2. Representation of a Slater Determinant

We wish to represent a general Slater determinant $|\Phi\rangle$ for a system of $N$ particles by use of creation and annihilation operators in a particular representation. The operator $a_i^+$ creates a particle with wave function $\varphi_i$ and the operator $a_i$ annihilates a particle with wave function $\varphi_i$. We denote by $|\Phi_0\rangle$ the configuration in which the first $N$-levels are occupied, so that

$$|\Phi_0\rangle = (\prod_{i=1}^N a_i^+)|0\rangle,$$

where $|0\rangle$ denotes the vacuum, in which no particles are present. Written in this form, $|\Phi_0\rangle$ is normalized to unity.

**Theorem.** Any $N$-particle Slater determinant $|\Phi\rangle$ which is not orthogonal to $|\Phi_0\rangle$ can be written in the form

$$|\Phi\rangle = [\prod_{i=1}^N \prod_{m=N+1}^{\infty} (1 + C_{mi} a_m^+ a_i)]|\Phi_0\rangle$$

$$= [\exp(\sum_{i=1}^N \sum_{m=N+1}^{\infty} C_{mi} a_m^+ a_i)]|\Phi_0\rangle,$$

where the coefficients $C_{mi}$ are uniquely determined. Conversely, any wave function written in the form of eq. (2), with $|\Phi_0\rangle$ defined by eq. (1), is an $N$-particle Slater determinant.

Problem: Demonstrate that this representation is correct.
Thouless theorem, fermion number conserving states

Every even product state, non-orthogonal to $|0\rangle$ can be uniquely written in the form:

$$|\Phi\rangle_{even} = \mathcal{N} \exp \left( -\frac{1}{2} \sum_{\mu\nu} Z_{\mu\nu} a_\mu^+ a_\nu^+ \right) |0\rangle$$

$$Z^T = -Z$$

Thouless theorem for particle-number conserving states

$$|\Phi_0\rangle = \prod_{h=1}^{A} a_h^+ |0\rangle$$

$$\alpha_{\mu} = \begin{cases} a_p^+ & \text{for } \mu = p \\ a_h & \text{for } \mu = h \end{cases}$$

$$\alpha_\mu |\Phi_0\rangle = 0$$

empty (particle, $p$) states

occupied (hole, $h$) states

independent-particle ground-state

quasi-particle vacuum!
According to the Thouless theorem, any product state, non orthogonal to the independent-particle ground state, can be written as

\[ |\Phi\rangle = N \exp \left( \frac{1}{2} \sum_{\mu\nu} Z^*_{\mu\nu} \alpha^+_{\mu} \alpha^+_{\nu} \right) |\Phi_0\rangle \]

\[ = N \exp \left( \sum_{p=A+1}^{M} \sum_{h=1}^{A} Z^*_{ph} a^+_p a_h \right) |\Phi_0\rangle \]
Hartree-Fock method

Based on the Ritz variational principle:

\[ |\Psi\rangle \quad \text{- trial (variational) wave function. Should be as rich and realistic as possible} \]

\[ \delta \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0 \quad \text{Energy of the system is minimized} \]

In the Hartree-Fock method, the trial wave function is the particle-number conserving product state. That’s it!

\[ |\tilde{Z}\rangle = \exp \left( \sum_{ph} \tilde{Z}_{p}^{*} a_{p}^{+} a_{h} \right) a_{1}^{+} \ldots a_{A}^{+} |0\rangle \]

\((M-A)A\) complex variables (<< size of the Hilbert space)

\[ \delta E_{HF} = 0 \quad E_{HF} \equiv \frac{\langle \tilde{Z} | \hat{H} | \tilde{Z} \rangle}{\langle \tilde{Z} | \tilde{Z} \rangle} \]

variation:

\[ \delta \equiv \sum_{ph} \delta \tilde{Z}_{p}^{*} \frac{\partial}{\partial \tilde{Z}_{p}^{*}} \]

\[ |\delta \tilde{Z}\rangle \equiv \delta |\tilde{Z}\rangle \]
Hartree-Fock method, Lipkin Model