Ring and Schuck theorem

Every even-particle-number product state can be written as

$$|\Phi\rangle_{\text{even}} = e^{i\phi} \exp\left(\frac{i}{2} \sum_{\mu\nu} \{T^{+}_{\mu\nu} a^{+}_{\mu} a^{+}_{\nu} + T_{\mu\nu} a_{\mu} a_{\nu}\} \right) |0\rangle$$

where $T^T = -T$

(there is no need to introduce *Y*-matrices)

Note that in the above one can replace a by α and |0> by |Φ>

Thouless theorem (1960)

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

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

$$Z^T = -Z$$

normalization constant

Thouless matrix

$$\cos(T^{+}T)^{1/2} = (1 + Z^{+}Z)^{-1/2}$$

1.A

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STABILITY CONDITIONS AND NUCLEAR ROTATIONS IN THE HARTREE-FOCK THEORY

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Abstract: An expression for a general Slater determinant is written in the notation of second quantization. This expression has just the right number of arbitrary coefficients, so no subsidiary conditions are required, and the expression for a particular determinant is unique. This notation is used to study two problems. Firstly, a condition for a particular solution of the Hartree-Fock equations to minimize the expectation value of the Hamiltonian is derived. This condition is equivalent to the condition for stability of collective modes in the random phase approximation. Secondly, the determinant which minimizes the expectation value of the Hamiltonian while giving a particular value to the expectation value of a component of angular momentum is found. In this way, an expression for the moment of inertia of an axially symmetric system is derived within the framework of the Hartree-Fock theory. The expression for a determinant is generalized to include the type of wave functions used in the theory of superconductivity.

Generalized coherent states

$$|Z\rangle = \exp\left(\frac{1}{2}\sum_{\mu\nu} Z^*_{\mu\nu} a^+_\mu a^+_\nu\right)|0\rangle$$

A product state in the Thouless representation but not normalized

$$\langle Z|0\rangle = 1$$ a phase convention…

Onishi Theorem

$$\langle Z'|Z\rangle = \det{}^{1/2}(1 + Z'Z^+)$$

Thouless theorem for odd-N states

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

blocked single-particle state

where

$$Z^T = -Z$$

$$Z_{1\mu} = -Z_{\mu 1} = 0 \quad \text{for all } \mu$$

Thouless theorem and density matrix

$$
\begin{aligned}
\rho_{\mu\nu} &= \langle\Phi|a^{+}_{\nu} a_{\mu}|\Phi\rangle = \overline{a^{+}_{\nu} a_{\mu}} \\
\kappa_{\mu\nu} &= \langle\Phi|a_{\nu} a_{\mu}|\Phi\rangle = \overline{a_{\nu} a_{\mu}}
\end{aligned}
$$

$$
\begin{aligned}
\rho^{+} &= \rho, \\
\kappa^{T} &= -\kappa
\end{aligned}
$$

In principle, by measuring various one- and many-body observables, one can extract the whole density matrix.

$$\langle\Phi|\hat{F}|\Phi\rangle = \sum_{\mu\nu} F_{\mu\nu}\rho_{\nu\mu} = \mathrm{Tr}F\rho$$

$$\langle\Phi|\hat{F}|\Phi\rangle = \sum_{\mu\mu'\nu\nu'} F_{\mu\mu'\nu\nu'}\left(\frac{1}{2}\rho_{\nu\mu}\rho_{\nu'\mu'} + \frac{1}{4}\kappa^{+}_{\mu'\mu}\kappa_{\nu'\nu}\right)$$

In terms of the matrix Bogoliubov transformation:

$$
\begin{aligned}
\rho &= B^{*}B^{T}, \\
\kappa &= B^{*}A^{T}
\end{aligned}
$$

The conditions

$$
\begin{aligned}
\rho^{2} + \kappa\kappa^{+} &= \rho, \\
\rho\kappa - \kappa\rho^{*} &= 0
\end{aligned}
$$

is equivalent to the unitarity conditions between matrices *A* and *B*.

Density matrix for N-even states

Let us use the Onishi theorem and differential calculus:

$$\langle Z|a_\nu a_\mu|Z\rangle = \frac{\partial}{\partial Z_{\mu\nu}}\langle Z|Z\rangle$$

$$\kappa_{\mu\nu} = \frac{\partial}{\partial Z_{\mu\nu}} \log\langle Z|Z\rangle = \frac{\partial}{\partial Z_{\mu\nu}} \log \det{}^{1/2}(1+ZZ^+)$$

$$\begin{aligned}\left(a_\nu - \sum_{\nu'} Z^*_{\nu\nu'} a^+_{\nu'}\right)|Z\rangle &= 0 \\ \langle Z|\left(a^+_\nu - \sum_{\nu'} Z_{\nu\nu'} a_{\nu'}\right) &= 0\end{aligned}$$

This gives

$$\langle Z|a^+_\nu a_\mu|Z\rangle = \sum_{\nu'} Z_{\nu\nu'}\langle Z|a_{\nu'} a_\mu|Z\rangle$$

$$\boxed{\rho = -\kappa Z}$$

$$\boxed{\begin{aligned}\rho &= Z^+(1+ZZ^+)^{-1}Z \\ \kappa &= -Z^+(1+ZZ^+)^{-1}\end{aligned}}$$

Alternative expression:

$$\begin{aligned}\rho &= (1+Z^+Z)^{-1}Z^+Z \\ \kappa &= -(1+Z^+Z)^{-1}Z^+\end{aligned}$$

Density matrix for N-odd states

$$\begin{aligned}\rho_{11} &= 1, \\ \rho_{\mu 1} = \rho^*_{1\mu} &= 0 \quad \text{for} \quad \mu \neq 1 \\ \rho_{\mu\nu} &= \left(Z^+(1+ZZ^+)^{-1}Z\right)_{\mu\nu} \quad \text{for} \quad \mu \neq 1, \nu \neq 1, \\ \kappa_{\mu 1} = -\kappa_{1\mu} &= 0 \\ \kappa_{\mu\nu} &= -\left(Z^+(1+ZZ^+)^{-1}\right)_{\mu\nu} \quad \text{for} \quad \mu \neq 1, \nu \neq 1.\end{aligned}$$

Generalized density matrix

$$\mathcal{R}^+ = \mathcal{R}$$
$$\mathcal{R}^2 = \mathcal{R}$$

$$\mathcal{F}\mathcal{R}\mathcal{F} = 1 - \mathcal{R}^*$$

$$\mathcal{R} = \begin{pmatrix} B^* B^T & B^* A^T \\ A^* B^T & A^* A^T \end{pmatrix} = \begin{pmatrix} B^* \\ A^* \end{pmatrix} \begin{pmatrix} B^T & A^T \end{pmatrix}$$

$$\begin{aligned} \mathcal{R} &= \varphi\varphi^+ \\ \mathcal{R}\varphi &= \varphi \end{aligned} \qquad \varphi \equiv \begin{pmatrix} B^* \\ A^* \end{pmatrix}$$

$$\begin{aligned} 1 - \mathcal{R} &= \chi\chi^+ \\ \mathcal{R}\chi &= 0 \end{aligned} \qquad \chi \equiv \begin{pmatrix} A \\ B \end{pmatrix}$$

$$\varphi^+\varphi = \chi^+\chi = 1$$
$$\varphi^+\chi = \chi^+\varphi = 0$$

$$\varphi\varphi^+ + \chi\chi^+ = 1$$

Product states with fixed particle number

$$\begin{aligned} \langle\Phi|\hat{N}|\Phi\rangle &= Tr(\rho) \\ \sigma_N^2 \equiv \langle\Phi|\hat{N}^2|\Phi\rangle - \langle\Phi|\hat{N}|\Phi\rangle^2 &= 2Tr(\kappa\kappa^+) \end{aligned}$$

For such states, pairing tensor has to vanish and

$$\rho^2 = \rho$$

Single-particle states

occupied (hole) states

$$\begin{aligned} \rho &= xx^+ \\ \rho x &= x \end{aligned}$$

empty (particle) states

$$\begin{aligned} 1-\rho &= yy^+ \\ \rho y &= 0 \end{aligned}$$

$$\begin{aligned} x^+x = 1 \quad &, \quad y^+y = 1 \\ x^+y = 0 \quad &, \quad y^+x = 0 \end{aligned}$$

$$|\Phi\rangle = \prod_{h=1}^{A} \left(\sum_{\mu} x^T_{h\mu} a^+_\mu \right) |0\rangle = \prod_{h=1}^{A} \left(a^+ x\right)_h |0\rangle$$

$h = 1, \ldots, A$ **hole states**

$p = A+1, \ldots, M$ **particle states**

Particle and hole configurations (many-body states)

Hole configuration $(x^{+}a)_h|\Phi\rangle$

Particle configuration $(a^{+}y)_p|\Phi\rangle$

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