

Hartree-Fock-Bogoliubov (HFB) Theory

This Lecture closely follows parts of chapter 7 in Ring & Schuck *The nuclear many-body problem*.

HFB provides a generalized single-particle theory that unifies Hartree-Fock and BCS. It thus can be used to describe aspects of deformations (i.e. long range part of nucleon-nucleon force) as well as pairing correlations due to short ranged attraction.

Let's consider M single-particle orbitals with creation operators $\hat{a}^\dagger = (\hat{a}_1^\dagger, \dots, \hat{a}_M^\dagger)$. The most general transformation of the single-particle basis is

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} \equiv W^\dagger \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix}$$

For unitary $WW^\dagger = 1$, the quasi-particle operators fulfill canonical anti-commutation rules $\{\beta_k, \beta_l^\dagger\} = \delta_{kl}$.

Bloch & Messiah: The W matrix can be decomposed as

$$W = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}$$

Properties of HFB state

Def.: HFB ground state $|\Phi\rangle = \prod_k \beta_k |-\rangle$, where the product runs over a maximal number of operators such that $\beta_k |\Phi\rangle = 0$ for all $k = 1, \dots, M$.

HFB state determined in terms of density matrix ρ_{kl} and pairing tensor κ_{kl} .

$$\rho_{kl} = \langle \Phi | \hat{a}_l^\dagger \hat{a}_k | \Phi \rangle, \quad \kappa_{kl} = \langle \Phi | \hat{a}_l \hat{a}_k | \Phi \rangle.$$

Properties:

$$\begin{aligned} \rho &= \rho^\dagger, & \rho &= V^* V^T = D \bar{V}^2 D \\ \kappa^T &= -\kappa, & \kappa &= -U V^\dagger = D \bar{U} \bar{V} D^T \\ \rho^2 - \rho &= -\kappa \kappa^\dagger, & \rho \kappa &= \kappa \rho^* \end{aligned}$$

Thus, ρ is diagonal in the canonical basis.

HFB Equations

Two-body Hamiltonian

$$H = \sum_{k,l \neq 0} t_{kl} \hat{a}_k^\dagger \hat{a}_l + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

We have to vary the energy expectation value with respect to the matrices U, V . This is rather inconvenient. An alternative approach is based on the following theorem:

Thouless: Let $|\Phi\rangle$ be a single-particle state of HFB-type. Any other HFB state $|\Phi'\rangle$ that is not orthogonal to $|\Phi\rangle$ can be obtained via

$$|\Phi'\rangle = |\Phi\rangle + |\delta\Phi\rangle = \exp \left\{ \sum_{k<l} Z_{kl} \beta_l^\dagger \beta_k^\dagger \right\} |\Phi\rangle.$$

Note: $Z = 0$ yields $|\Phi'\rangle = |\Phi\rangle$.

Approach: Expand energy expectation value $\langle\Phi'|H|\Phi'\rangle/\langle\Phi'|\Phi'\rangle$ up to quadratic order in Z_{kl} . The terms linear in Z have to vanish at the variational extremum, and the quadratic term is the stability matrix. Require also that the resulting single-particle Hamiltonian is diagonal. This yields the HFB equations

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

where

$$h_{kl} = t_{kl} + \sum_{ij} \bar{v}_{kilj} \rho_{ij},$$
$$\Delta_{kl} = \frac{1}{2} \sum_{ij} \bar{v}_{klij} \kappa_{ij}.$$

are the HFB Hamiltonian and pairing field, respectively. Here U_k is the k^{th} column of the matrix U . Recall that ρ and κ are also given in terms of U and V .

Note: The HFB equations constitute a $2M$ dimensional eigenvalue problem, but only M of its solutions are independent. For any eigenvalue E_k and eigenvector (U_k, V_k) there is also an eigenvalue $-E_k$ with eigenvector (V_k, U_k) .

Numerical solution of HFB equations:

1. by iteration
2. gradient method (steepest decent): Use Thouless theorem and consider those variations of an initial HFB state that lower the energy and keep the average particle number fixed.

HFB calculations are particularly valuable to compute bulk properties for nuclei (masses, deformations, radii, etc.) across the nuclear chart, and are used to determine the nuclear energy density functional.