Thouless, Nucl. Phys. 21 (1960) 225

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 φ_i and the operator a_i annihilates a particle with wave function φ_i. We denote by $|\Phi_0\rangle$ the configuration in which the first N-levels are occupied, so that

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

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

$$\begin{aligned} |\Phi\rangle &= [\prod_{i=1}^{N} \prod_{m=N+1}^{\infty} (1+C_{mi}a^\dagger{}_m a_i)]|\Phi_0\rangle \\ &= [\exp(\sum_{i=1}^{N} \sum_{m=N+1}^{\infty} C_{mi}a_m{}^\dagger a_i)]|\Phi_0\rangle, \end{aligned} \tag{2}$$

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

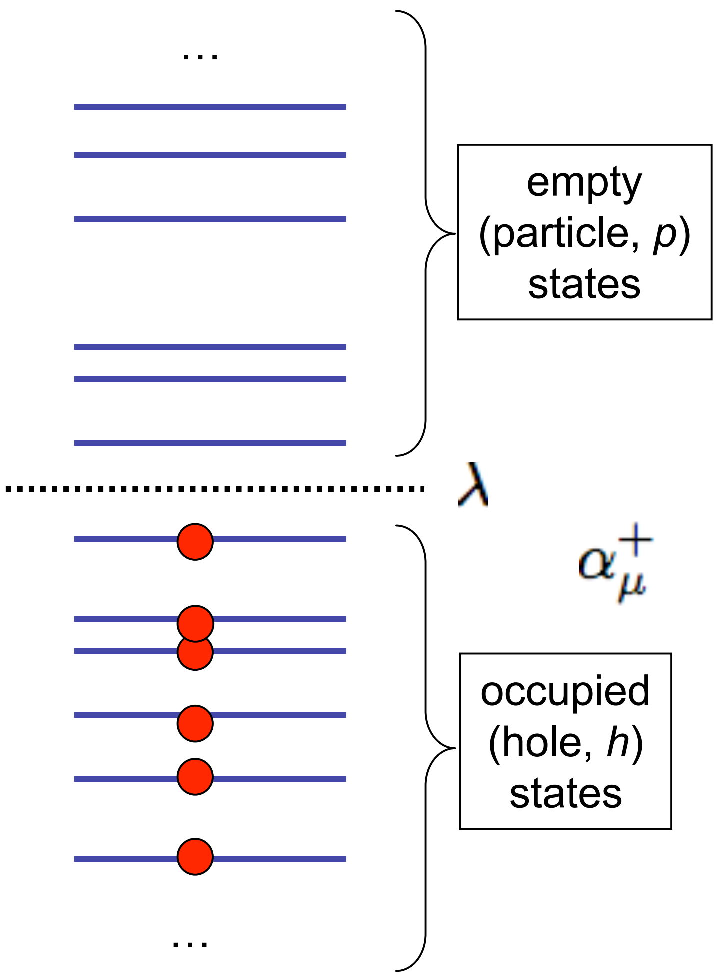
Thouless theorem, fermion number conserving states

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

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

$$Z^T = -Z$$

Thouless theorem for particle-number conserving states



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

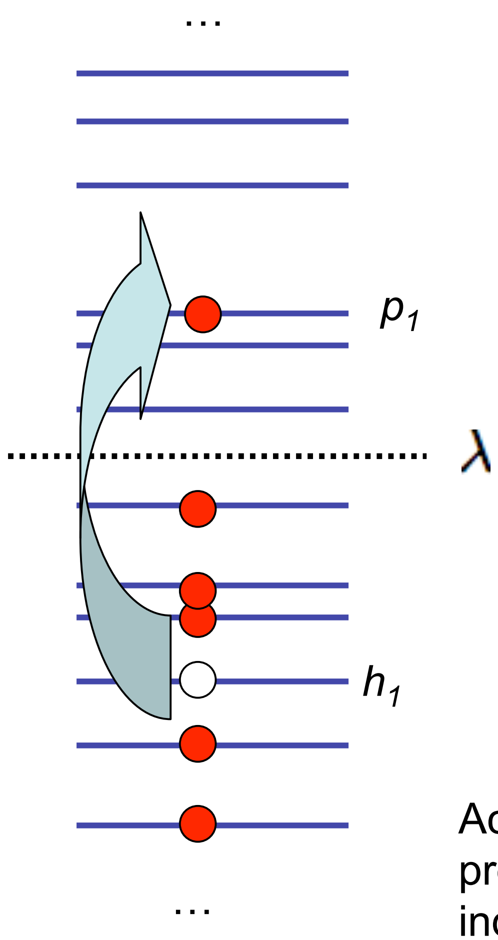
independent-particle ground-state

$$\alpha^{+}_{\mu} = \begin{cases} a^{+}_{p} & \text{for } \mu = p \\ a_{h} & \text{for } \mu = h \end{cases}$$

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

quasi-particle vacuum!

A particle-hole excitation



particle-hole

$$
\begin{aligned}
|\Phi_{p_1 h_1}\rangle &= a^+_{p_1} a_{h_1} |\Phi_0\rangle \\
&= \alpha^+_{p_1} \alpha^+_{h_1} |\Phi_0\rangle
\end{aligned}
$$

two-quasiparticle

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

$$
\begin{aligned}
|\Phi\rangle &= \mathcal{N} \exp\left(\frac{1}{2} \sum_{\mu\nu} Z^*_{\mu\nu} \alpha^+_\mu \alpha^+_\nu \right) |\Phi_0\rangle \\
&= \mathcal{N} \exp\left(\sum_{p=A+1}^{M} \sum_{h=1}^{A} Z^*_{ph} a^+_p a_h \right) |\Phi_0\rangle
\end{aligned}
$$

Hartree-Fock method

Based on the Ritz variational principle:

$|\Psi\rangle$ - trial (variational) wave function. Should be as rich and realistic as possible

$$\delta \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$$

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!

$$|\tilde{Z}\rangle = \exp\left(\sum_{ph} \tilde{Z}^*_{ph} a^+_p a_h \right) a^+_1 \ldots a^+_A |0\rangle$$

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

$$\delta E_{\mathrm{HF}} = 0 \qquad E_{\mathrm{HF}} \equiv \frac{\langle \tilde{Z} | \hat{H} | \tilde{Z} \rangle}{\langle \tilde{Z} | \tilde{Z} \rangle}$$

variation: $$\delta \equiv \sum_{ph} \delta \tilde{Z}^*_{ph} \frac{\partial}{\partial \tilde{Z}^*_{ph}}$$

$$|\delta \tilde{Z}\rangle \equiv \delta |\tilde{Z}\rangle$$

Hartree-Fock method, Lipkin Model