[2] Fermions

Slater Determinant

- The second quantization formution of the fermionic systems goes in much the same way as the bosonic case.

- The space of the fermionic wave function is the set of anti-symmetric wave function that yields the parity representation of S_N. It can be spanned by the anti-symmetrized product state:

$$\Phi(\mathbb{X}) = \sum_{\varkappa} a_{\varkappa} \, \Phi^{(a)}_{\varkappa}(\mathbb{X}) \quad \left(\leftarrow \text{an arbitrary fermionic state} \right)$$

$$\Phi^{(a)}_{\varkappa}(\mathbb{X}) \equiv \sum_{P \in S_N} (-1)^P P \underbrace{\Phi_{\varkappa}(\mathbb{X})}_{\phi_{\varkappa_1}(x_1) \cdots \phi_{\varkappa_N}(x_N)} \quad \left((-1)^P \cdots \text{the parity of the permutation } P \right)$$

$$= \det \begin{vmatrix} \phi_{\varkappa_1}(x_1) & \phi_{\varkappa_1}(x_2) & \cdots & \phi_{\varkappa_1}(x_N) \\ \phi_{\varkappa_2}(x_1) & \phi_{\varkappa_2}(x_2) & \cdots & \phi_{\varkappa_2}(x_N) \\ \vdots & \vdots & & \vdots \\ \phi_{\varkappa_N}(x_1) & \phi_{\varkappa_N}(x_2) & \cdots & \phi_{\varkappa_N}(x_N) \end{vmatrix}$$

Slater determinant

- Apart from the over-all sign, we can specify the Slater determinant by the occupation number, $\mathbf{n}$, where $n_{\varkappa}$ is the number of times $\varkappa$ appears in the list $\boldsymbol{\varkappa}$. To remove the sign ambiguity, we introduce the ordering rule (arbitrary, but fixed) in $\boldsymbol{\varkappa}$-space, and define

$$|\mathbf{n}\rangle \equiv \Phi^{(a)}_{\boldsymbol{\varkappa}} \quad (\boldsymbol{\varkappa} \text{ is ordered})$$

- Because of the antisymmetric nature, $n_{\varkappa} = 0, 1$ for all $\varkappa$. (Pauli's exclusion principle)

- We introduce the innerproduct in the fermionic states:

$$\langle \Psi_1 | \Psi_2 \rangle = \int' d\mathbf{x}\ \Psi_1^*(\mathbf{x}) \Psi_2(\mathbf{x}) = \frac{1}{N!} \int d\mathbf{x}\ \Psi_1^*(\mathbf{x}) \Psi_2(\mathbf{x})$$

- Then, one can show that

$$\langle m' | m \rangle = \delta_{m' m} \qquad (\text{Show it!})$$

Proof: $\langle m' | m \rangle = \int' d\mathbf{x} \sum_{P,Q} (-1)^{PQ} (P\, \Phi^*_{\mathbf{n}'}(\mathbf{x}))(Q\, \Phi_{\mathbf{n}}(\mathbf{x}))$

where $\mathbf{n}'$ and $\mathbf{n}$ are ordered list of labels corresponding to m' and m, respectively.

$$\langle m' | m \rangle = \frac{1}{N!} \int d\mathbf{x} \sum_{P,Q} (-1)^{PQ} \Phi^*_{P\mathbf{n}'}(\mathbf{x}) \Phi_{Q\mathbf{n}}(\mathbf{x})$$

$$= \frac{1}{N!} \sum_{P,Q} (-1)^{PQ} \delta_{P\mathbf{n}', Q\mathbf{n}}$$

Here we notice that $\delta_{P\mathbf{n}', Q\mathbf{n}} = \delta_{P,Q}\, \delta_{\mathbf{n}', \mathbf{n}}$ because if two ordered list are not equal we can't make them equal by any permutation and, if $\mathbf{n}' = \mathbf{n}$, we must choose $P = Q$ to make $P\mathbf{n} = Q\mathbf{n}$. Therefore,

$$\langle m' | m \rangle = \frac{1}{N!} \sum_{PQ} (-1)^{PQ} \delta_{P,Q}\, \delta_{m', m}$$

$$= \frac{1}{N!} \sum_{P} \delta_{m' m} = \delta_{m' m}$$

Creation / Annihilation Operators

- The operators can be defined in much the same way as bosons. Since we can't have more than one particle in the same one-particle state, we do not need the factor $\sqrt{n_\kappa !}$ in the present case. Instead, we need the sign factor.

- Definition $\quad c_k |\mathfrak{n}\rangle = 0 \quad (\text{if } n_k = 0)$

Suppose $\varkappa \equiv (\kappa_1\, \kappa_2 \cdots \kappa_N)$ is ordered, and $\mathfrak{n}$ is the corresponding occupation number vector;

$$|\mathfrak{n}\rangle = \Phi^{(a)}_{\varkappa}(\mathbb{X}) = \begin{vmatrix} \phi_{\kappa_1}(x_1) & \cdots & \phi_{\kappa_N}(x_1) \\ \vdots & \ddots & \vdots \\ \phi_{\kappa_1}(x_N) & \cdots & \phi_{\kappa_N}(x_N) \end{vmatrix}$$

Then we define $c^\dagger_\kappa$ as the operator that adds the ϕ_κ-column and the x_{N+1} row, i.e.,

$$c^\dagger_\kappa |\mathfrak{n}\rangle = \begin{vmatrix} \phi_{\kappa_1}(x_1) & \cdots & \phi_{\kappa_N}(x_1) & \cdots \phi_{\kappa_N}(x_1) \\ \vdots & \ddots & \vdots & \vdots \\ \phi_{\kappa_1}(x_N) & \cdots & \phi_{\kappa_N}(x_N) & \phi_\kappa(x_N) \\ \phi_{\kappa_1}(x_{N+1}) & \cdots & \phi_{\kappa_N}(x_{N+1}) & \phi_\kappa(x_{N+1}) \end{vmatrix}$$

Obviously, this wave function can be expressed as

$$c^\dagger_\kappa |\mathfrak{n}\rangle = \Phi^{(a)}_{(\varkappa,\kappa)}\left(\begin{pmatrix} \mathbb{X} \\ x_{N+1} \end{pmatrix}\right) = (-1)^P\, \Phi^{(a)}_{P(\varkappa,\kappa)}\begin{pmatrix} \mathbb{X} \\ x_{N+1} \end{pmatrix}.$$

where $(\varkappa,\kappa)$ is the list we obtain by appending κ to $\varkappa$.
To make $\varkappa' \equiv P(\varkappa,\kappa)$ have the right order ($\kappa'_i < \kappa'_j$ for all $i<j$), P must be the permutation

that brings x to the right place in the list $\mathbb{X}$, which is already ordered. When $x_i < x < x_{i+1}$, P swaps x with all x_js for $j \geq i+1$.
Therefore $(-1)^P = (-1)^m$ where m is the number of x_js in $\mathbb{X}$ that are larger than x. In terms of $\mathbb{n}$, this means

- Definition of fermionic creation op.

$$c_x^\dagger |\mathbb{n}\rangle = (-1)^{\gamma(x|\mathbb{n})} |\mathbb{n} + \mathbb{1}_x\rangle \quad \text{④} \quad \left(\begin{array}{l}\text{if } n_x = 0, \\ \text{otherwise} \\ c_x^\dagger|\mathbb{n}\rangle = 0\end{array}\right)$$

where $\gamma(x|\mathbb{n}) \equiv \sum_{\substack{x' \\ (x'>x)}} n_{x'} = \left(\begin{array}{l}\text{the number of } x_i\text{s} \\ \text{in } \mathbb{X} \text{ larger than } x\end{array}\right)$

- The annihilation operator c_x is defined as

$$c_x |\mathbb{n} + \mathbb{1}_x\rangle = (-1)^{\gamma(x|\mathbb{n})} |\mathbb{n}\rangle$$

or

$$c_x |\mathbb{n}\rangle = (-1)^{\gamma(x|\mathbb{n})} |\mathbb{n} - \mathbb{1}_x\rangle \quad \left(\begin{array}{l}\text{if } n_x = 1, \\ \text{otherwise} \\ c_x|\mathbb{n}\rangle = 0\end{array}\right)$$

- From these definitions, the anti-commutation relation follows

$$\{c_{x'}, c_x^\dagger\} \equiv c_{x'} c_x^\dagger + c_x^\dagger c_{x'} = \delta_{x'x} \quad \text{— ①}$$

(Prove it!)

- As in the bosonic case, $\hat{n}_x \equiv c_x^\dagger c_x$ is the occupation number operator:

$$\hat{n}_x |\mathbb{n}\rangle = n_x |\mathbb{n}\rangle$$

- Proof of ①

The equation to be proved is symmetric under swapping $x \leftrightarrow x'$. Therefore it suffices to prove when $x \le x'$. When $x = x'$, for $\mathbf{n}$ with $n_x = 0$

$$
\begin{aligned}
(c_x c_x^{+} + c_x^{+} c_x)|\mathbf{n}\rangle &= c_x c_x^{+} |\mathbf{n}\rangle \\
&= c_x (-1)^{\gamma(x|\mathbf{n})} |\mathbf{n} + \mathbb{1}_x\rangle \\
&= (-1)^{\gamma(x|\mathbf{n})} (-1)^{\gamma(x|\mathbf{n}+\mathbb{1}_x)} |\mathbf{n}\rangle = |\mathbf{n}\rangle
\end{aligned}
$$

and also for $\mathbf{n}$ with $n_x = 1$, similarly we can show

$$(c_x c_x^{+} + c_x^{+} c_x)|\mathbf{n}\rangle = |\mathbf{n}\rangle .$$

Therefore, $c_x c_x^{+} + c_x^{+} c_x = 1$

Unless this condition is satisfied, obviously $(c_x c_{x'}^{+} + c_{x'}^{+} c_x)|\mathbf{n}\rangle = 0$

When $x < x'$, for $\mathbf{n}$ with $\underline{n_x = 1 \text{ and } n_{x'} = 0}$

$$
\begin{aligned}
c_x c_{x'}^{+} |\mathbf{n}\rangle &= c_x (-1)^{\gamma(x'|\mathbf{n})} |\mathbf{n} + \mathbb{1}_{x'}\rangle \\
&= (-1)^{\gamma(x'|\mathbf{n})} (-1)^{\gamma(x|\mathbf{n}+\mathbb{1}_{x'})} |\mathbf{n} + \mathbb{1}_{x'} - \mathbb{1}_x\rangle \\
&= (-1)^{\gamma(x'|\mathbf{n}) + \gamma(x|\mathbf{n}) + 1} |\mathbf{n} + \mathbb{1}_{x'} - \mathbb{1}_x\rangle
\end{aligned}
$$

$$
\begin{aligned}
c_{x'}^{+} c_x |\mathbf{n}\rangle &= c_{x'}^{+} (-1)^{\gamma(x|\mathbf{n})} |\mathbf{n} - \mathbb{1}_x\rangle \\
&= (-1)^{\gamma(x|\mathbf{n})} (-1)^{\gamma(x'|\mathbf{n} - \mathbb{1}_x)} |\mathbf{n} + \mathbb{1}_{x'} - \mathbb{1}_x\rangle \\
&= (-1)^{\gamma(x|\mathbf{n}) \gamma(x'|\mathbf{n})} |\mathbf{n} + \mathbb{1}_{x'} - \mathbb{1}_x\rangle
\end{aligned}
$$

Therefore, $(c_x c_{x'}^{+} + c_{x'}^{+} c_x)|\mathbf{n}\rangle = 0$ for any $|\mathbf{n}\rangle$.

Field Operators

- The field operator is defined as

$$\hat{\psi}(x) \equiv \sum_{\mu} \phi_{\mu}(x) c_{\mu}$$

- It inherits the anticommutation relation of c_{μ}:

$$\{\hat{\psi}(x), \hat{\psi}^{\dagger}(x')\} = \delta(x-x')$$

$$\{\hat{\psi}(x), \hat{\psi}(x')\} = 0$$

(The proof is exactly like the one for bosons.)

Question In ⊛ (in 2-2-②) (the defining equation of the creation operator), we have the sign factor. Why can we not get rid of this complication? (It's just a definition. So why can we not define the creation op. with no sign?)

Answer The definition without the sign factor would be inconvenient and therefore useless. The creation operator defined without the sign would not satisfy either commutation or anticommutation relation. Such a mixed relation would not be inherited by the field operators. In other words, such a mixed relation is not invariant under unitary transformation.

ex If we define c'_k and c'^{+}_k by

$$c'^{+}_k |n\rangle = \begin{cases} |n + 1_k\rangle & (\text{if } n_k = 0) \\ 0 & (\text{if } n_k = 1) \end{cases}$$

Then, obviously

$$[c'_k, c'^{+}_{k'}] = 0 \quad (\text{for } k \neq k') \quad \text{just like bosons}$$

However,

$$[c'_k\, c'^{+}_k] |n\rangle = \begin{cases} |n\rangle & (\text{if } n_k = 0) \\ -|n\rangle & (\text{if } n_k = 1) \end{cases}$$

Therefore, we have neither

$$[c'_k\, c'^{+}_{k'}] = \delta_{kk'} \quad \text{or} \quad \{c'_k, c'^{+}_{k'}\} = \delta_{kk'}.$$

Hamiltonian of Non-Interacting Fermions

- As we have seen in the bosonic case, the hamiltonian

$$\mathcal{H} = \sum_i K(x_i) \qquad \left(K(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + w(x) \right)$$

can be expressed in the 2-nd quantization formalism as

$$\hat{\mathcal{H}} = \int dx \; \hat{K}(x) \qquad \left(\hat{K}(x) \equiv \hat{\psi}^{+}(x)\, K(x)\, \hat{\psi}(x) \right)$$

- If we choose the single-particle eigenstate of the Schrödinger equation as $\phi_\kappa(x)$ we have

$$\hat{\mathcal{H}} = \sum_\kappa \epsilon_\kappa c_\kappa^{+} c_\kappa \qquad \text{—— (1)}$$

$$\left(U(x)\, \phi_\kappa(x) = \epsilon_\kappa \phi_\kappa(x) \right)$$

- Example: Non-interacting electrons confined in the void space ($u=0$).

Assuming that the space is a cube of size L with the periodic boundary condition, the single particle states and the corresponding eigenenergies are

$$\phi_{\mathbb{k},\sigma}(x) = \frac{1}{\sqrt{\Omega}} e^{i\mathbb{k}\cdot x} \qquad \Omega = L^3 \qquad k^\alpha = \frac{2\pi}{L} \times (\text{integer}) \quad (\alpha = x, y, z)$$

$$\sigma = \pm 1$$

$$(\kappa = (\mathbb{k}, \sigma))$$

$$\epsilon_{\mathbb{k},\sigma} = \frac{\hbar^2}{2m}\mathbb{k}^2$$

The Ground State of Non-Interacting Fermions

- From 2-4-①, it is obvious that all eigenvectors of the non-interacting fermionic Hamiltonian are single Slater determinants $|n\rangle$ and

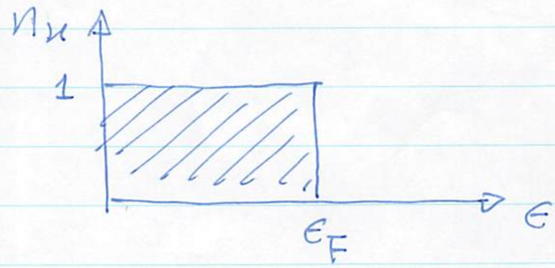
$$\hat{\mathcal{H}}|n\rangle = E(n)|n\rangle \qquad E(n) = \sum_{\kappa} \epsilon_\kappa n_\kappa$$

- Obviously, the ground state is $|n\rangle$ with n such that

$n_\kappa = 1$ for the N smallest ϵ_κ and
$n_\kappa = 0$ for all the other states.

- The single-particle energy of the highest occupied single-particle state is called the Fermi level (or the Fermi energy), and denoted as ϵ_F

(Ferm Sea)



Free Electrons at Finite Temperature

- A real electron has an "orbital" degee of freedom and a "spin" degree of freedom. (Here, orbital means a conventional orbital for an electron in an atom, while it is just the energy level in other circumstances.) In some cases, the two degrees of freedom are not mixed by the Hamiltonian. In such cases, the general label $\varkappa$ we have been using so far is $\varkappa = (\alpha, \sigma)$ where α and $\sigma = \pm 1$ are the orbital and the spin indices, respectively.

- As in the bosonic case, the density operator is

$$\hat{\rho} \equiv Z^{-1} e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} \quad \left(Z = \mathrm{Tr}\, e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} \right)$$

- For the non-interacting electrons $\left(\mathcal{H} = \sum_{\varkappa} \epsilon_\varkappa c_\varkappa^\dagger c_\varkappa \right)$

$$\hat{\rho} = Z^{-1} e^{-\beta \sum_{\varkappa} (\epsilon_\varkappa - \mu) c_\varkappa^\dagger c_\varkappa}$$

- The expected occupation number is

$$f_\varkappa \equiv \langle c_\varkappa^\dagger c_\varkappa \rangle = \frac{1}{e^{\beta(\epsilon_\varkappa - \mu)} + 1} \quad \left(\begin{array}{c} \text{Fermi} \\ \text{distribution} \end{array} \right)$$

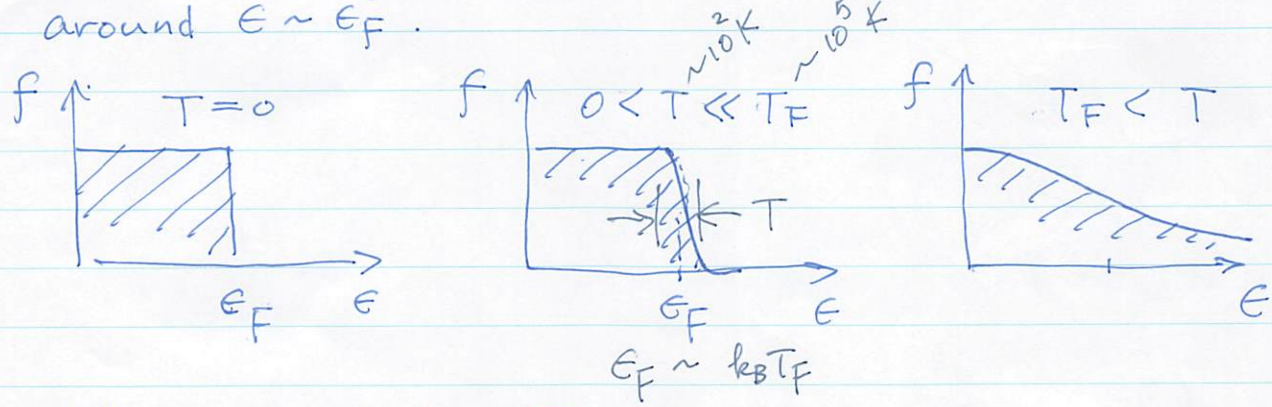
- With the total particle number fixed to be N, as we decrease the temperature, we can show

$$\mu \to \epsilon_F \qquad f_\varkappa \longrightarrow \theta(\epsilon_F - \epsilon_\varkappa)$$

as we anticipate.

Fermi Temperature

- Starting from $T=0$, as we increase the temperature, the Fermi distribution is relaxed from the rigid step function on the boundary, i.e., around $\epsilon \sim \epsilon_F$.



- However, before T becomes comparable to "the Ferm temperature" defined by $T_F \equiv \epsilon_F / k_B$, the finite-$T$ effect is restricted to the boundary region (i.e. near the Fermi surface).

- Free electrons. As we have seen before, the single-particle eigenenergy is $\epsilon_{k\sigma} = \frac{\hbar^2}{2m} k^2$, with $k^x, k^y, k^z = \frac{2\pi}{L} \times$ (integer).
  This means that in the k-space volume d^3k, we have

$$2 \times \frac{d^3 k}{\left(\frac{2\pi}{L}\right)^3} = \frac{\Omega}{4\pi^3} d^3 k \quad \left(\leftarrow \text{The factor 2 comes from the spin degree of freedom}\right)$$

single-particle states. When the Fermi energy is ϵ_F, the k-space volume below ϵ_F is

$$\int_0^{k_F} d^3 k = \frac{4\pi}{3} k_F^3 \quad \left(\frac{\hbar^2}{2m} k_F^2 \equiv \epsilon_F\right)$$

Therefore, $N = \frac{\Omega}{3\pi^2} k_F^3 \rightarrow \epsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{\Omega}\right)^{\frac{2}{3}}$.

(Compute the Fermi temperature for the Avogadro's number of free electrons confined in a cube of $1\,\text{cm}^3$.)

A remark on Slater determinant

From the derivation, there is no reason to expect that an arbitrary state can be expressed as a »single« Slater determinant. In fact, the set of single Slater determinants has zero measure in the space of general N-fermion wave functions, i.e., the vast majority of N-fermion wave functions cannot be expressed as single Slater determinants. they are rather expressed as linear combinations of many Slater determinants.

Nonetheless, students, once including myself, are often confused with this fact, probably because most of the many-body wave functions disscussed in the introductory lectures are single Slater determinants, such as the wave functions of the non-interacting fermions, the variational wave function in the Hartree-Fock approximation, wave functions in the simplest band theory, etc.

In fact, it is easy to see that the single Slater determinants are rather special wave functions, by counting the number of parameters we need to specify a single Slater determinant.

Suppose we have N fermions. Also suppose that the one-particle state space is $M (< \infty)$ dimensional, e.g., every fermion can take only M positions.

To make a Slater determinant, we need N one-particle states ϕ_i $(i=1,\cdots,N)$. Each ϕ_i is a complex vector in M dimensional space. Therefore we need $2M$ real parameters to specify ϕ_i. (To be precise, we need less because of the redundancy with respect to the over-all phase factor and the normalization condition $\langle \phi_i | \phi_i \rangle = 1$. But we only count the leading order term.) Therefore, we need, at most, $2MN$ real parameters to specify a single Slater determinant.

On the other hand, we need much more parameters to specify a general N-fermion wave function. There are ${}_MC_N$ independent Slater determinants. To specify a wave function we must specify ${}_MC_N$ complex coefficient in the linear combination, which means we need $2 \times {}_MC_N$ real parameters. When $M \gg N$, this is

$$2\,{}_MC_N \sim 2M^N/N!$$

Obviously, for $1 \ll N \lesssim M$, we have $2M^N/N! \gg 2MN$ which means that the set of Slater determinant is much "smaller" than the whole state space.

Question: Suppose we have 4 independent (mutually orthogonal) single-particle wave functions $\phi_i(x)$ $(i=1\cdots 4)$. Consider

$$|\psi\rangle = (|12\rangle + |34\rangle)/\sqrt{2}$$

where $|ij\rangle \equiv \begin{vmatrix} \phi_i(x_1) & \phi_j(x_1) \\ \phi_i(x_2) & \phi_j(x_2) \end{vmatrix}$.

Can we express $|\psi\rangle$ as a single Slater determinant, like $|\psi\rangle = \begin{vmatrix} \chi_1(x_1) & \chi_2(x_1) \\ \chi_1(x_2) & \chi_2(x_2) \end{vmatrix}$ by choosing χ_1 and χ_2 ?

Simple examples of 2-body fermionic wave functions.

Let N (M in the previous page) be the dimension of the space of the single particle wave functions.

① The case $N=2$ ---- We have only two independent single-particle states, ϕ_1 and ϕ_2. So, essentially we can create only one Slater determinant : $|\phi_1\phi_2\rangle_a$. So, any fermionic 2-body fn. can be expressed by a single Slater determinant.

$$\left(\equiv \phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2) \right)$$

② The case $N=3$

Consider the wave function

$$\psi \equiv |\chi_1\chi_2\rangle_a + |\chi_3\chi_4\rangle_a \quad \left(\begin{array}{l} \chi_1 \sim \chi_4 \text{ are} \\ \text{arbitrary s.p.s.} \end{array} \right)$$

Since $\chi_1 \cdots \chi_4$ can't be all independent, at least one of them can be expressed by a linear combination of the other three. So, let χ_4 be a linear combination of χ_1 χ_2 and χ_3 :

$$\chi_4 = \xi_1\chi_1 + \xi_2\chi_2 + \xi_3\chi_3$$

Then, $\psi = |\chi_1\chi_2\rangle_a + |\chi_3, \xi_1\chi_1 + \xi_2\chi_2 + \xi_3\chi_3\rangle_a$

$$= |\chi_1\chi_2\rangle_a + |\chi_3, \xi_1\chi_1 + \xi_2\chi_2\rangle_a$$

$$= |\chi_1, \chi_2 - \xi_1\chi_3\rangle_a + \xi_2|\chi_3, \chi_2\rangle_a$$

$$= |\chi_1, \chi_2 - \xi_1\chi_3\rangle_a + \xi_2|\chi_3, \chi_2 - \xi_1\chi_3\rangle_a$$

$$= | \chi_1 - \xi_2 \chi_3 \, , \, \chi_2 - \xi_1 \chi_3 \rangle_a$$

This means any linear combination of any two Slater determinants can be expressed by a single Slater determinant. By applying this repeatedly we can show that any fermionic wave function can be expressed as a single Slater determinant.

③ The case $N \geq 4$

Consider an arbitrary s.p.s. $\theta(x)$ and the mapping generated by $\theta(x)$ as

$$f_\theta : \psi(x_1 x_2) \longrightarrow (f_\theta \psi)(x_2) \equiv \int dx_1 \, \theta^*(x_1) \psi(x_1 x_2)$$

Assuming that ψ can be expressed as a single Slater det., if we apply this mapping to this Slater determinant we obtain for $\psi = |\chi_1 \chi_2\rangle_a$

$$f_\theta |\chi_1 \chi_2\rangle_a = \langle \theta | \chi_1 \rangle \chi_2 - \langle \theta | \chi_2 \rangle \chi_1$$

Therefore, the space

$$\left\{ f_\theta \psi \;\middle|\; \theta \in \begin{pmatrix} \text{the set of} \\ \text{all s.p.s.s} \end{pmatrix} \right\}$$

is spanned by χ_1 and χ_2. So, it is at most 2-dimensional.

However, if we consider the wave function (#) with $\chi_1 \cdots \chi_4$ are all independent,

$$f_\theta \psi = \langle\theta|\chi_1\rangle \chi_2 - \langle\theta|\chi_2\rangle \chi_1 + \langle\theta|\chi_3\rangle \chi_4 - \langle\theta|\chi_4\rangle \chi_3$$

it forms a 4-dimensional space when θ runs over $N(\geq 4)$-dimensional space of s.p.s.s. Therefore the wave function (#) cannot be expressed as a single Slater determinant.

(An example of such a state is the ground state of the 2-site system discussed in "magnons and spin waves". The singlet ground state Ψ_4 has the form of (#) with 4 independent single-particle states.)