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When can an A-particle fermion wavefunction be written as a Slater determinant?

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Abstract. A simple necessary and sufficient condition which tells when an A-particle fermion wavefunction can be written as a Slater determinant is proven.

1. Introduction

In calculations of fermion many-body wavefunctions, it is often assumed that the A-particle wavefunction $\psi(x_1, \ldots, x_A)$ is an antisymmetrized product of A one-particle wavefunctions $\phi_1, \ldots, \phi_A$. This is generally expressed by writing $\psi(x_1, \ldots, x_A)$ as a Slater determinant, i.e.

$$\psi(x_1, \ldots, x_A) = \det \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_1(x_A) \\ \vdots & & \vdots \\ \phi_A(x_1) & \cdots & \phi_A(x_A) \end{pmatrix}. \tag{1}$$

By $x_1, x_2, \ldots,$ we mean generalized coordinates, which can contain three-dimensional space coordinates, spin coordinates, etc. For some particular A-particle wavefunctions, equation (1) can be an exact relation. However, in most cases it will be an approximation which implies the loss of correlations between the particles [1]. One can derive a necessary and sufficient condition for ψ which tells when relation (1) will be exact or not. In the literature, one finds the condition [2]

$$\rho^2 = \rho \tag{2}$$

where ρ is the one-particle density matrix of the A-particle system

$$\rho(x, x') := \langle\psi|a^+(x')a(x)|\psi\rangle. \tag{3}$$

In section 2, we derive an equivalent but purely algebraic condition which immediately gives a set of A one-particle wavefunctions $\phi_1, \ldots, \phi_A$. In section 3, we simplify this condition to an expression with a limited number of terms, independent of the number of particles A. To show the equivalence between this condition and the condition of section 2, we derive a third equivalent algebraic condition. In section 4, we show the equivalence between the algebraic conditions of section 3 and (2).

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2. An algebraic condition

Suppose that ψ can be written as a Slater determinant of A one-particle functions $\phi_1, \ldots, \phi_A$ such that (1) holds. If we define M_{ij} as the minor of the element $\phi_i(x_j)$ of the determinant in expression (1) and develop this determinant to the jth column we get

$$\psi(x_1, \ldots, x_A) = \sum_{i=1}^{A} M_{ij}\phi_i(x_j). \tag{4}$$

We can replace x_j by another value, say y_j, and use expression (4) with i, j varying from 1 to A to get

$$\begin{pmatrix} M_{11} & \cdots & M_{A1} \\ \vdots & & \vdots \\ M_{1A} & \cdots & M_{AA} \end{pmatrix} \begin{pmatrix} \phi_1(y_1) & \cdots & \phi_1(y_A) \\ \vdots & & \vdots \\ \phi_A(y_1) & \cdots & \phi_A(y_A) \end{pmatrix} = \begin{pmatrix} \psi(X_{(x_1\to y_1)}) & \cdots & \psi(X_{(x_1\to y_A)}) \\ \vdots & & \vdots \\ \psi(X_{(x_A\to y_1)}) & \cdots & \psi(X_{(x_A\to y_A)}) \end{pmatrix}. \tag{5}$$

The notation $\psi(X_{(x_i\to y_j)})$ stands for $\psi(x_1, \ldots, x_{i-1}, y_j, x_{i+1}, \ldots, x_A)$. Taking the determinant of both sides we get the condition

$$(\psi(x_1, \cdots, x_A))^{A-1}\psi(y_1, \cdots, y_A) = \det \begin{pmatrix} \psi(X_{(x_1\to y_1)}) & \cdots & \psi(X_{(x_1\to y_A)}) \\ \vdots & & \vdots \\ \psi(X_{(x_A\to y_1)}) & \cdots & \psi(X_{(x_A\to y_A)}) \end{pmatrix}. \tag{6}$$

We made use of the fact that

$$\begin{pmatrix} M_{11} & \cdots & M_{A1} \\ \vdots & & \vdots \\ M_{1A} & \cdots & M_{AA} \end{pmatrix} = \det \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_1(x_A) \\ \vdots & & \vdots \\ \phi_A(x_1) & \cdots & \phi_A(x_A) \end{pmatrix} \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_1(x_A) \\ \vdots & & \vdots \\ \phi_A(x_1) & \cdots & \phi_A(x_A) \end{pmatrix}^{-1}. \tag{7}$$

As such, equation (6) is a necessary condition for an A-particle wavefunction to be a Slater determinant. It must hold for all values of the coordinates $x_1, 1 \ldots, x_A, y_1, \ldots, y_A$. It is also a sufficient condition if we consider $x_1, \ldots, x_A$ as constants, then equation (6) gives the Slater determinant expression of $\psi(y_1, \ldots, y_A)$. Apart from the normalization, the one-particle wavefunctions are given by

$$\phi_i : \phi_i(y) = \psi(X_{(x_i\to y)}) \qquad \forall y. \tag{8}$$

To get an orthonormal set of one-particle wavefunctions, one can apply a Gramm–Schmidt orthogonalization procedure, which does not affect the determinant, and multiply each row with a suitable normalization factor. If ψ is correctly normalized, the product of all the normalization factors will cancel with the factor $(\psi(x_1, \ldots, x_A))^{A-1}$.

3. Equivalent conditions

If $\psi(x_1, \ldots, x_A) \neq 0$, we can simplify equation (6) by replacing $(y_3, \ldots, y_A)$ by $(x_3, \ldots, x_A)$ and (x_1, x_2) by (y_3, y_4), respectively. This gives

$$\psi(y_1, y_2, x_3, \ldots, x_A)\psi(y_3, y_4, x_3, \ldots, x_A) + \psi(y_2, y_3, x_3, \ldots, x_A)\psi(y_1, y_4, x_3, \ldots, x_A) \\ + \psi(y_3, y_1, x_3, \ldots, x_A)\psi(y_2, y_4, x_3, \ldots, x_A) = 0 \tag{9}$$

for all values of $y_1, \ldots, y_4, x_3, \ldots, x_A$. This expression can be written in the more compact form

$$\sum_{k,l,m,n=1\cdots 4} \varepsilon_{klmn} \psi(y_k, y_l, x_3, \ldots, x_A)\psi(y_m, y_n, x_3, \ldots, x_A) = 0 \tag{10}$$

where ε_{klmn} is the fully antisymmetric tensor in the indices k, l, m, n. Equation (9) can be generalized to

$$\psi(y_1, \ldots, y_A)\psi(x_1, \ldots, x_A) = \sum_{i=1}^{A} \psi(Y_{(y_i \to x_j)})\psi(X_{(x_j \to y_i)}). \tag{11}$$

This expression is fully equivalent to equation (9).

Proof. Equation (9) can easily be derived from equation (11) by replacing $(y_3, \ldots, y_A)$ by $(x_3, \ldots, x_A)$. On the other hand, we can prove equation (11) by induction, starting from equation (9). Let N be the number of y-coordinates that differ from any of the x-coordinates. In the case $N = 0$, expression (11) is trivial since the antisymmetry of the fermion wavefunction ψ implies that $\psi(X_{(x_i \to x_j)}) = 0$ for $i \neq j$. Suppose that equation (11) holds for $N = n-1$. Now we consider the case where $N = n$. Without loss of generality, we can take $(y_{n+1}, \ldots, y_A) = (x_{n+1}, \ldots, x_A)$. To clarify the following reasoning, we introduce the notation

$$\chi(y, x) = \psi(y_1, \ldots, y_{n-2}, y, x, x_{n+1}, \ldots, x_A). \tag{12}$$

Now we can work out the following product explicitly:

$$\begin{aligned} &\psi(x_1, \ldots, x_A)\psi(y_1, \ldots, y_n, x_{n+1}, \ldots, x_A)\psi(y_1, \ldots, y_{n-1}, x_n, \ldots, x_A) \\ &\quad = \psi(x_1, \ldots, x_A)\chi(y_{n-1}, y_n)\chi(y_{n-1}, x_n) \\ &\quad = \sum_{i=1}^{n-1} \psi(X_{(x_i \to y_{n-1})})\chi(y_{n-1}, y_n)\chi(x_i, x_n). \end{aligned} \tag{13}$$

Applying equation (9) to (13) gives

$$\begin{aligned} &\psi(x_1, \ldots, x_A)\chi(y_{n-1}, y_n)\chi(y_{n-1}, x_n) \\ &\quad = \sum_{i=1}^{n-1} \psi(X_{(x_i \to y_{n-1})})[\chi(y_{n-1}, x_n)\chi(x_i, y_n) + \chi(y_{n-1}, x_i)\chi(y_n, x_n)] \end{aligned} \tag{14}$$

$$\begin{aligned} &\quad = \chi(y_{n-1}, x_n)\sum_{i=1}^{n-1} \psi(X_{(x_i \to y_{n-1})})\chi(x_i, y_n) \\ &\qquad + \chi(y_n, x_n)\sum_{i=1}^{n-1} \psi(X_{(x_i \to y_{n-1})})\chi(y_{n-1}, x_i). \end{aligned} \tag{15}$$

The second term in (15) can be simplified after interchanging some coordinates

$$\sum_{i=1}^{n-1} \psi(X_{(x_i \to y_{n-1})})\chi(y_{n-1}, x_i) = \sum_{i=1}^{n-1} \psi(X_{(x_n \to y_{n-1}, x_i \to x_n)})\chi(x_i, y_{n-1}) \tag{16}$$

$$= -\psi(X_{(x_n \to y_{n-1})})\chi(y_{n-1}, x_n). \tag{17}$$

We were allowed to apply equation (11) to (16), since the arguments of the two wavefunctions contained only $n-1$ different coordinates. Substituting (17) into (15) gives

$$\psi(x_1,\ldots,x_A)\chi(y_{n-1},y_n)\chi(y_{n-1},x_n) \\ = \chi(y_{n-1},x_n)\left[\sum_{i=1}^{n-1}\psi(X_{(x_i\to y_{n-1})})\chi(x_i,y_n)+\psi(X_{(x_n\to y_{n-1})})\chi(x_n,y_n)\right]. \quad (18)$$

If $\psi(x_1,\ldots,x_n,y_{n+1},\ldots,y_A)\neq 0$, we can suppose without loss of generality that equation (18) can be reduced to

$$\psi(x_1,\ldots,x_A)\psi(y_1,\ldots,y_n,x_{n+1},\ldots,x_A) \\ = \sum_{i=1}^{n}\psi(X_{(x_i\to y_{n-1})})\psi(y_1,\ldots,y_{n-2},x_i,y_n,x_{n+1},\ldots,x_A). \quad (19)$$

This is equation (11) for $N=n$. By induction, we obtain that equation (11) holds for $N=0,1,\ldots,A$. This proves the equivalence between equation (11) and equation (9). □

We have shown that (6) leads to (9) and that (9) is equivalent to (11). To establish the equivalence between (6) and (9), it is sufficient to show that (11) leads to (6). This will be proved in the following paragraph.

Proof. First, we introduce the notation

$$D(X;y_1,\ldots,y_A):=\det\begin{pmatrix}\psi(X_{(x_1\to y_1)}) & \cdots & \psi(X_{(x_1\to y_A)})\\ \vdots & & \vdots\\ \psi(X_{(x_A\to y_1)}) & \cdots & \psi(X_{(x_A\to y_A)})\end{pmatrix}. \quad (20)$$

With this notation, equation (6) can be written as

$$(\psi(x_1,\ldots,x_A))^{A-1}\psi(y_1,\ldots,y_A)=D(X;y_1,\ldots,y_A). \quad (21)$$

Let N again denote the number of y-coordinates that differ from any of the x-coordinates. Since $\psi(X_{(x_i\to x_j)})=0$ for $i\neq j$, it is easy to see that $D(X;x_1,\cdots,x_A)=(\psi(x_1,\ldots,x_A))^A$. In other words, equation (21) holds for $N=0$. Suppose that equation (21) holds for $N=n-1$. Now we consider the case where $N=n$. Without loss of generality, we can take $(y_{n+1},\ldots,y_A)=(x_{n+1},\ldots,x_A)$. Expanding $D(X;y_1,\ldots,y_{n-1},y,x_{n+1},\ldots,x_A)$ to the nth column gives

$$D(X;y_1,\ldots,y_{n-1},y,x_{n+1},\ldots,x_A)=\sum_{i=1}^{n}\psi(X_{(x_i\to y)})m_{in} \quad (22)$$

where m_{in} stands for the minor of the element on the ith row in the nth column in the determinant of (20). For $y=x_j$, $j\leqslant n$, we get

$$D(X;y_1,\ldots,y_{n-1},x_j,x_{n+1},\ldots,x_A)=\psi(x_1,\ldots,x_A)m_{jn}. \quad (23)$$

In this case $N=n-1$, so equation (21) holds. Combining (23) and (21) we obtain, if $\psi(x_1,\ldots,x_A)\neq 0$,

$$m_{jn}=(\psi(x_1,\ldots,x_A))^{A-2}\psi(y_1,\ldots,y_{n-1},x_j,x_{n+1},\ldots,x_A). \quad (24)$$

Inserting this expression for m_{jn} in (22) gives

$$D(X; y_1, \ldots, y_{n-1}, y, x_{n+1}, \ldots, x_A) = (\psi(x_1, \ldots, x_A))^{A-2} \sum_{i=1}^{n} \psi(X_{(x_i \to y)}) \psi(y_1, \ldots, y_{n-1}, x_i, x_{n+1}, \ldots, x_A). \quad (25)$$

Applying equation (11) results in

$$D(X; y_1, \ldots, y_{n-1}, y, x_{n+1}, \ldots, x_A) = (\psi(x_1, \ldots, x_A))^{A-1} \psi(y_1, \ldots, y_{n-1}, y, x_{n+1}, \ldots, x_A). \quad (26)$$

This is expression (6) for $N = n$. By induction, we obtain that expression (6) must hold for $N = 0, 1, \ldots, A$.

This proves the equivalence between the expressions (6), (9) and (11). Note that the number of terms in expression (9) is independent of the number of particles A. □

4. Idempotence of the one-particle density matrix

It is known that (2) is a necessary and sufficient condition which tells whether ψ can be written as a Slater determinant [2]. So (2) has to be equivalent with the conditions derived in the previous sections. Indeed, equation (2) can easily be derived from equation (11).

$$\psi(y_1, \ldots, y_A) \psi(x_1, \ldots, x_A) = \sum_{i=1}^{A} \psi(Y_{(y_i \to x_1)}) \psi(X_{(x_1 \to y_i)}) \quad (27)$$

$$\Downarrow$$

$$\int \psi^*(y_1, \ldots, y_A) \psi^*(x_1', x_2, \ldots, x_A) \psi(y_1, \ldots, y_A) \psi(x_1, x_2, \ldots, x_A) \, \mathrm{d}y_1 \cdots \mathrm{d}y_A \, \mathrm{d}x_2 \cdots \mathrm{d}x_A$$
$$= \sum_{i=1}^{A} \int \psi^*(y_1, \ldots, y_A) \psi^*(x_1', x_2, \ldots, x_A) \times \psi(Y_{(y_i \to x_1)}) \psi(X_{(x_1 \to y_i)}) \, \mathrm{d}y_1 \cdots \mathrm{d}y_A \, \mathrm{d}x_2 \cdots \mathrm{d}x_A. \quad (28)$$

The integration symbol stands for integrating over all the continuous components and for summing over all the discrete components of the coordinates. We assume that ψ is normalized according to $\langle \psi | \psi \rangle = A$. Rearranging the variables in the ith term of the summation

$$y_1 := y_i, y_i := y_{i-1}, \ldots, y_2 := y_1 \quad (29)$$

and dividing both sides of (28) by A leads to

$$\int \psi^*(x_1', x_2, \ldots, x_A) \psi(x_1, x_2, \ldots, x_A) \, \mathrm{d}x_2 \cdots \mathrm{d}x_A$$
$$= \int \left[\int \psi^*(x_1', x_2, \ldots, x_A) \psi(y, x_2, \ldots, x_A) \, \mathrm{d}x_2 \cdots \mathrm{d}x_A \times \int \psi^*(y, y_2, \ldots, y_A) \psi(x_1, y_2, \ldots, y_A) \, \mathrm{d}y_2 \cdots \mathrm{d}y_A \right] \mathrm{d}y. \quad (30)$$

This precisely matches the first-quantization expression for the one-particle density matrix

$$\rho(x_1, x_1') = \int \rho(x_1, y)\rho(y, x_1')\,\mathrm{d}y \tag{31}$$

or

$$\rho^2 = \rho. \tag{32}$$

We do not know a direct way to extract (6), (9) or (11) from equation (32).

5. Conclusions

An A-particle fermion wavefunction can be written as a Slater determinant if, and only if, one (and consequently all) of the following conditions is (are) fullfilled:

$$(\psi(x_1, \cdots, x_A))^{A-1}\psi(y_1, \cdots, y_A) = \det\begin{pmatrix} \psi(X_{(x_1\to y_1)}) & \cdots & \psi(X_{(x_1\to y_A)}) \\ \vdots & & \vdots \\ \psi(X_{(x_A\to y_1)}) & \cdots & \psi(X_{(x_A\to y_A)}) \end{pmatrix} \tag{33}$$

for all values of the coordinates $x_1, \ldots, x_A, y_1, \ldots, y_A$; or

$$\begin{aligned}\psi(y_1, y_2, x_3, \ldots, x_A)\psi(y_3, y_4, x_3, \ldots, x_A) + \psi(y_2, y_3, x_3, \ldots, x_A)\psi(y_1, y_4, x_3, \ldots, x_A) \\ + \psi(y_3, y_1, x_3, \ldots, x_A)\psi(y_2, y_4, x_3, \ldots, x_A) = 0\end{aligned} \tag{34}$$

for all values of the coordinates $x_3, \ldots, x_A, y_1, \ldots, y_4$; or

$$\psi(y_1, \ldots, y_A)\psi(x_1, \ldots, x_A) = \sum_{i=1}^{A}\psi(Y_{(y_i\to x_j)})\psi(X_{(x_j\to y_i)}) \tag{35}$$

for all values of the coordinates $x_1, \ldots, x_A,\ y_1, \ldots, y_A$ and for $j = 1, \cdots, A$; or if

$$\rho^2 = \rho. \tag{36}$$

The question can be raised whether similar conditions apply to boson many-particle wavefunctions.

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