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1987 J. Phys. A: Math. Gen. 20 121

(http://iopscience.iop.org/0305-4470/20/1/021)

J. Phys. A: Math. Gen. **20** (1987) 121-131. Printed in the UK

Boson representation of Fermi systems: nature and properties of subsidiary conditions

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Received 17 February 1986, in final form 13 May 1986

Abstract. Based on Girardeau's composite-particle theory the PPP (extended Hubbard) Hamiltonian is represented in terms of ideal-boson operators. A major unsolved problem was to find (approximate) eigenstates of the Hamiltonian which, at the same time, satisfy certain subsidiary conditions. The latter are necessary to ensure that the mapping of the fermion space into the space of boson states is unique. In the present paper a partial solution to the above mentioned problem is presented by using some arguments from the representation theory of the symmetric group. The results are of immediate practical relevance for all calculations dealing with the eigenvalue problem of the Hamiltonian in ideal-boson space.

1. Introduction

In recent years electron-pair theories have become popular in various branches of physics. In solid-state theory, for example, pair theory concepts are presently used to study exciton systems at high density and the related problem of Bose-Einstein condensation of excitons (Rashba and Sturge 1982). Another field, where pair theories might be useful, is the theory of the metal-insulator transition (Mott 1974). In this context a pair-theory approach to the Hubbard (1963) Hamiltonian has been formulated by the present author (Barentzen 1983, hereafter referred to as I). More recently a variational treatment of the Hubbard model based on similar ideas has been worked out by Katsnelson and Irkhin (1984).

Electron pairs are sometimes denoted as quasibosons, since the commutation relations of fermion-pair operators resemble those of elementary (ideal) bosons. The basic idea of the pair-theory method is to represent the fermion Hamiltonian by ideal-boson operators and to diagonalise it in a boson space. Mathematically this corresponds to a mapping of the fermion space into a space of boson states. Such mappings can be performed in a variety of ways; a good account of several of these methods is given in the monograph by Ring and Schuck (1980).

A particularly simple and elegant formulation of the many-body problem for composite particles has been worked out by Girardeau (1963). In his method the Hamiltonian $\hat{H}$ in boson space takes a rather simple and familiar form. The price one pays for the simplicity of the Hamiltonian is that all eigenstates $|\Psi_M)$ of $\hat{H}$ are required to be simultaneous eigenstates of a certain exchange operator $\hat{K}$, which commutes with $\hat{H}$ and the pair occupation number operator $\hat{N}$:

$$\hat{K}|\Psi_M) = -\tfrac{1}{2}M(M-1)|\Psi_M). \tag{1.1}$$

0305-4470/87/010121+11$02.50

This subsidiary condition, where M ($M = 1, 2, \ldots$) are the eigenvalues of $\hat{N}$, guarantees that only those boson states $|\Psi_M)$ are considered, which satisfy the Pauli principle. The same condition is also necessary to ensure that the mapping of the fermion space into the space of boson states is unique. In practical calculations, for example, variational treatments, the fulfilment of the subsidiary condition causes severe problems, because each trial vector has to be chosen *a priori* such that condition (1.1) is satisfied. So far the problem has not been solved in a satisfactory manner and this is probably the reason why no calculations based on the pair-theory method have been published so far.

The aim of the present paper is to derive the most general eigenvector $|\Psi_M)$ of equation (1.1) for arbitrary M, and thus to provide a partial solution to the problem outlined above. The essential elements of the pair-theory method are summarised in §§ 2 and 3, the treatment there being mainly based on Girardeau's (1963) composite-particle theory. The method will be illustrated by choosing the PPP (extended Hubbard) model as an example. The eigenvalue problem (1.1) is studied in § 4. The eigenvalues as well as the general form of the eigenvectors of $\hat{K}$ have already been obtained by Girardeau (1963, appendix). For $-M(M-1)/2$, the lowest eigenvalue of $\hat{K}$, the most general eigenvector satisfying equation (1.1) is then derived in an obvious way by using techniques from the representation theory of the symmetric group (Boerner 1963). From the most general $|\Psi_M)$ a special eigenvector will be obtained, which might be a good trial vector for a variational treatment of $\hat{H}$. Finally the main results of the present work are summarised in § 5.

2. The overcompleteness problem

The main features of the pair-theory method can be more easily understood by referring to a particular model. The Hamiltonian to be chosen here is the well known PPP Hamiltonian (Parr 1963, Koutecký *et al* 1985), often also denoted as extended Hubbard model. In the usual Fock-space representation the Hamiltonian may be written as

$$H = \sum_{\sigma k} \varepsilon_k a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_{qkk'} U(q) a^{\dagger}_{k+q,\uparrow} a^{\dagger}_{k'-q,\downarrow} a_{k'\downarrow} a_{k\uparrow} + \tfrac{1}{2} \sum_{\sigma} \sum_{qkk'} \tilde{U}(q) a^{\dagger}_{k+q,\sigma} a^{\dagger}_{k'-q,\sigma} a_{k'\sigma} a_{k\sigma} \tag{2.1}$$

where the $a^{\dagger}_{k\sigma}$ and $a_{k\sigma}$ are, respectively, the creation and annihilation operators for an electron with spin σ and reduced wavevector k. The one-particle part of (2.1) is the usual hopping term, while the remaining terms represent the Coulomb interactions. Here $U(q)$ and $\tilde{U}(q) = U(q) - U/N$ denote the two-electron Coulomb repulsion integrals, where U describes the on-site interaction. Since the precise analytical forms of the matrix elements are irrelevant for our purposes, they will not be given here. The Hubbard (1963) model is related to the PPP Hamiltonian (2.1) and can be recovered from the latter by replacing $U(q)$ by U/N. Hereafter it will be assumed that the total number N_e of electrons equals the number N of lattice sites (half-filled band case).

The PPP Hamiltonian possesses several constants of motion. They need not all be listed here, since they have been exhaustively discussed in the recent paper by Koutecký *et al* (1985). The only constants of motion needed in the following are the number operators $N_\sigma = \Sigma_k a^{\dagger}_{k\sigma} a_{k\sigma}$ where, because of the relation $N_\uparrow + N_\downarrow = N$, it suffices to consider only $N_\downarrow$ and its associated eigenvalues M ($M = 0, 1, 2, \ldots$). The Hamiltonian

(2.1) will now be rewritten in terms of particle-hole (p-h) operators. To this end a new vacuum state is introduced by

$$|\Psi_0\rangle = \prod_k a_{k\uparrow}^\dagger |0\rangle \tag{2.2}$$

where the product extends over all wavevectors of the reduced zone and the $a_{k\sigma}$ are redefined as

$$a_{k\sigma} = \begin{cases} b_k & \text{for } \sigma = \downarrow \text{ (particles)} \\ c_k^\dagger & \text{for } \sigma = \uparrow \text{ (holes).} \end{cases} \tag{2.3}$$

The b_k and c_k both annihilate the new vacuum and all particle operators anticommute with all hole operators because they refer to different spin components. Moreover, $|\Psi_0\rangle$ is an eigenvector of both $N_\downarrow$ and H with respective eigenvalues $M = 0$ and $E_0 = N^2\tilde{U}(0)/2$.

The new fermion operators are now used to construct the p-h operators; they are defined by

$$\rho_k(q) = c_{k+q} b_k \qquad \rho_k^\dagger(q) = b_k^\dagger c_{k+q}^\dagger. \tag{2.4}$$

Unfortunately these operators satisfy rather complicated commutation relations, as was shown by Girardeau (1963) and in paper I. Since they resemble those of elementary (ideal) bosons, fermion pairs are sometimes also denoted as quasibosons. To obtain H in terms of the p-h operators, let $\mathcal{U}_M$ denote the subspace spanned by all eigenvectors of $N_\downarrow$ for some fixed eigenvalue $M > 0$ of $N_\downarrow$ (the trivial case $M = 0$ will be excluded here and in the following, since it has already been solved above). An arbitrary vector $|\Psi_M\rangle$ of $\mathcal{U}_M$ has the form

$$|\Psi_M\rangle = \frac{1}{M!} \sum_{k_1 \ldots k_M} \sum_{q_1 \ldots q_M} \psi_{k_1 \ldots k_M}(q_1 \ldots q_M) |(k_1 q_1) \ldots (k_M q_M)\rangle \tag{2.5a}$$

where

$$|(k_1 q_1) \ldots (k_M q_M)\rangle = \rho_{k_1}^\dagger(q_1) \ldots \rho_{k_M}^\dagger(q_M) |\Psi_0\rangle \tag{2.5b}$$

and ψ is an arbitrary coefficient function. Then, by using the same arguments as in paper I, we find that on any subspace $\mathcal{U}_M$ the p-h number operator $N_\downarrow$ takes the form

$$N_\downarrow = \frac{1}{M} \sum_{qk} \rho_k^\dagger(q) \rho_k(q) \tag{2.6}$$

while the PPP Hamiltonian is obtained as

$$H_M = E_0 + H_{M1} + H_{M2} \tag{2.7a}$$

where

$$H_{M1} = \sum_{qkk'} \left(\frac{1}{M} \omega_k(q) \delta_{kk'} - U(k - k') \right) \rho_k^\dagger(q) \rho_{k'}(q) \tag{2.7b}$$

and

$$H_{M2} = \tfrac{1}{2} \sum_q \tilde{U}(q) (\Gamma_1^\dagger(q) \Gamma_1(q) + \Gamma_2^\dagger(q) \Gamma_2(q)). \tag{2.7c}$$

The p-h energies $\omega_k(q)$ in (2.7*b*) are defined by

$$\omega_k(q) = U + \varepsilon_k - \varepsilon_{k+q} \tag{2.8}$$

while the operators $\Gamma_t(q)$ in (2.7*c*) are given by

$$\Gamma_1(q) = \frac{1}{M} \sum_{kk'} \rho^+_{k'}(k+q)\rho_{k'}(k) \tag{2.9a}$$

$$\Gamma_2(q) = \frac{1}{M} \sum_{kk'} \rho^+_{k'}(k+q)\rho_{k'+q}(k). \tag{2.9b}$$

In view of the complicated form of the p-h commutators it would be highly desirable to see, if there is a possibility of expanding the quasiboson operators $\rho_k(q)$ in terms of ideal-boson operators $B_k(q)$, possibly at the cost of some additional terms in the Hamiltonian. This is the basic idea of the pair-theory method. For this purpose it would be necessary to map the spaces $\mathcal{U}_M$ together with their associated operators into a space of ideal-boson states. Before this can be done, however, a serious mathematical obstacle has to be overcome, which is inherent in all composite-particle theories. Namely, it generally turns out that the set of all product states (2.5*b*) is overcomplete for all $M \geq 2$. Since the problem has been discussed in detail by Girardeau (1963) and the present author (paper I), only the main arguments will be provided here without proof. Overcompleteness implies, of course, that a given vector $|\Psi_M\rangle$ of $\mathcal{U}_M$ ($M \geq 2$) does not possess a unique expansion in terms of the product states (2.5*b*) and, hence, would have many images in ideal-boson space.

There are several ways how to overcome the overcompleteness problem; some of these methods have been reviewed by Ring and Schuck (1980). In Girardeau's (1963) composite-particle theory on which the present work is based, the problem is solved by imposing subsidiary conditions on the space of coefficient functions ψ (equation (2.5*a*)) so that the latter all represent physically admissible many-pair states, i.e. states having the correct symmetry under exchange of fermions between different pairs, and thus satisfying the Pauli principle. The subsidiary conditions imposed by Girardeau (1963) are

$$K_{ij}\psi_{k_1 \ldots k_M}(q_1 \ldots q_M) = -\psi_{k_1 \ldots k_M}(q_1 \ldots q_M) \qquad 1 \leq i < j \leq M \tag{2.10a}$$

where $K_{ij}\psi$ is defined by (see paper I)

$$K_{ij}\psi_{k_1 \ldots k_M}(q_1 \ldots q_M) = \psi_{k_1 \ldots k_M}(q_1 \ldots q_j + k_j - k_i \ldots q_i + k_i - k_j \ldots q_M). \tag{2.10b}$$

While it is not difficult to show that any coefficient function satisfying (2.10) also obeys the Pauli principle, it requires more effort to prove that *the same conditions just suffice to remove the overcompleteness of the product states* (2.5*b*). For a proof of this assertion the reader is again referred to Girardeau's (1963) paper. In summary, any given vector $|\Psi_M\rangle$ of $\mathcal{U}_M$ can be uniquely represented by an expansion such as (2.5*a*), provided the coefficient function ψ satisfies the subsidiary conditions (2.10).

The functions ψ and $K_{ij}\psi$ only differ by a fermion interchange (either particles or holes) between pairs i and j ($1 \leq i < j \leq M$). This can be more easily seen in the Wannier representation. The latter is obtained by means of the relation

$$\rho^+_k(q) = \sum_{mn} (mn|kq)\rho^+_m(n) \tag{2.11}$$

the $\rho^+_m(n)$ denoting the p-h creation operators in the Wannier representation. The Fourier coefficients $(mn|kq)$ are defined by

$$(mn|kq) = (kq|mn)^* = N^{-1} \exp\{\mathrm{i}[kR_n - (k+q)R_m]\} \tag{2.12}$$

where R_n and R_m are lattice vectors. With the help of (2.11) the p-h operators in (2.5*a*) are now expressed in terms of the $\rho_m^\dagger(n)$. This yields the following relation for the coefficient function ψ in the Wannier representation:

$$\psi_{m_1\ldots m_M}(n_1\ldots n_M)=\sum_{k_1\ldots k_M}\sum_{q_1\ldots q_M}(m_1n_1|k_1q_1)\ldots(m_Mn_M|k_Mq_M)\psi_{k_1\ldots k_M}(q_1\ldots q_M). \tag{2.13}$$

The counterpart of equation (2.10*b*) in the Wannier representation is then obtained on multiplying (2.13) by K_{ij} and inserting the RHS of (2.10*b*) for $K_{ij}\psi$. A little manipulation gives

$$\begin{aligned}K_{ij}\psi_{m_1\ldots m_M}(n_1\ldots n_M)&\\ &=\psi_{m_1\ldots m_M}(n_1\ldots n_j\ldots n_i\ldots n_M)\\ &=\psi_{m_1\ldots m_j\ldots m_i\ldots m_M}(n_1\ldots n_M)\qquad 1\leqslant i<j\leqslant M\end{aligned} \tag{2.14}$$

where the second line of (2.14) follows from the fact that ψ is invariant with respect to interchanges of whole pairs (see paper I). By equations (2.14) the K_{ij} operators are now easily recognised as fermion interchanges; these expressions will also be useful later in § 4.

Rather than picking out one particular pair of indices i and j, it is most convenient for the subsequent development to sum over all pairs (ij) and to state the subsidiary conditions (2.10) in form of the eigenvalue equation

$$K\psi_{k_1\ldots k_M}(q_1\ldots q_M)=-\tfrac{1}{2}M(M-1)\psi_{k_1\ldots k_M}(q_1\ldots q_M) \tag{2.15a}$$

where

$$K=\sum_{1\leqslant i<j\leqslant M}K_{ij} \tag{2.15b}$$

will be referred to as exchange operator. The eigenvalue problem (2.15) is the main object of the present paper; its solution will be presented in § 4.

3. Boson expansion of the Hamiltonian

The results of the preceding section enable us to perform the mapping of the spaces $\mathcal{U}_M$ and their associated operators into a space of ideal-boson states. In paper I such a mapping has already been carried out for the Hubbard model, and the arguments presented there can be readily extended to the more general case under consideration.

The boson space is constructed by means of a boson vacuum $|\Psi_0\rangle$ and boson creation and annihilation operators $B_k^\dagger(q)$ and $B_k(q)$, respectively, satisfying the commutation relations

$$[B_k(q),B_{k'}(q')]=0\qquad[B_k(q),B_{k'}^\dagger(q')]=\delta_{kk'}\delta_{qq'} \tag{3.1}$$

together with the condition $B_k(q)|\Psi_0\rangle=0$. The ideal-state space $\hat{\mathcal{U}}_M$ is then constructed as follows. For any vector $|\Psi_M\rangle$ of $\mathcal{U}_M$, whose coefficient function ψ has been made unique by imposition of the subsidiary condition (2.15), we define its unique image in $\hat{\mathcal{U}}_M$ by

$$|\Psi_M\rangle=\frac{1}{\sqrt{M!}}\sum_{k_1\ldots k_M}\sum_{q_1\ldots q_M}\psi_{k_1\ldots k_M}(q_1\ldots q_M)|(k_1q_1)\ldots(k_Mq_M)\rangle \tag{3.2a}$$

where the coefficient function is the *same* as in $|\Psi_M\rangle$ and

$$|(k_1q_1)\ldots(k_Mq_M))=B^{\dagger}_{k_1}(q_1)\ldots B^{\dagger}_{k_M}(q_M)|\Psi_0). \tag{3.2b}$$

The ideal-state space $\hat{\mathcal{U}}_M$ is then defined to be the set of all such states $|\Psi_M)$ as $|\Psi_M\rangle$ runs over all of $\mathcal{U}_M$.

The subsidiary condition (2.15) can now be reformulated as an eigenvalue problem in $\hat{\mathcal{U}}_M$. As has already been shown in paper I, the ideal-space representation of (2.15) is given by

$$\hat{K}|\Psi_M)=-\tfrac{1}{2}M(M-1)|\Psi_M) \tag{3.3a}$$

where $\hat{K}$ is defined as follows:

$$\hat{K}=\tfrac{1}{2}\sum_{qq'}\sum_{kk'}B^{\dagger}_{k'}(q)B^{\dagger}_{k'+k}(q')B_{k'+k}(q-k)B_{k'}(q'+k). \tag{3.3b}$$

A comparison of equations (3.3) and (2.15) reveals that K and $\hat{K}$ both represent the same exchange operator, but in different spaces. Hence, only those vectors $|\Psi_M)$ satisfying (3.3*a*) can be vectors of the ideal-state space $\hat{\mathcal{U}}_M$. This implies, for example, that the product states (3.2*b*) themselves are not contained in $\hat{\mathcal{U}}_M$, because they obviously do not satisfy (3.3*a*). Thus the latter condition leads to a restriction of the space of all possible M-boson states to a proper subspace.

The next problem is to express H_M, equations (2.7), in terms of ideal-boson operators. Quite generally, the correspondence between operators O on $\mathcal{U}_M$ and those $\hat{O}$ on $\hat{\mathcal{U}}_M$ is determined by expressing first $O|\Psi_M\rangle$ in the form (2.5*a*), then using (3.2), and finally identifying the result as some operator $\hat{O}$ acting on $|\Psi_M)$. The first task, therefore, is to calculate $H_M|\Psi_M\rangle$. A somewhat lengthy calculation paralleling that already performed in I (appendix B) for the Hubbard model yields

$$H_M|\Psi_M\rangle=\frac{1}{M!}\sum_{k_1\ldots k_M}\sum_{q_1\ldots q_M}\{H_M\psi_{k_1\ldots k_M}(q_1\ldots q_M)\}|(k_1q_1)\ldots(k_Mq_M)\rangle \tag{3.4}$$

where the expression in curly brackets is given by

$$H_M\psi_{k_1\ldots k_M}(q_1\ldots q_M)=(E_0+H_{M1}+H_{M2})\psi_{k_1\ldots k_M}(q_1\ldots q_M) \tag{3.5a}$$

and the operators are defined by

$$\begin{aligned}H_{M1}\psi_{k_1\ldots k_M}(q_1\ldots q_M)&\\ =\sum_{i=1}^{M}\omega_{k_i}(q_i)\psi_{k_1\ldots k_M}(q_1\ldots q_M)&\\ -\sum_{i,j=1}^{M}\sum_{q}U(q)\psi_{k_1\ldots k_i+q\ldots k_M}(q_1\ldots q_i-q\ldots q_j+q\ldots q_M)&\end{aligned} \tag{3.5b}$$

$$\begin{aligned}H_{M2}\psi_{k_1\ldots k_M}(q_1\ldots q_M)&\\ =\tfrac{1}{2}\sum_{i,j=1}^{M}\sum_{q}\tilde{U}(q)[\psi_{k_1\ldots k_M}(q_1\ldots q_i-q\ldots q_j+q\ldots q_M)&\\ +\psi_{k_1\ldots k_i+q\ldots k_j-q\ldots k_M}(q_1\ldots q_i-q\ldots q_j+q\ldots q_M)].&\end{aligned} \tag{3.5c}$$

To $H_M|\Psi_M\rangle$ there corresponds a vector $\hat{H}|\Psi_M)$ in $\hat{\mathcal{U}}_M$ given by

$$\hat{H}|\Psi_M)=\frac{1}{\sqrt{M!}}\sum_{k_1\ldots k_M}\sum_{q_1\ldots q_M}\{H_M\psi_{k_1\ldots k_M}(q_1\ldots q_M)\}|(k_1q_1)\ldots(k_Mq_M)) \tag{3.6}$$

where the coefficient function $H_M\psi$ has to be the *same* as in (3.4). One may now ask what operator $\hat{H}$, expressed as an explicit function of the ideal operators $B_k(q)$ and $B_k^\dagger(q)$, leads to equation (3.6) with expressions (3.5) for $H_M\psi$. Such an operator has already been constructed for the Hubbard Hamiltonian in paper I. By a slight extension of the arguments presented there one readily verifies that the following operator has the desired properties:

$$\hat{H} = E_0 + \hat{H}_1 + \hat{H}_2 \tag{3.7a}$$

where

$$\hat{H}_1 = \sum_{qkk'} W_{kk'}(q) B_k^\dagger(q) B_{k'}(q) - \sum_{qq'} \sum_{kk'p} U(k) B_{k'}^\dagger(q) B_p^\dagger(q') B_p(q'+k) B_{k'+k}(q-k) \tag{3.7b}$$

$$\hat{H}_2 = \tfrac{1}{2} \sum_{qq'} \sum_{kk'p} \tilde{U}(k) B_{k'}^\dagger(q) B_p^\dagger(q') [B_p(q'+k) B_{k'}(q-k) + B_{p-k}(q'+k) B_{k'+k}(q-k)] \tag{3.7c}$$

and

$$W_{kk'}(q) = \omega_k(q)\delta_{kk'} - U(k-k'). \tag{3.7d}$$

In the same way the ideal-space image of the pair occupation number operator (2.6) is obtained as

$$\hat{N} = \sum_{qk} B_k^\dagger(q) B_k(q). \tag{3.8}$$

Equations (3.3), (3.7) and (3.8) represent the ideal-space formulation of the PPP Hamiltonian. One realises that $\hat{H}$ is Hermitian and the quantum number M no longer explicitly occurs. Since $\hat{N}$ is derived from (2.6), it clearly commutes with $\hat{H}$. Moreover, since $\hat{H}$ and $\hat{N}$ are defined on $\mathfrak{U}_M$ and any vector of that space has to satisfy (3.3), $\hat{H}$, $\hat{N}$ and $\hat{K}$ must possess common eigenvectors. This, in turn, is only possible if all these operators commute:

$$[\hat{H}, \hat{K}] = [\hat{N}, \hat{K}] = [\hat{H}, \hat{N}] = 0. \tag{3.9}$$

A somewhat lengthy but straightforward calculation shows that (3.9) is in fact fulfilled.

Since the main object of the present paper is to investigate the properties of the exchange operator, no attempt will be made here to find the (approximate) eigenstates and eigenvalues of $\hat{H}$. As far as the Hubbard Hamiltonian is concerned, some arguments have been provided in I indicating that its boson transcription is really the faithful image of the original Hamiltonian, both yielding identical spectra. So far, in all practical calculations, for example, variational treatments, the fulfilment of the subsidiary condition (3.3) has caused severe problems, since any trial vector has to be chosen *a priori* such that (3.3) is satisfied. This clearly shows why it is worthwhile first to study carefully the properties of the exchange operator.

4. Properties of the subsidiary condition

The problem of finding the eigenstates of the exchange operator is closely related to the representation theory of the symmetric group $\mathcal{S}_M$, i.e. the group of all permutations of M objects. This is due to the fact that, according to (2.15*b*), K is the sum over all interchanges (transpositions) K_{ij} and, hence, an element of the symmetric group algebra (Boerner 1963). This connection has already been clearly recognised by Girardeau (1963, appendix) and part of the subsequent development follows his treatment of the subject.

The analysis is simplest in the space of coefficient functions ψ, the latter being given in the Wannier representation. As was shown in § 2, in this representation the eigenvalue problem is

$$K\psi_{m_1 \ldots m_M}(n_1 \ldots n_M) = -\tfrac{1}{2}M(M-1)\psi_{m_1 \ldots m_M}(n_1 \ldots n_M) \tag{4.1a}$$

where K is given as in (2.15b) and

$$K_{ij}\psi_{m_1 \ldots m_M}(n_1 \ldots n_M) = \psi_{m_1 \ldots m_M}(n_1 \ldots n_j \ldots n_i \ldots n_M) \qquad 1 \leq i < j \leq M. \tag{4.1b}$$

Subsequently a few elementary facts and notions from the representation theory of $\mathcal{S}_M$ will be needed, which will now be briefly summarised. For the details the reader is referred to Boerner's (1963) monograph (see, in particular, chapter IV).

Let $\mathcal{D}^{(\mu)}$ denote the Young diagram corresponding to the partition $(\mu) = (\mu_1, \mu_2, \ldots, \mu_n)$ of M and let $\mathcal{T}_i^{(\mu)}$ $(i = 1, \ldots, M!)$ denote the Young tableaux corresponding to $\mathcal{D}^{(\mu)}$. For a given tableau $\mathcal{T}^{(\mu)}$ (now dropping the subscript) one defines two kinds of permutations, the row and the column permutations (Boerner 1963, ch IV). The former only permute the numbers of each row among themselves and constitute a subgroup $\mathcal{P}$ of $\mathcal{S}_M$ of order $\mu_1! \ldots \mu_n!$, the μ_i denoting the lengths of the rows of $\mathcal{D}^{(\mu)}$. Similarly, the column permutations only permute the numbers of each column among themselves; they also form a subgroup $\mathcal{Q}$ of $\mathcal{S}_M$ of order $\bar{\mu}_1! \ldots \bar{\mu}_m!$, where the $\bar{\mu}_i$ denote the lengths of the columns of $\mathcal{D}^{(\mu)}$. To each tableau $\mathcal{T}^{(\mu)}$ one can now associate a Young operator $Y^{(\mu)}$ as follows

$$Y^{(\mu)} = \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{Q}} (-1)^q pq \tag{4.2}$$

where the symbol $(-1)^q$ denotes, as usual, the parity of the permutation q. The Young operators will play an important role in the subsequent development.

The derivation of the spectrum of K rests upon a famous theorem by J von Neumann, which will be stated here without proof (see Boerner 1963, p 108 for a proof of the theorem). Let

$$A = \sum_{s \in \mathcal{S}_M} a(s)s \tag{4.3}$$

be an element of the symmetric group algebra with the property

$$pAq = (-1)^q A \tag{4.4}$$

for all $p \in \mathcal{P}$ and all $q \in \mathcal{Q}$ of a given Young tableau $\mathcal{T}^{(\mu)}$. The theorem then states that there exists a number $\Lambda^{(\mu)}$ such that

$$A = \Lambda^{(\mu)} Y^{(\mu)} \tag{4.5}$$

where $Y^{(\mu)}$ is the Young operator associated with the tableau $\mathcal{T}^{(\mu)}$.

It can now be proved that the operator

$$A = KY^{(\mu)} \tag{4.6}$$

where K is the exchange operator (2.15b), satisfies the requirements of von Neumann's theorem. Since a detailed proof of this assertion has been given by Girardeau (1963, appendix), it will be omitted here. Then, since A of equation (4.6) satisfies the condition (4.4), the theorem is applicable and yields

$$KY^{(\mu)} = \Lambda^{(\mu)} Y^{(\mu)}. \tag{4.7}$$

This important relation (Girardeau 1963, equation (A21)) immediately yields the eigenfunctions of K. As is evident from (4.7), any coefficient function of the form

$$\psi_{m_1 \ldots m_M}(n_1 \ldots n_M) = Y^{(\mu)} \chi_{m_1 \ldots m_M}(n_1 \ldots n_M) \tag{4.8}$$

where χ may be arbitrary, is an eigenfunction of K, provided that ψ does not identically vanish. The eigenvalues $\Lambda^{(\mu)}$ of K have also been obtained by Girardeau (1963, appendix) and are given by

$$\Lambda^{(\mu)} = \tfrac{1}{2} \sum_{k=1}^{n} \mu_k(\mu_k - 1) - \tfrac{1}{2} \sum_{l=1}^{m} \bar{\mu}_l(\bar{\mu}_l - 1). \tag{4.9}$$

He also showed that the $\Lambda^{(\mu)}$ obtained are the only eigenvalues of K for any given M and (μ). Equation (4.9) implies that all eigenvalues are integers and lie on the interval $[-\frac{1}{2}M(M-1), \frac{1}{2}M(M-1)]$. For illustration, the possible partitions (μ) and the corresponding eigenvalues $\Lambda^{(\mu)}$ for $M = 2$ to 4 are listed below:

$M=2$	(μ)	(2)	(1^2)			
	$\Lambda^{(\mu)}$	1	-1			
$M=3$	(μ)	(3)	(2, 1)	(1^3)		
	$\Lambda^{(\mu)}$	3	0	-3		
$M=4$	(μ)	(4)	(3, 1)	(2^2)	$(2, 1^2)$	(1^4)
	$\Lambda^{(\mu)}$	6	2	0	-2	-6.

Although (4.9) gives a precise prescription how to calculate the eigenvalues for any given M and (μ), this formula is hardly applicable even for moderately large M, as one may readily verify. Therefore, any treatment based on projection operators (Löwdin 1962) is highly unpractical, since the method requires the knowledge of all $\Lambda^{(\mu)}$ for any given M. The latter technique has been applied by Girardeau (1971) to construct a projected 'effective' Hamiltonian, in which the subsidiary condition (3.3a) is incorporated as an additional exchange interaction. Due to the problems outlined above, such a treatment is limited to very low M, and only the case $M = 2$ has been treated in this manner (Girardeau 1971). In summary, so far the problem of finding (approximate) eigenstates of $\hat{H}$ which are, at the same time, exact eigenstates of $\hat{K}$ satisfying (3.3a), has not been solved in a satisfactory way.

The method to be presented here is rather simple and obvious and works equally well for any number M of pairs. It is based on the fact that condition (3.3a) needs to be solved only for the lowest eigenvalue of $\hat{K}$ for a given M, i.e. for $\Lambda^{(\mu)} = -M(M-1)/2$. Therefore, as equation (4.8) shows, all we need to know is the Young operator corresponding to this particular eigenvalue.

Now it follows from (4.9) that the lowest eigenvalue is attained for $\mu_k = 1$ ($k = 1, \ldots, n$) and $\bar{\mu}_l = M\delta_{l1}$ ($l = 1, \ldots, m$) and thus belongs to the Young diagram consisting of one column only (of length M). Hence, the corresponding Young operator is just (apart from a factor $1/\sqrt{M!}$) the familiar antisymmetriser usually denoted as

$$A_M = \frac{1}{\sqrt{M!}} \sum_{p \in \mathcal{S}_M} (-1)^p p. \tag{4.10}$$

The eigenfunction belonging to the lowest eigenvalue is then obtained by combining equations (4.8) and (4.10):

$$\psi_{m_1 \ldots m_M}(n_1 \ldots n_M) = A_M \chi_{m_1 \ldots m_M}(n_1 \ldots n_M)$$

$$= \frac{1}{\sqrt{M!}} \sum_{p \in \mathcal{S}_M} (-1)^p \chi_{m_1 \ldots m_M}(n_{p1} \ldots n_{pM}) \tag{4.11}$$

where $p1, \ldots, pM$ is the permuted set of indices $1, \ldots, M$. Hence, any function of the form (4.11), where χ is still arbitrary (only subject to the condition that ψ is not identically zero), is a solution of the eigenvalue equation (4.1a). Clearly, the function χ itself can be obtained only by solving the eigenvalue problem of the Hamiltonian. If, in particular, χ is assumed to be of the product form

$$\chi_{m_1 \ldots m_M}(n_1 \ldots n_M) = \prod_{i=1}^{M} \chi_{m_i}(n_i) \tag{4.12}$$

equation (4.11) can be written as the determinant

$$\psi_{m_1 \ldots m_M}(n_1 \ldots n_M) = \frac{1}{\sqrt{M!}} \begin{vmatrix} \chi_{m_1}(n_1) & \chi_{m_1}(n_2) & \ldots & \chi_{m_1}(n_M) \\ \chi_{m_2}(n_1) & \chi_{m_2}(n_2) & \ldots & \chi_{m_2}(n_M) \\ & \ldots & & \\ \chi_{m_M}(n_1) & \chi_{m_M}(n_2) & \ldots & \chi_{m_M}(n_M) \end{vmatrix}. \tag{4.13}$$

The determinantal form (4.13) might be a good starting point for a variational treatment. Here it may also be mentioned that a similar form of trial wavefunction is used in valence bond theory (Gerratt 1971) and in the AGP method (Linderberg 1980).

So far the discussion has been restricted to the Wannier representation. In order to link the results of this section with those obtained in § 3, the analogue of (4.11) in the Bloch representation is needed. A straightforward calculation yields

$$\psi_{k_1 \ldots k_M}(q_1 \ldots q_M) = \frac{1}{\sqrt{M!}} \sum_{p \in \mathcal{S}_M} (-1)^p \chi_{k_1 \ldots k_M}(q_{p1} + k_{p1} - k_1, \ldots, q_{pM} + k_{pM} - k_M) \tag{4.14}$$

where use has been made of equations (2.12) and (2.13). The same arguments as those used in connection with (4.11) show that any function of the form (4.14), which is not identically zero, is a solution of (2.15a). Hence, as follows from the discussion in § 3, any vector $|\Psi_M)$ of the form of equation (3.2a), where ψ is now given by (4.14), is an eigenvector of equation (3.3a). The problem to find the most general vector $|\Psi_M)$, which satisfies the subsidiary condition (3.3a), is thus completely solved.

5. Conclusion

Based on Girardeau's composite-particle theory the PPP (extended Hubbard) Hamiltonian has been represented in terms of ideal-boson operators. As is the case with all boson representations of Fermi systems, the Hamiltonian $\hat{H}$ in boson space is defined on a proper subspace of the space of all possible M-boson states ($M = 1, 2, \ldots$). In Girardeau's theory the restriction of $\hat{H}$ to the proper subspace is effected by means of the subsidiary condition (1.1). So far the problem to find (approximate) eigenstates of $\hat{H}$ which are, at the same time, exact eigenstates of equation (1.1) has not been solved in a satisfactory manner. In the present work a partial solution to this problem

has been achieved. We were able to derive the most general eigenvector $|\Psi_M)$ of equation (1.1) by using techniques commonly employed in the representation theory of the symmetric group. From the most general $|\Psi_M)$ a special eigenvector can be obtained, in which the coefficient function takes the form of an antisymmetrised product of pair orbitals. The latter form might be a good starting point for a variational treatment of $\hat{H}$ and relates the pair-theory approach to the valence bond theory and the AGP method.

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