]}=\tfrac{1}{2}b^{(S)}f(S)[U^{(S)}(I)\times 0+U^{(S)}(P_{21})\times(-1)^{-l^a-l^b-\gamma+L}]\\&\qquad=\tfrac{1}{2}b^{(S)}f(S)(-1)^{-l^a-l^b-\gamma+L+S}.\end{aligned} \tag{7.10}$$

After the proper normalisation, equations (6.16′) and (7.10) give

$$\begin{aligned}&\mathcal{S}^{L,M_L;(S)}(\beta=\gamma,\tau=\{(l^a)^1(l^b)^1\}|\Omega)\\&\qquad=(1/\sqrt{2})\{S^{L,M_L}(\gamma,[l^a,l^b]|\Omega)+(-)^{-l^a-l^b-\gamma+L+S}S^{L,M_L}(\gamma,[l^b,l^a]|\Omega).\end{aligned} \tag{7.11}$$

Both equations (7.8) and (7.10) satisfy equation (6.18) and our results are correct. In fact, equations (7.9) and (7.11) are exactly the same as the expression given in Macek (1967). The total antisymmetry-adapted wavefunctions are now given by

$$\Psi^{L,M_L;S,M_s}(n,\beta,\tau|\boldsymbol{r},\boldsymbol{\sigma})=\mathcal{R}(n,\lambda|r)\mathcal{S}^{L,M_L;(S)}(\beta,\tau|\Omega)\Theta^{S,M_s}(\boldsymbol{\sigma}). \tag{7.12}$$

From equations (2.2), (4.16) and (7.9), the ground state of our model system is identified as

$$\Psi^{L=0,M_L=0;S=0,M_s=0}(n=\tfrac{5}{2},\beta=0,\tau=\{s^2\}|\boldsymbol{r},\boldsymbol{\sigma}).$$

8. Antisymmetry-adapted wavefunctions for N = 3

For $N\geqslant 3$, if we use the functions (5.3*a*), it is rather tedious to investigate their transformation properties under the operations of permutations. But using functions in the form in equation (5.3*b*), we can easily see their transformation properties, and the construction of the antisymmetric wavefunctions is straightforward. However, it is difficult to obtain a closed expression which can describe all the possible antisymmetric states. We therefore present a class of antisymmetric wavefunctions which consists of all the ground states, all the first excited states and the states obtained by the hyperradial

excitations of these. The construction procedure given in § 6 will be followed. The results are given below.

$$\Psi(L=1, M_L; S=\tfrac{1}{2}, M_s: n, \beta=0, \tau=\{s^2p\}\,|\,\boldsymbol{r}, \boldsymbol{\sigma})$$
$$= \text{const}\,\mathcal{R}(n, \lambda=1\,|\,r)\{-\sqrt{3}[\sin\eta_3\cos\eta_2 Y(1, M_L\,|\,\omega_2)$$
$$-\sin\eta_3\sin\eta_2 Y(1, M_L\,|\,\omega_1)]\Theta(s=\tfrac{1}{2}, M_s; S_2=1\,|\,\boldsymbol{\sigma})$$
$$+[2\cos\eta_3 Y(1, M_L\,|\,\omega_3)-\sin\eta_3\cos\eta_2 Y(1, M_L\,|\,\omega_2)$$
$$-\sin\eta_3\sin\eta_2 Y(1, M_L\,|\,\omega_1)]\Theta(s=\tfrac{1}{2}, M_s; S_2=0\,|\,\boldsymbol{\sigma})\}, \tag{8.1}$$

where $n=5, 6, 7, 8, \ldots,$

$$\Psi(L=0, M_L=0; S=\tfrac{1}{2}, M_s: n, \beta=1, \tau=\{s^3\}\,|\,\boldsymbol{r}, \boldsymbol{\sigma})$$
$$= \text{constant}\,\mathcal{R}(n, \lambda=2\,|\,r)[-\sqrt{3}\sin^2\eta_3(1-2\sin^2\eta_2)\Theta(S=\tfrac{1}{2}, M_s; S_2=1\,|\,\boldsymbol{\sigma})$$
$$+(2-3\sin^2\eta_3)\Theta(S=\tfrac{1}{2}, M_s; S_2=0\,|\,\boldsymbol{\sigma})], \tag{8.2}$$

where $n=6, 7, 8, \ldots,$

$$\Psi(L=1, M_L; S=\tfrac{3}{2}, M_s: n, \beta=0, \tau=\{sp^2\}\,|\,\boldsymbol{r}, \boldsymbol{\sigma})$$
$$= \text{constant}\,\mathcal{R}(n, \lambda=2\,|\,r)[\sin\eta_3\cos\eta_2\cos\eta_3\mathcal{Y}(1, 1; 1, M_L\,|\,\omega_2, \omega_3)$$
$$-\sin\eta_3\sin\eta_2\cos\eta_3\mathcal{Y}(1, 1; 1, M_L\,|\,\omega_1, \omega_3)$$
$$+\sin^2\eta_3\sin\eta_2\cos\eta_2\mathcal{Y}(1, 1; 1, M_L\,|\,\omega_1, \omega_2)]\Theta(S=\tfrac{3}{2}, M_s\,|\,\boldsymbol{\sigma}), \tag{8.3}$$

where $n=6, 7, 8, \ldots,$

$$\Psi(L=0 \text{ or } 2, M_L; S=\tfrac{1}{2}, M_s: n, \beta=0, \tau=\{sp^2\}\,|\,\boldsymbol{r}, \boldsymbol{\sigma})$$
$$= \text{constant}\,\mathcal{R}(n, \lambda=2\,|\,r)\{\sqrt{3}[\sin\eta_3\cos\eta_2\cos\eta_3\mathcal{Y}$$
$$\times(1, 1; L=0 \text{ or } 2, M_L\,|\,\omega_2, \omega_3)-\sin\eta_3\sin\eta_2\cos\eta_3\mathcal{Y}$$
$$\times(1, 1; L=0 \text{ or } 2, M_L\,|\,\omega_1, \omega_3)]\Theta(S=\tfrac{1}{2}, M_s; S_2=1\,|\,\boldsymbol{\sigma})$$
$$-[\sin\eta_3\cos\eta_2\cos\eta_3\mathcal{Y}(1, 1; L=0 \text{ or } 2, M_L\,|\,\omega_2, \omega_3)$$
$$+\sin\eta_3\sin\eta_2\cos\eta_3\mathcal{Y}(1, 1; L=0 \text{ or } 2, M_L\,|\,\omega_1, \omega_3)$$
$$-2\sin^2\eta_3\sin\eta_2\cos\eta_2\mathcal{Y}(1, 1; L=0 \text{ or } 2, M_L\,|\,\omega_1, \omega_2)]$$
$$\times\Theta(S=\tfrac{1}{2}, M_s; S_2=0\,|\,\boldsymbol{\sigma})\} \tag{8.4}$$

where $n=6, 7, 8, \ldots,$

$$\Psi(L=1, M_L; S=\tfrac{1}{2}, M_S: n, \beta=0, \tau=\{sp^2\}\,|\,\boldsymbol{r}, \boldsymbol{\sigma})$$
$$= \text{constant}\,\mathcal{R}(n, \lambda=2\,|\,r)\{[\sin\eta_3\cos\eta_2\cos\eta_3\mathcal{Y}(1, 1; L=1, M_L\,|\,\omega_2, \omega_3)$$
$$-\sin\eta_3\sin\eta_2\cos\eta_3\mathcal{Y}(1, 1; L=1, M_L\,|\,\omega_1, \omega_3)$$
$$-2\sin^2\eta_3\sin\eta_2\cos\eta_2\mathcal{Y}(1, 1; L=1, M_L\,|\,\omega_1, \omega_2)]$$
$$\times\Theta(S=\tfrac{1}{2}, M_s; S_2=1\,|\,\boldsymbol{\sigma})$$
$$+\sqrt{3}[\sin\eta_3\cos\eta_2\cos\eta_3\mathcal{Y}(1, 1; L=1, M_L\,|\,\omega_2, \omega_3)$$
$$+\sin\eta_3\sin\eta_2\cos\eta_3\mathcal{Y}(1, 1; L=1, M_L\,|\,\omega_1, \omega_3)]$$
$$\times\Theta(S=\tfrac{1}{2}, M_s; S_2=0\,|\,\boldsymbol{\sigma})\}, \tag{8.5}$$

where $n = 6, 7, 8, \ldots,$

$$\Psi(L=2, M_L; S=\tfrac{1}{2}, M_s: n, \beta=0, \tau=\{s^2d\}|\boldsymbol{r}, \boldsymbol{\sigma})$$
$$= \text{constant} \times \mathscr{R}(n, \lambda=2|r)\{-\sqrt{3}[\sin^2\eta_3 \cos^2\eta_2 Y(2, M_L|\omega_2)$$
$$-\sin^2\eta_3 \sin^2\eta_2 Y(2, M_L|\omega_1)]\Theta(S=\tfrac{1}{2}, M_s; S_2=1|\boldsymbol{\sigma})$$
$$\times[2\cos^2\eta_3 Y(2, M_L|\omega_3) - \sin^2\eta_3 \cos^2\eta_2 Y(2, M_L|\omega_2)$$
$$-\sin^2\eta_3 \sin^2\eta_2 Y(2, M_L|\omega_1)]\Theta(S=\tfrac{1}{2}, M_s; S_2=0|\boldsymbol{\sigma})\}. \tag{8.6}$$

where $n = 6, 7, 8, \ldots.$
In equations (8.1)–(8.6), $\Theta(S, M_s: S_2|\boldsymbol{\sigma})$ are the spin functions which satisfy

$$\mathscr{S}^2\Theta(S, M_s; S_2|\boldsymbol{\sigma}) = S(S+1)\Theta(S, M_s; S_2|\boldsymbol{\sigma}), \tag{8.7}$$

$$\mathscr{S}_z\Theta(S, M_s; S_2|\boldsymbol{\sigma}) = S_z\Theta(S, M_s; S_2|\boldsymbol{\sigma}), \tag{8.8}$$

$$\mathscr{S}_2^2\Theta(S, M_s; S_2|\boldsymbol{\sigma}) = S_2(S_2+1)\Theta(S, M_s; S_2|\boldsymbol{\sigma}), \tag{8.9}$$

where

$$\mathscr{S}_2 = s_1 + s_2, \qquad \mathscr{S} = \mathscr{S}_2 + s_3. \tag{8.10}$$

and s_i are one-particle spin operators. Explicit expressions of Θ are given in equation (6.2). The functions $\mathscr{Y}$ are defined as

$$\mathscr{Y}(l_1, l_2; L, M_L|\omega_1, \omega_2)$$
$$= \sum_{m_1} Y(l_1, m_1|\omega_1) Y(l_2, M_L - m_1|\omega_2)(l_1, m_1, l_2, M_L - m_1|l_1, l_2, L, M_L). \tag{8.11}$$

We list all the possible antisymmetry-adapted ground and first excited states in table 1.

Table 1.

η	S	λ	β	ξ	τ	L	S	Term	Equation	
(4	0	0	0	0	S^3	0)		No antisymmetry adapted state is allowed		
5	0	1	0	1	S^2p	1	$\frac{1}{2}$	^2P	(8.1)	Ground states
6	0	2	1	0	S^3	0	$\frac{1}{2}$	^2S	(8.2)	1st excited states
6	0	2	0	2	Sp^2	1	$\frac{3}{2}$	^4P	(8.3)	
6	0	2	0	2		0	$\frac{1}{2}$	^2S	(8.4)	
6	0	2	0	2		1	$\frac{1}{2}$	^2P	(8.5)	
6	0	2	0	2		2	$\frac{1}{2}$	^2D	(8.4)	
6	0	2	0	2	S^2d	2	$\frac{1}{2}$	^2D	(8.6)	
6	1	1	0	1	S^2d	1	$\frac{1}{2}$	^2P	(8.1)	

9. Applications and concluding remarks

As we mentioned in § 1, our exactly soluble model systems provide a new starting point for a perturbation theory to realistic systems. This idea was considered by White and Stillinger (1970) for the ground state of two-electron atoms ($N = 2$). They took the

exactly soluble model system described by the Hamiltonian (1.1) as the unperturbed starting point. The parameter ζ in the unperturbed Hamiltonian (1.1) was obtained by averaging the actual electron–electron and electron–nucleus potentials over all the $3N-1=5$ hyperspherical angles in the configuration space. In spite of the crudeness of the zeroth-order model, they obtained a reasonable value for the energy expectation value by the second-order correction. There is another method to determine the value of the parameter ζ for the zeroth-order model.

For a system defined by

$$H = \tfrac{1}{2}(\boldsymbol{p}_1^2 + \ldots + \boldsymbol{p}_N^2) + U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N), \tag{9.1}$$

we separate the Hamiltonian into two parts:

$$H = H_0(\zeta) + H'(\zeta), \tag{9.2}$$

where

$$H_0(\zeta) = \tfrac{1}{2}(\boldsymbol{p}_1^2 + \ldots + \boldsymbol{p}_N^2) - \zeta/(\boldsymbol{r}_1^2 + \ldots + \boldsymbol{r}_N^2)^{1/2} \tag{9.3}$$

and

$$H'(\zeta) = U(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) - [-\zeta/(\boldsymbol{r}_1^2 + \ldots + \boldsymbol{r}_N^2)^{1/2}]. \tag{9.4}$$

The eigenvalue problem

$$(H - E)\Psi = 0 \tag{9.5}$$

is approached by perturbation expansions of the eigenfunctions and eigenvalues:

$$\begin{aligned} \Psi(\zeta) &= \psi_0(\zeta) + \xi\psi_1(\zeta) + \ldots, \\ E(\zeta) &= E_0(\zeta) + \xi E_1(\zeta) + \xi^2 E_2(\zeta) + \ldots. \end{aligned} \tag{9.6}$$

An appropriate value of ζ can be determined by the variational requirement

$$\frac{\partial}{\partial\zeta}\left[\frac{\langle\Phi(\zeta)|H|\Phi(\zeta)\rangle}{\langle\Phi(\zeta)|\Phi(\zeta)\rangle}\right] = 0, \tag{9.7}$$

where

$$\Phi(\zeta) = \psi_0(\zeta) + \xi^i\psi_i(\zeta). \tag{9.8}$$

The $\xi^i\psi_i(\zeta)$ is the lowest-order correction to the $\psi_0(\zeta)$.

In any case, it is essential to know the physically acceptable zeroth-order states which satisfy the Pauli principle. The zeroth-order states cannot always give good approximations to realistic systems; however, this kind of approach has certain advantages. The zeroth-order states here correspond (contrary to the usual practice) to strongly coupled particle states. The global quantum numbers of the model system can provide a useful classification of the states of a quantum system with strong particle correlations. In fact the study of two-electron atoms based on the idea of Fano (1976), Macek (1968) and Lin (1974) (Klar and Klar 1980; for three-electron systems, see Clark and Greene (1980)) showed that the quantum numbers related to the model system are very useful for the classification of the doubly excited states of He. Our model system may also give some useful insight into the periodicity of atoms (periodic table). With the independent particle model, one cannot explain the Aufbau principle whose characteristic is due to a symmetry breaking by particle interactions. It is interesting to study the Aufbau scheme from another end, starting from an exactly

soluble interacting model like the one shown in this paper. This problem is now under investigation.

In summary, we have discussed a class of exactly soluble quantum systems of N interacting identical spin-$\frac{1}{2}$-fermions. The classification of the state vectors is based on the dynamical group $O(3N+1, 2)$ and its subgroups. The Casimir operators of the subgroups are expressed in terms of hyperspherical coordinates, and the group theoretical interpretation of the corresponding quantum numbers is exhibited. We have presented a systematic procedure of constructing the Pauli antisymmetry-adapted wavefunctions. This procedure works in principle for the system of any number of spin-$\frac{1}{2}$-fermions. The resulting antisymmetric states are labelled by conserved good quantum numbers. For $N = 2$ and 3, these antisymmetric wavefunctions are explicitly constructed. For $N = 2$, the ground state of our model system is designated by $^1S(s^2)$ (analogous to the ground state of atomic helium or deuteron, in the nuclear physics context). For $N = 3$, however, the ground state of our model system is labelled by $^2P(s^2p)$. The ground state of atomic lithium is $^2S(s^3)$. For our model system, the state $^2S(s^3)$ appears in its first excited level ($n = 6$). No state with $n = 4$ is allowed by the Pauli exclusion principle. Note however, that the quantum numbers in the model and in atomic physics notation do not have exactly the same meaning, but one can establish a correspondence.

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