# Hartree-Fock-Bogoliubov

**A. Two-body (density-dependent) interaction:**

$$\hat{H} = \sum_{ij} t_{ij} c_i^+ c_j + \tfrac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} c_i^+ c_j^+ c_l c_k$$

**B. Variational principle:**

$$\delta E[\Psi] = 0; \quad E[\Psi] = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}; \quad E[\Psi] > E_0$$

**C. Trial wave functions: product states**

$$\beta_K^+ = \sum_i \left( u_{iK} c_i^+ + v_{iK} c_i \right)$$

general Bogoliubov transformation

$$|\Psi\rangle = \prod_K \beta_K |-\rangle; \quad \beta_K |\Psi\rangle = 0$$

HFB wave function is the quasuparticle vacuum

- HFB - quasiparticles incorporated into the HF formalism
- HFB wave function - the most general product wave function consisting of independently moving quasiparticles (in HF: particles)
- Selfconsistent description of coupling between p-h an p-p channels

# HFB - density matrix and pairing tensor

**HFB density matrix**

**HFB pairing tensor**

$$\rho_{ij} \equiv \langle \Psi | c_j^+ c_i | \Psi \rangle, \quad \kappa_{ij} \equiv \langle \Psi | c_j c_i | \Psi \rangle$$

$$\hat{\rho} = v^* v^T, \quad \hat{\kappa} = v^* u^T$$

$$\hat{\rho}^2 - \hat{\rho} = -\hat{\kappa}\hat{\kappa}^+, \quad \hat{\rho}\hat{\kappa} = \hat{\kappa}\hat{\rho}$$

$$\hat{\Re} = \begin{pmatrix} \hat{\rho} & \hat{\kappa} \\ -\hat{\kappa}^* & 1 - \hat{\rho}^* \end{pmatrix}, \quad \hat{\Re}^2 = \hat{\Re}$$

$$\hat{\Re}\begin{pmatrix} u_K \\ v_K \end{pmatrix} = 0, \quad \hat{\Re}\begin{pmatrix} v_K^* \\ u_K^* \end{pmatrix} = \begin{pmatrix} v_K^* \\ u_K^* \end{pmatrix}$$

**Generalized density matrix**

**Eigenvalues are 0 or 1 (thus defining occupations of quasiparticle states)**

$$\hat{H}(c^+, c) \Rightarrow \hat{H}(\beta^+, \beta) = E_0 + \hat{H}_{20} + \hat{H}_{11} + \hat{H}_{\text{int}}$$

**Independent quasiparticle Hamiltonian ($H_{HFB}$)**

**Quasiparticle interaction**

$$\left[\hat{H}, \hat{N}\right] = 0, \quad \text{but} \quad \left[\hat{H}_{HFB}, \hat{N}\right] \neq 0$$

$$\text{However, we require that } \left\langle \hat{N} \right\rangle = N \Rightarrow \hat{H}' = \hat{H} - \lambda \hat{N}$$

# HFB equations

$$\hat{K} = \begin{pmatrix} \hat{h} - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}^* + \lambda \end{pmatrix}$$

HFB Hamiltonian

$$h_{ij} = t_{ij} + \Gamma_{ij}$$

HF Hamiltonian

$$\Gamma_{ij} = \sum_{kl} \bar{v}_{iljk} \rho_{kl}$$

Selfconsistent HF field

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \bar{v}_{ijkl} \kappa_{kl}$$

Selfconsistent pair field

**HFB equations**

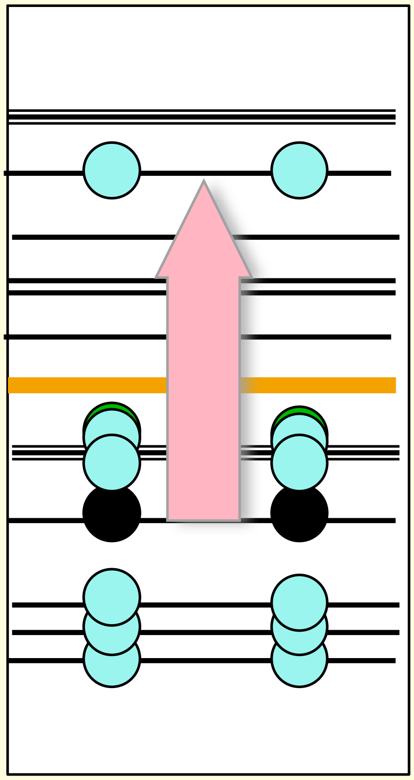
$$\begin{pmatrix} \hat{h} - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}^* + \lambda \end{pmatrix} \begin{pmatrix} u_K \\ v_K \end{pmatrix} = E_K \begin{pmatrix} u_K \\ v_K \end{pmatrix}$$

$$\left[\hat{K}, \hat{\mathfrak{R}}\right] = 0$$

Complicated eigenvalue problem

- HFB equations treat p-h and p-p on the same footing
- $\Delta$ is a state-dependent field. In general, it depends on density and has a kinetic term
- The generalized density matrix and the HFB Hamiltonian can be diagonalized simultaneously
- Fermi level determined from the particle number equation
- Often it is convenien to express the HFB equations in the canonical basis

# Independent quasiparticle approach



$$\alpha_k^+ = u_k c_k^+ - v_k c_{\bar{k}}$$
$$\alpha_{\bar{k}}^+ = u_k c_{\bar{k}}^+ + v_k c_k$$

Bogoliubov-Valatin Transformation

phase convention: $u_{\bar{k}} = u_k > 0, \quad v_k = -v_{\bar{k}} > 0$

$\varepsilon_F$

$$\{\alpha_k, \alpha_j\} = 0, \quad \{\alpha_k^+, \alpha_j^+\} = 0,$$
$$\{\alpha_k, \alpha_j^+\} = \delta_{ij} \Rightarrow u_k^2 + v_k^2 = 1$$

$$|0\rangle = |BCS\rangle = \prod_{k>0} \left(u_k + v_k c_k^+ c_{\bar{k}}^+\right) |-\rangle$$

$$\alpha_k |0\rangle = 0$$

BCS wave function is the quasiparticle vacuum!

$$|0\rangle \propto \exp\left(A^+\right) |-\rangle = \sum_{n=0}^{\infty} \tfrac{1}{n!} \left(A^+\right)^n |-\rangle$$

$$A^+ = \sum_{k>0} \frac{u_k}{v_k} c_k^+ c_{\bar{k}}^+$$

BCS function is a superposition of different number of pairs

- ❏ Important ground-state correlations are included
- ❏ BCS wave function does not have a sharp particle number (an intrinsic wave function!)

# BCS equations

$$\hat{H}(c^+,c) \Rightarrow \hat{H}(\alpha^+,\alpha) = E_0 + \hat{H}_{20} + \hat{H}_{11} + \hat{H}_{\text{int}}$$

**Independent quasiparticle Hamiltonian ($H_{BCS}$)**

**Quasiparticle interaction**

$$\left[\hat{H},\hat{N}\right] = 0, \quad \text{but} \quad \left[\hat{H}_{BCS},\hat{N}\right] \neq 0$$

$$\text{However, we require that } \left\langle \hat{N} \right\rangle = N \Rightarrow \hat{H}' = \hat{H} - \lambda\hat{N}$$

**Particle number equation**

**Variational method**

$$\delta\left\langle 0\left|\hat{H}'\right|0\right\rangle = 0 \qquad N = \sum_{i>0} 2v_i^2$$

$$\tilde{\varepsilon}_k = \varepsilon_k + \sum_{i>0} \bar{v}_{k\bar{k}i\bar{i}} v_i^2 - \lambda \qquad \Delta_k = -\sum_{i>0} \bar{v}_{k\bar{k}i\bar{i}} u_i v_i$$

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\right)$$

**Pairing gap equation**