The Mathematics of Second Quantization for Systems of Fermions

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I. Introduction[1]

It is the practice in most textbooks in which the subject of second quantization of many-fermion systems is discussed to give "plausibility" arguments only for the equivalence of configuration-space and second-quantized formalisms. This is undoubtedly because the actual proofs, as first constructed by Jordan (*1*) and Jordan and Wigner (*2*), are rather too lengthy and intricate to repeat in detail.

In a previous International Spring School of the University of Naples this subject was discussed by J. G. Valatin (*3*) in a lecture entitled "Second Quantization and Configuration Space Method." In this lecture Valatin presented a treatment, which he had published some years earlier (*4*), that was much improved over that of Jordan and Wigner. Valatin's improvement was in laying stress on the exact mathematical nature of the equivalence, in which the operations of annihilation and creation and the second-quantized description of states arise naturally as operations and elements of a long-known algebra of Grassman.

In one essential sense, however, the work of Valatin is still as complicated to repeat as that of Jordan and Wigner. This is because the equivalences in both cases are established by detailed comparisons of the complete sets of matrix elements of the one- and two-particle operators in configuration space and second-quantized formalisms. This is still

[1] The content of these notes is essentially the same as that of a paper by this author in *Proc. Phys. Soc.* **81**, 427 (1963).

sufficiently tedious, in spite of the basic elegance of Valatin's work, to seem to dissuade its widespread adoption as introductory material.

It has seemed to me that such complication is out of proportion to the simplicity of the results required, and in particular that it should not be necessary to treat separately the one-particle and two-particle operators, but that the general result for an operator $\mathcal{O}$ depending symmetrically on the coordinates of f particles

$$\mathcal{O}^{(f)}(x^{s_1} \dots x^{s_f}) = \frac{1}{f!} \sum_{\substack{s_1 \dots s_f = 1 \\ s_1 \neq s_2 \neq \dots s_f}}^{N} O(x^{s_1} \dots x^{s_f}) , \tag{1}$$

should be derivable in a direct manner:

$$\mathcal{O}^{(f)} \equiv \frac{1}{f!} \sum_{\substack{s_1 \dots s_f \\ t_1 \dots t_f}} \langle t_1 \dots t_f \mid O \mid s_1 \dots s_f \rangle \, a_{t_1}^{\dagger} \dots a_{t_f}^{\dagger} \, a_{s_f} \dots a_{s_1} . \tag{2}$$

With the aid of a slightly different approach it is indeed possible to avoid the comparison of separate N-particle matrix elements, and Eq. (2) may be written down almost at sight (with some knowledge, of course, of exactly what is meant by second quantization) from an appropriate relation in configuration space. This relation [Eq. (7)] requires little effort to derive, but gives a new starting point for the second quantization of many-fermion systems that makes the comparison of the two formalisms almost trivially simple.

II. The Operation in Configuration Space

A complete specification of the operator $\mathcal{O}^{(f)}$ of Eq. (2) in the configuration space of an N-particle system can be given by either listing its matrix elements between a given set of basis wave functions in this space or, what can be almost the same thing, by writing down the result of the operation when performed on an arbitrary basis function. The latter specification is the one that we shall use; it does not necessarily require explicit calculation of the N-particle matrix elements, but can be written instead directly in terms of matrix elements between products of f single-particle wave functions.

The Hilbert space of N-fermion wave functions is built up from the space $\mathfrak{R}$ of single-particle wave functions ψ_r by antisymmetrizing the tensor product of N identical spaces. This space has several notations in the literature, for instance, $P_{s_n}\mathfrak{R}\otimes\mathfrak{R}\otimes$ — — $\otimes\mathfrak{R} = P_{s_n}\mathfrak{R}^{(N)}$ by Cook (*5, 6*) and $A\mathfrak{R}^{\otimes N}$ by Kastler (*7, 8*); its covariant space is denoted as $\overset{N}{\wedge}\mathfrak{R}$ by Valatin. We use Kastler's notation. A complete set of basis functions in this space is provided by the Slater determinants

$$\varphi_{r_1\ldots r_N}(x^1 \ldots x^N) = \frac{1}{\sqrt{N!}}\begin{vmatrix}\psi_{r_1}(x^1) & \ldots & \psi_{r_N}(x^1)\\ \ldots & \ldots & \ldots\\ \psi_{r_1}(x^N) & \ldots & \psi_{r_N}(x^N)\end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}}\sum_{\substack{\text{Perm}\\ x^1\ldots x^N}} \varepsilon^{x^1\cdots x^N}\, \psi_{r_1}(x^1)\ldots\psi_{r_N}(x^N)\,. \tag{3}$$

In Eq. (3) the determinant is written out using the Levi-Civita densities $\varepsilon^{x_1\cdots x_N}$ which take the values -1, 0, or $+1$ according as $x^1 \ldots x^N$ is ... odd, no, or an even permutation of the original order, respectively.

We operate with $\mathcal{O}^{(f)}(x^{s_1}\ldots x^{s_N})$ on an arbitrary Slater basis function of $A\mathfrak{R}^{\otimes N}$:

$$\mathcal{O}^{(f)}\varphi_{r_1\ldots r_N} = \frac{1}{f!}\sum_{\substack{s_1\ldots s_f=1\\ s_1\neq s_2\neq\cdots s_f}}^{N} O(x^{s_1}\ldots x^{s_f})\,\frac{1}{\sqrt{N!}}\sum_{\substack{\text{Perm}\\ x^1\cdots x^N}}\varepsilon^{x^1\cdots x^N}\,\psi_{r_1}(x^1)\ldots\psi_{r_N}(x^N). \tag{4}$$

Now $O(x^{s_1}\ldots x^{s_f})\,\psi_{r_{s_1}}(x^{s_1})\ldots\psi_{r_{s_f}}(x^{s_f})$ is some function of $x^{s_1}\ldots x^{s_f}$ with the same boundary conditions as the ψ_r's and can, therefore, be expanded in the set of functions $\psi_{t_1}(x^{s_1})\,\psi_{t_2}(x^{s_2})\ldots\psi_{t_f}(x^{s_f})$, which form a complete basis set for such functions:

$$O(x^{s_1}\ldots x^{s_f})\,\psi_{r_{s_1}}(x^{s_1})\ldots\psi_{r_{s_f}}(x^{s_f})$$
$$= \sum_{t_1'\ldots t_f'} F(t_1'\ldots t_f',\ r_{s_1}\ldots r_{s_f})\,\psi_{t_1'}(x^{s_1})\ldots\psi_{t_f'}(x^{s_f}). \tag{5}$$

Multiplication from the right by $\psi^*_{t_1}(x^{s_1})\ldots\psi^*_{t_f}(x^{s_f})$ and integration over all $x^{s_1}\ldots x^{s_f}$ gives

$$F(t_1\ldots t_f,\ r_{s_1}\ldots r_{s_f}) = \int\!\ldots\!\int \psi^*_{t_1}(x^{s_1})\ldots\psi^*_{t_f}(x^{s_f})\,O(x^{s_1}\ldots x^{s_f})\,\psi_{r_{s_1}}(x^{s_1})\ldots\psi_{r_{s_f}}(x^{s_f})\,dx^{s_1}\ldots dx^{s_f} \tag{6}$$
$$= \langle t_1\ldots t_f\,|\,O\,|\,r_{s_1}\ldots r_{s_f}\rangle\,.$$

Using this expression in Eq. (4) and the fact that O is invariant under permutations of the x's we obtain:

$$\mathscr{O}^{(f)}\varphi_{r_1\ldots r_N} = \frac{1}{f!}\sum_{\substack{s_1\ldots s_f=1\\ s_1\neq s_2\neq\ldots s_f}}^{N} \frac{1}{\sqrt{N!}} \sum_{\substack{\text{Perm}\\ x_1\ldots x_N}} \varepsilon^{x_1\cdots x_N} \sum_{t_1\ldots t_f} \langle t_1 \ldots t_f \mid O \mid r_{s_1} \ldots r_{s_f}\rangle$$

$$\times\ \psi_{r_1}(x^1)\ldots\psi_{t_1}(x^{s_1})\ldots\psi_{t_f}(x^{s_f})\ldots\psi_{r_N}(x^N) \tag{7}$$

$$= \frac{1}{f!}\sum_{\substack{s_1\ldots s_f=1\\ s_1\neq s_2\neq\ldots s_f}}^{N} \sum_{t_1\ldots t_f} \langle t_1 \ldots t_f \mid O \mid r_{s_1} \ldots r_{s_f}\rangle\, \varphi_{r_1\ldots t_1\ldots t_f\ldots r_N}.$$

Equation (7) gives a complete specification of the operator. The matrix elements of $\mathscr{O}$ between any pair of basis functions in $A\mathfrak{R}^{\otimes N}$ could be calculated, if required, from this equation. Tabulation of these is, in general, exceedingly complicated and Eq. (7) probably represents the most concise way of summarizing these properties. When $f = N$ we have the particular case:

$$\mathscr{O}^{(N)}(x^1 \ldots x^N) = \frac{1}{N!} \sum_{\substack{\text{Perm}\\ x^1\ldots x^N}} O(x^1 \ldots x^N) = O(x^1 \ldots x^N). \tag{8}$$

In this case Eq. (7) reduces to:

$$\mathscr{O}^{(N)}\varphi_{r_1\ldots r_N} = \sum_{s_1\ldots s_N} \langle s_1 \ldots s_N \mid O \mid r_1 \ldots r_N\rangle\, \varphi_{s_1\ldots s_N} \tag{9}$$

which can be shown by a straightforward calculation to be equal to

$$\mathscr{O}^{(N)}\varphi_{r_1\ldots r_N} = \sum_{s_1<s_2\ldots<s_N} \langle \varphi_{s_1\ldots s_N} \mid \mathscr{O} \mid \varphi_{r_1\ldots r_N}\rangle\, \varphi_{s_1\ldots s_N} \tag{10}$$

which is the usual representation.

III. The Operation in Second Quantization

The isomorphism between the elements e of the Grassman space algebra[2] $\mathscr{G}(\mathfrak{R})$ on $\mathfrak{R}$ (generated by taking the outer products 1, 2, 3, ...

[2] Sufficient knowledge of this algebra to understand second quantization can be obtained from the book by Littlewood (*9*).

at a time of a set of primitive elements a_r isomorphic with ψ_r), and the Slater basis functions of the complete fermion state space,

$$\bigotimes_{N=0}^{\infty} A\mathfrak{R}^{\otimes N},$$

[Fock (*10*)] has been demonstrated by Valatin. The outer product of two ordered elements e_i, e_j, is defined by the rule

$$e_i e_j = - e_j e_i . \tag{11}$$

In this isomorphism the Slater wave function $\varphi_{r_1 \ldots r_N}(x^1 \ldots x^N)$ corresponds 1 : 1 with the algebraic element $e_r^N = a_{r_1} a_{r_2} \ldots a_{r_N}$. This is the "occupation number representation" of second quantization. The outer product by a primitive element a_r is denoted by $\alpha_r^+ \mid$ and is the familiar creation operation for Fermi particles. The inner product by a_r, denoted $\alpha_r \mid$ or $(a_r$, is the annihilation operation. Interior multiplication of two ordered normalized elements e_i, e_j, is defined as follows. Given an element e_j such that e_i is a left factor, that is, there exists an element e_k such that

$$e_j = e_i e_k , \tag{12}$$

then the inner product is defined by

$$(e_i, e_j) = (e_i, e_i e_k) = (e_i, e_i) e_k = e_k \tag{13a}$$

if e_i is not a left factor of e_j then

$$(e_i, e_j) = 0 . \tag{13b}$$

This operation is the exact inverse of exterior multiplication.

Second quantization of Eq. (7) consists simply of rewriting it in its corresponding algebraic form. It thus becomes

$$e_r^N = \frac{1}{f!} \sum_{\substack{s_1 \ldots s_f = 1 \\ s_1 \neq s_2 \ldots \neq s_f}} \sum_{t_1 \ldots t_f} \langle t_1 \ldots t_f \mid O \mid r_{s_1} \ldots r_{s_f} \rangle \, a_{r_1} \ldots a_{t_1} \ldots a_{t_f} \ldots a_{r_N} . \tag{14}$$

By use of the multiplication rules (11) and (13) of the algebra, which are the familiar rules for using the creation and annihilation operators for

Fermi particles, Eq. (14) can be written in the alternative form:

$$e_r^N = \frac{1}{f!} \sum_{\substack{s_1 \ldots s_f = 1 \\ s_1 \neq s_2 \ldots \neq s_f}}^{N} \sum_{t_1 \ldots t_f} \langle t_1 \ldots t_f | O | r_{s_1} \ldots r_{s_f} \rangle \alpha_{t_1}^{\dagger} \alpha_{t_2}^{\dagger} \ldots \alpha_{t_f}^{\dagger} \alpha_{r_{s_f}} \ldots \alpha_{r_{s_2}} \alpha_{r_{s_1}} | e_r^N \quad (15)$$

The restrictions on the first sum may be removed since it may be seen by use of (11) and (13) that the additional terms are all zero. By a slight change of suffies Eq. (15) gives the final form of the operator as predicted in Eq. (2).

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