The Hartree-Fock-Bogoliubov Approach

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Introduction

Introduction

A two-body Hamiltonian of a system of fermions can be expressed in terms of a set of annihilation and creation operators $(c_l^\dagger, c_l)$

$$H = \sum_{l_1 l_2} t_{l_1 l_2} c_{l_1}^\dagger c_{l_2} + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c_{l_1}^\dagger c_{l_2}^\dagger c_{l_4} c_{l_3}, \tag{1}$$

where the anti-symmetrized two-body interaction matrix-elements are defined as

$$\bar{v}_{l_1 l_2 l_3 l_4} = \langle l_1 l_2 | v | l_3 l_4 \rangle - \langle l_1 l_2 | v | l_4 l_3 \rangle. \tag{2}$$

Introduction

In the Hartree-Fock-Bogoliubov (HFB) method, the ground-state wave function is defined as a quasiparticle vacuum

$$|\Phi(q)\rangle = \prod_{k=1}^{M} \beta_k(q) |0\rangle , \quad \beta_k(q) |\Phi(q)\rangle = 0, \tag{3}$$

where $|0\rangle$ denotes the particle vacuum.

The $(\beta_k, \beta_k^\dagger)$ are quasiparticle creation and annihilation operators.

The Bogoliubov transformation

The Bogoliubov transformation

The quasiparticle operators $(\beta_k, \beta_k^\dagger)$ are connected to the particle operators $(c_l, c_l^\dagger)$ via a linear Bogoliubov transformation

$$\beta_k^\dagger = U_{lk} c_l^\dagger + V_{lk} c_l, \tag{4}$$

$$\beta_k = U_{lk}^* c_l + V_{lk}^* c_l^\dagger, \tag{5}$$

namely,

$$\begin{pmatrix} \beta_k^\dagger \\ \beta_k \end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix} c_l^\dagger \\ c_l \end{pmatrix} \tag{6}$$

The unitary transformation matrix $\mathcal{W}^\dagger$ is defined by

$$\mathcal{W}^\dagger = \begin{pmatrix} U^T & V^T \\ V^\dagger & U^\dagger \end{pmatrix}, \tag{7}$$

satisfying the condition,

$$\mathcal{W}\mathcal{W}^\dagger = \mathcal{W}^\dagger\mathcal{W} = 1. \tag{8}$$

The Bogoliubov transformation

namely the matrix U and V satisfy the following relations:

$$\begin{cases} V^\dagger V + U^\dagger U = 1, \\ U^T V + V^T U = 0, \end{cases} \tag{9}$$

and

$$\begin{cases} UU^\dagger + V^* V^T = 1, \\ UV^\dagger + V^* U^T = 0. \end{cases} \tag{10}$$

The inverse transformation of (4) is

$$\begin{pmatrix} c_l^\dagger \\ c_l \end{pmatrix} = \mathcal{W} \begin{pmatrix} \beta_k^\dagger \\ \beta_k \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U^* & V \\ V^* & U \end{pmatrix}. \tag{11}$$

where

$$c_l^\dagger = U_{lk}^* \beta_k^\dagger + V_{lk}\beta_k, \tag{12}$$

$$c_l = V_{lk}^* \beta_k^\dagger + U_{lk}\beta_k. \tag{13}$$

The Bogoliubov transformation

Homework 1: Prove that the quasiparticle operators defined in (4) satisfy the following relations:

$$\{\beta_k^\dagger, \beta_{k'}\} = \delta_{kk'}, \quad \{\beta_k^\dagger, \beta_{k'}^\dagger\} = \{\beta_k, \beta_{k'}\} = 0. \tag{14}$$

Quasiparticle representation

The H in the quasiparticle representation

Applying transformation (11) to the one-body operator

$$\begin{aligned}
\sum_{l_1 l_2} t_{l_1 l_2} c^\dagger_{l_1} c_{l_2} &= \sum_{l_1 l_2} t_{l_1 l_2} \Big[U^*_{l_1 k_1} U_{l_2 k_2} \beta^\dagger_{k_1} \beta_{k_2} + V_{l_1 k_1} V^*_{l_2 k_2} \beta_{k_1} \beta^\dagger_{k_2} \\
&\quad + U^*_{l_1 k_1} V^*_{l_2 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + V_{l_1 k_1} U_{l_2 k_2} \beta_{k_1} \beta_{k_2} \Big] \\
&= \sum_{l_1 l_2} t_{l_1 l_2} \Big[V_{l_1 k_1} V^*_{l_2 k_2} \delta_{k_1 k_2} + (U^*_{l_1 k_1} U_{l_2 k_2} - V_{l_1 k_2} V^*_{l_2 k_1}) \beta^\dagger_{k_1} \beta_{k_2} \\
&\quad + \frac{1}{2} (U^*_{l_1 k_1} V^*_{l_2 k_2} - U^*_{l_1 k_2} V^*_{l_2 k_1}) \beta^\dagger_{k_1} \beta^\dagger_{k_2} + \frac{1}{2} (U_{l_1 k_1} V_{l_2 k_2} - U_{l_1 k_2} V_{l_2 k_1}) \beta_{k_2} \beta_{k_1} \Big] \\
&= T^0 + \sum_{k_1 k_2} T^{11}_{k_1 k_2} \beta^\dagger_{k_1} \beta_{k_2} + \frac{1}{2} \sum_{k_1 k_2} \Big[T^{20}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + h.c. \Big] \qquad (15)
\end{aligned}$$

where,

$$T^0 = \sum_{l_1 l_2} t_{l_1 l_2} V_{l_1 k_1} V^*_{l_2 k_2} \delta_{k_1 k_2} = \mathrm{Tr}(t V^* V^T), \qquad (16)$$

$$T^{11}_{k_1 k_2} = \sum_{l_1 l_2} t_{l_1 l_2} (U^*_{l_1 k_1} U_{l_2 k_2} - V_{l_1 k_2} V^*_{l_2 k_1}) = (U^\dagger t U - V^\dagger t^T V)_{k_1 k_2}, \qquad (17)$$

$$T^{20}_{k_1 k_2} = \sum_{l_1 l_2} t_{l_1 l_2} (U^*_{l_1 k_1} V^*_{l_2 k_2} - U^*_{l_1 k_2} V^*_{l_2 k_1}) = (U^\dagger t V^* - V^\dagger t^T U^*)_{k_1 k_2}. \qquad (18)$$

The H in the quasiparticle representation

$$
\begin{aligned}
H &= \sum_{l_1 l_2} t_{l_1 l_2} c^\dagger_{l_1} c_{l_2} + \frac{1}{4}\sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3} \\
&= H^0 + \sum_{k_1 k_2} H^{11}_{k_1 k_2} \beta^\dagger_{k_1}\beta_{k_2} + \frac{1}{2}\sum_{k_1 k_2}\left[H^{20}_{k_1 k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + h.c.\right] \\
&\quad + \sum_{k_1 k_2 k_3 k_4} H^{40}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_4}\beta^\dagger_{k_3} + h.c. \\
&\quad + \sum_{k_1 k_2 k_3 k_4} H^{31}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta_{k_4} + h.c. \\
&\quad + \frac{1}{4}\sum_{k_1 k_2 k_3 k_4} H^{22}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta_{k_4}\beta_{k_3}
\end{aligned} \tag{19}
$$

where,

$$
\begin{aligned}
H^0 &= \mathrm{Tr}\left(t\rho + \frac{1}{2}\Gamma\rho - \frac{1}{2}\Delta\kappa^*\right) = \mathrm{Tr}(t\rho) + \frac{1}{2}\mathrm{Tr}(\rho\bar{v}\rho) + \frac{1}{4}\mathrm{Tr}\left(\kappa^*\bar{v}\kappa\right) \\
H^{11} &= U^+ h U - V^+ h^T V + U^+ \Delta V^* - V^+ \Delta^* U \\
H^{20} &= U^+ h V^* - V^+ h^T U^* + U^+ \Delta U^* - V^+ \Delta^* V^*
\end{aligned}
$$

The H in the quasiparticle representation

The density matrices

In the above expressions, we introduce density matrices in the particle basis

$$\rho_{ll'} = \langle \Phi \left| c_{l'}^{+} c_l \right| \Phi \rangle , \quad \kappa_{ll'} = \langle \Phi \left| c_{l'} c_l \right| \Phi \rangle , \quad \kappa_{ll'}^{*} = \left\langle \Phi \left| c_l^{\dagger} c_{l'}^{\dagger} \right| \Phi \right\rangle$$

or in matrix notation

$$\rho = V^* V^T, \quad \kappa = V^* U^r = -UV^+,$$

ρ is hermitian $\left(\rho^+ = \rho\right)$ and κ is skew symmetric $\left(\kappa^T = -\kappa\right)$.

The single-particle matrix elements

We also introduce the mean-field matrix elements:

$$h = t + \Gamma$$

$$\Gamma_{lm} = \sum_{pq} \bar{v}_{lqmp} \rho_{pq} \quad := \mathrm{Tr}(\bar{v}\rho)$$

$$\Delta_{lm} = \frac{1}{2} \sum_{pq} \bar{v}_{lmpq} \kappa_{pq} := -\frac{1}{2} \mathrm{Tr}(\bar{v}\kappa)$$

The H in the quasiparticle representation

The following quasiparticle interacting terms are usually negligible:

$$
\begin{aligned}
H^{40}_{k_1k_2k_3k_4} &= \frac{1}{4}\sum_{l_1l_2l_3l_4} \bar{v}_{l_1l_2l_3l_4} U^*_{l_1k_1} U^*_{l_2k_2} V^*_{l_3k_3} V^*_{l_4k_4}, \\
H^{31}_{k_1k_2k_3k_4} &= \frac{1}{2}\sum_{l_1l_2l_3l_4} \bar{v}_{l_1l_2l_3l_4} \left[U^*_{l_1k_1} U^*_{l_2k_2} V^*_{l_4k_4} U_{l_3k_3} + U^*_{l_1k_1} V_{l_2k_3} V^*_{l_4k_2} V^*_{l_3k_4} \right], \\
H^{22}_{k_1k_2k_3k_4} &= \sum_{l_1l_2l_3l_4} \bar{v}_{l_1l_2l_3l_4} \left[U^*_{l_1k_1} U^*_{l_2k_2} U_{l_4k_4} U_{l_3k_3} + V_{l_1k_4} V_{l_2k_3} V^*_{l_4k_2} V^*_{l_3k_2} \right. \\
&\quad + U^*_{l_1k_1} V_{l_2k_4} U_{l_4k_3} V^*_{l_3k_2} + V^*_{l_1k_4} U^*_{l_2k_1} V^*_{l_4k_2} U_{l_3k_3} \\
&\quad \left. - U^*_{l_1k_1} V_{l_2k_2} V^*_{l_4k_2} U_{l_3k_3} - V_{l_1k_4} U^*_{l_2k_1} U_{l_4k_3} V^*_{l_3k_2} \right].
\end{aligned}
$$

The H in the quasiparticle representation

Thus, the Hamiltonian in quasi-particle representation is

$$H \simeq H^0 + \sum_{k_1 k_2} H^{11}_{k_1 k_2} \beta^\dagger_{k_1} \beta_{k_2} + \frac{1}{2} \sum_{k_1 k_2} \left[H^{20}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + h.c. \right] \tag{20}$$

The HFB equation is to find the matrix $\mathcal{W}$ which diagonalizes the H^{11} and drives $H^{20} = 0$, in which case, one has

$$H \simeq H^0 + \sum_k E_k \beta^\dagger_k \beta_k, \tag{21}$$

where E_k is the so-called quasiparticle energy.

The HFB equation

The HFB equation

Starting from the variational principle

$$\delta \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi \mid \Phi \rangle} = 0, \quad H = H_0 - \lambda N$$

According to Thouless theorem, one can express the function $|\Phi'\rangle = |\Phi\rangle + |\delta\Phi\rangle$ as

$$\left|\Phi'\right\rangle = \exp\left(\sum_{k<k'} Z_{kk'} \beta_k^+ \beta_{k'}^+\right) |\Phi\rangle$$

which is not orthogonal to $|\Phi\rangle$.
The variables $Z_{kk'}$ $(with k < k')$ are independent variables.

The HFB equation

We write the H as

$$H = E_0 + \sum_{k_1 k_2} H^{11}_{k_1 k_2} \beta^+_{k_1} \beta_{k_2} + \sum_{k_1 < k_2} \left(H^{20}_{k_1 k_2} \beta^+_{k_1} \beta^+_{k_2} + \text{h.c.} \right) + H_{\text{int}}$$

where

$$\frac{\langle \Phi' | H | \Phi' \rangle}{\langle \Phi' \mid \Phi' \rangle} = H^0 + \left(H^{20^*} H^{20} \right) \begin{pmatrix} Z \\ Z^* \end{pmatrix} + \frac{1}{2} (Z^* Z) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Z \\ Z^* \end{pmatrix}$$

where the index of the vectors and matrices runs over all pairs ($k < k$) and

$$\begin{aligned} H^0 &= \langle \Phi | H | \Phi \rangle, & A_{kk'll'} &= \left\langle \Phi \left| \left[\beta_{k'} \beta_k, \left[H, \beta_l{}^+ \beta_{l'}{}^+ \right] \right] \right| \Phi \right\rangle \\ H^{20}_{kk'} &= \langle \Phi \left| [\beta_{k'} \beta_k, H] \right| \Phi \rangle, & B_{kk'll'} &= - \langle \Phi \left| [\beta_{k'} \beta_k, [H, \beta_{l'} \beta_l]] \right| \Phi \rangle \end{aligned}$$

The variation principle leads to

$$\frac{\partial}{\partial Z^*_{kk'}} \frac{\langle \Phi' | H | \Phi' \rangle}{\langle \Phi' \mid \Phi' \rangle} \bigg|_{z=0} = H^{20}_{kk'} = 0$$

The HFB equation

Therefore, the variational equation, together with the diagonalization of the H^{11}, is equivalent to diagonalize the following matrix

$$K = \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix} = \begin{pmatrix} \langle \Phi | \{[\beta_k, H], \beta^+_{k'}\} | \Phi \rangle & \langle \Phi | \{[\beta_k, H], \beta_{k'}\} | \Phi \rangle \\ \langle \Phi | \{[\beta^+_k, H], \beta^+_{k'}\} | \Phi \rangle & \langle \Phi | \{[\beta^+_k, H], \beta_{k'}\} | \Phi \rangle \end{pmatrix}$$

In the space of the basis operators c_l, c^+_l this matrix has the form

$$h_{\mathrm{HFB}} \equiv \mathcal{W} K \mathcal{W}^\dagger = \mathcal{W} \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix} \mathcal{W}^\dagger = \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* - \lambda \end{pmatrix}$$

with

$$h_{ll'} = \langle \Phi | \{[c_l, H], c^+_{l'}\} | \Phi \rangle, \quad \Delta_{ll'} = \langle \Phi | \{[c_l, H], c_{l'}\} | \Phi \rangle$$

Applying Wick's theorem,

$$h = t + \Gamma; \quad \Gamma_{ll'} = \sum_{qq'} \bar{v}_{lq'l'q} \rho_{qq'}; \quad \Delta_{ll'} = \frac{1}{2} \sum_{qq'} \bar{v}_{ll'qq'} \kappa_{qq'}$$

The HFB equation

Diagonalizing the matrix H_{HFB} leads to the HFB equation

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

where the columns U_k, V_k of the matrices U and V determine the quasi-particle operator β_k^+. The value of λ is determined to ensure the conservation of particle number.
Note: the above equation produces $2M$ eigenvalues, where

- the M eigenvalues of E_k and HFB wave functions (U, V)
- the M eigenvalues of $-E_k$ and HFB wave functions (V^*, U^*)

The HFB equation (alternative way to detive)

Using the Wick theorem,

$$\hat{H} = \hat{H}_0 - \lambda\hat{N} = \sum_{k_1 k_2}(t^{k_1}_{k_2} - \lambda\delta^{k_1}_{k_2})A^{k_1}_{k_2} + \frac{1}{4}\sum_{k_1 k_2 k_3 k_4} \bar{v}^{k_1 k_2}_{k_3 k_4} A^{k_1 k_2}_{k_3 k_4}$$

where $A^{k_1}_{k_2} \equiv c^\dagger_{k_1} c_{k_2}$. According to the Wick theorem, one can write the operators in terms of normal-ordered ones

$$\begin{aligned}
A^{k_1}_{k_2} &= \{A^{k_1}_{k_2}\} + \langle\Phi|A^{k_1}_{k_2}|\Phi\rangle, \\
A^{k_1 k_2}_{k_3 k_4} &= \{A^{k_1 k_2}_{k_3 k_4}\} + (1-\hat{P}_{12})(1-\hat{P}_{34})\{A^{k_1}_{k_3}\}\langle\Phi|A^{k_2}_{k_4}|\Phi\rangle + (1-\hat{P}_{34})\langle\Phi|A^{k_1}_{k_3}|\Phi\rangle\langle\Phi|A^{k_2}_{k_4}|\Phi\rangle \\
&\quad + \{A^{k_1 k_2}\}\langle\Phi|A_{k_3 k_4}|\Phi\rangle + \{A_{k_3 k_4}\}\langle\Phi|A^{k_1 k_2}|\Phi\rangle
\end{aligned}$$

Using the definitions for Γ and Δ, we immediately find

$$H = E^0 + \frac{1}{2}\left\{ (c^+, c) \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^* - \lambda \end{pmatrix} \begin{pmatrix} c \\ c^+ \end{pmatrix} \right\} + \frac{1}{4}\sum_{k_1 k_2 k_3 k_4} \Gamma^{k_1 k_2}_{k_3 k_4}\{A^{k_1 k_2}_{k_3 k_4}\}$$

The HFB equation (alternative way to derive)

The second term can be rewritten by transforming the single-particle basis $(c^\dagger, c)$ into quasiparticle $(\beta^\dagger, \beta)$ representation via the Bogoliubov transformation (U, V), which transform it into the following form

$$\frac{1}{2}\left\{ (c^+, c) \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*-\lambda \end{pmatrix} \begin{pmatrix} c \\ c^+ \end{pmatrix} \right\} = \sum_k E_k \{\beta_k^\dagger \beta_k\}.$$

It is equivalent to the following eigenvalue problem,

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

where the Bogoliubov transformation was introduced before as follows

$$c_l^\dagger = U_{lk}^* \beta_k^\dagger + V_{lk}\beta_k, \quad (22)$$

$$c_l = V_{lk}^* \beta_k^\dagger + U_{lk}\beta_k. \quad (23)$$

The HFB in canonical basis

Decomposition of the Bogoliubov transformation

Theorem of Bloch and Messiah

A unitary matrix of the form $\mathcal{W}$ can always be decomposed into three matrices of very special form:

$$\mathcal{W} \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix} \tag{24}$$

or

$$U = D\bar{U}C, \quad V = D^* \bar{V} C$$

$$\bar{U} = \begin{bmatrix} 0 & & & & & & & & 0 \\ & \ddots & & & & & & & \\ & & 0 & & & & & & \\ & & & \boxed{\begin{matrix} u_1 & 0 \\ 0 & u_1 \end{matrix}} & & & & & \\ & & & & \ddots & & & & \\ & & & & & \boxed{\begin{matrix} u_n & 0 \\ 0 & u_n \end{matrix}} & & & \\ & & & & & & 1 & & \\ & & & & & & & \ddots & \\ 0 & & & & & & & & 1 \end{bmatrix}, \quad \bar{V} = \begin{bmatrix} 1 & & & & & & & & 0 \\ & \ddots & & & & & & & \\ & & 1 & & & & & & \\ & & & \boxed{\begin{matrix} 0 & v_1 \\ -v_1 & 0 \end{matrix}} & & & & & \\ & & & & \ddots & & & & \\ & & & & & \boxed{\begin{matrix} 0 & v_n \\ -v_n & 0 \end{matrix}} & & & \\ & & & & & & 0 & & \\ & & & & & & & \ddots & \\ 0 & & & & & & & & 0 \end{bmatrix}$$

Decomposition of the Bogoliubov transformation

$$\left.\begin{matrix} c \to a \\ c^{+} \to a^{+} \end{matrix}\right\} \to \left\{\begin{matrix} \alpha \to \beta \\ \alpha^{+} \to \beta^{+} \end{matrix}\right.$$

$$D \qquad \bar{U}, \bar{V} \qquad C$$

1. The D transformation among single-particle operators $(c_l^\dagger, c_l)$: which diagonalizes the one-body density ρ

$$a_k^\dagger = \sum_l D_{lk} c_l^\dagger \tag{25}$$

The new basis defined by $\{a_k^\dagger, a_k\}$ is called canonical basis.

2. The special Bogoliubov transformation defined by $\bar{U}$, $\bar{V}$, which mixes the creation and annihilation operators of "paired" levels $(u_p > 0, v_p > 0)$,

$$\begin{aligned} \alpha_p^+ &= u_p a_p^+ - v_p a_{\bar{p}} \\ \alpha_{\bar{p}}^+ &= u_p a_{\bar{p}}^+ + v_p a_p \end{aligned} \tag{26}$$

3. The C transformation among quasi-particle operators $(\alpha_k^\dagger, \alpha_k)$:

$$\beta_k^\dagger = \sum_{k'} C_{k'k} \alpha_{k'}^\dagger. \tag{27}$$

The constraint HFB calculation

The HFB equation with constraints

- Unrestricted HF/HFB calculations give only one point on the energy surface, i.e., the local minimum.
- The energy surface (energy as a function of collective parameter, like deformation parameters) can be obtained by imposing certain subsidiary conditions.
- The Hamiltonian becomes

$$H' = H - \lambda Q \tag{28}$$

where Q is a certain single-particle operator with a fixed expectation value,

$$\langle \Phi | Q | \Phi \rangle = q. \tag{29}$$

The Lagrange multiplier is the derivative of the energy with respect to q,

$$\lambda = \frac{dE}{dq}. \tag{30}$$

The HFB equation with constraints

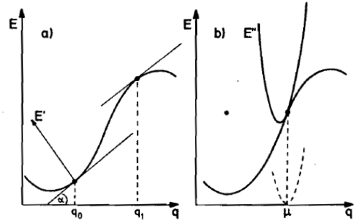


Figure 7.2. Schematic representation of an energy surface showing the methods of linear (a) and (b) quadratic constraint.

- The linear constraint works as long as the function $E(q)$ has a positive second derivative. it does not work in the cases where the curve is downwards.
- The use of a quadratic constraint can avoid the above problem

$$H' = H - \lambda(Q - q)^2 \tag{31}$$

from which one finds the variation of energy

$$\delta\langle H'\rangle = \delta\langle H\rangle - \lambda(Q - q)\delta\langle Q\rangle = 0$$

The constraint term is changing automatically during the iteration.

The HFB equation with constraints

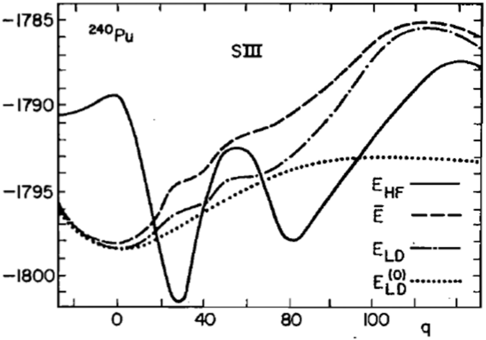
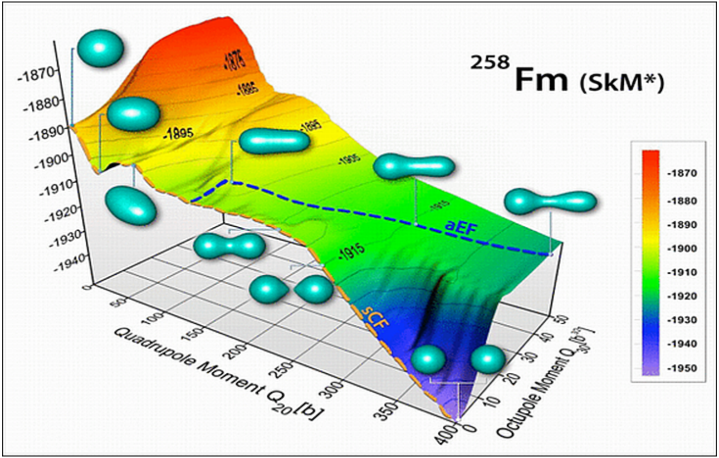


Figure 7.4. Deformation energy curves of ^{240}Pu obtained with the Skyrme III interaction as a function of the mass quadrupole moment q. The details are explained in the text. (From [BQ 75a].)

The HFB equation with constraints



The multi-quasiparticle states

The even-even nuclei

The HFB wave function of an even-even nucleus is simply the quasiparticle vacuum

$$|\Phi_0\rangle = \prod_{k=1}^{M} \beta_k |0\rangle = \beta_1\beta_2\ldots\beta_M|0\rangle \tag{32}$$

with even number parity. It means that

$$\beta_k |\Phi_0\rangle = 0, \quad k = 1, 2, \cdots M$$

The exact wave function of an even-even nucleus can be expanded in terms of the following basis:

$$|\Phi_0\rangle, \quad \beta^\dagger_k\beta^\dagger_{k'} |\Phi_0\rangle, \quad \beta^\dagger_k\beta^\dagger_{k'}\beta^\dagger_{k''}\beta^\dagger_{k'''} |\Phi_0\rangle, \cdots$$

The odd-mass nuclei

For odd-mass nuclei, we have to make sure that we use coefficients U and V which guarantee odd number parity for the wave function $|\Phi_1\rangle$ that is, $|\Phi_1\rangle$ can be written as a one quasi-particle state based on a properly chosen ground state $|\Phi_0\rangle$
The one-quasi-particle state

$$|\Phi_1\rangle = \beta_1^+ |\Phi_0\rangle$$

is a vacuum to the operators $\left(\tilde{\beta}_1, \tilde{\beta}_2, \ldots, \tilde{\beta}_M\right)$ with

$$\tilde{\beta}_1 = \beta_1^+, \tilde{\beta}_2 = \beta_2, \ldots, \tilde{\beta}_M = \beta_M$$

The exchange of a quasi-particle creation operator β_1^+ with the corresponding annihilation operator β_1 means that we have replaced columns 1 in the matrices U and V by the corresponding columns in the matrices V^*, U^*:

$$(U_{l1}, V_{l1}) \leftrightarrow (V_{l1}^*, U_{l1}^*)$$

Thus by making such a replacement we change the number parity of the corresponding vacuum and go over to a one-quasi-particle state.
The exact wave function of an even-odd nucleus can be expanded in terms of the following basis:

$$\beta_k^\dagger |\Phi_0\rangle, \quad \beta_k^\dagger \beta_{k'}^\dagger \beta_{k''}^\dagger |\Phi_0\rangle, \cdots$$

The temperature-dependent HFB in rotating frame

The temperature-dependent HFB in rotating frame

The CTHFB equations have formally the same structure as ordinary cranked HFB equations. We can write them down in the form of a nonlinear eigenvalue problem given by Baranger [20]):

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = E_k \begin{pmatrix} U \\ V \end{pmatrix}_k . \tag{1}$$

The CTHFB matrix contains the potential h in the ph channel,

$$h = \varepsilon - \lambda_p N_p - \lambda_n N_n - \omega J_x + \Gamma , \tag{2}$$

with single-particle energies ε, Coriolis field ωJ_x, number operators for protons and neutrons, N_p and N_n, and selfconsistent field

$$\Gamma_{kk'} = \sum_{ll'} v_{kl'k'l} \rho_{ll'} . \tag{3}$$

The pairing potential in the pp channel is defined as usual

$$\Delta_{kk'} = \tfrac{1}{2} \sum_{ll'} v_{kl'l'l} \kappa_{ll'} . \tag{4}$$

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The difference from simple HFB equations consists in the densities which are now thermal averages over a statistical ensemble of multi-quasiparticle states:

$$\rho_{kk'} = \left(UfU^{\dagger} + V^{*}(1-f)V^{\mathrm{T}}\right)_{kk'}, \tag{5}$$

$$\kappa_{kk'} = \left(UfV^{\dagger} + V^{*}(1-f)U^{\mathrm{T}}\right)_{kk'}. \tag{6}$$

They contain the temperature-dependent occupation factors for quasiparticles,

$$f_k = 1/\left(1+\exp(E_k/T)\right), \tag{7}$$

which are zero for normal HFB theory.

The diagonalization of the HFB matrix gives us quasiparticle energies E_k and a quasiparticle basis, i.e. the HFB coefficients U_{mk} and V_{mk}, which define the quasiparticle operators via the general Bogoliubov transformation

$$\alpha_k^{\dagger} = \sum_m U_{mk} C_m^{\dagger} + V_{mk} C_m. \tag{8}$$

Having this basis we can calculate the densities ρ and κ in eqs. (5) and (6) and the potentials Γ and Δ.

To obtain a closed system we finally have to specify the constraints, which determine the Lagrange parameters λ_{p}, λ_{n} and ω:

$$\langle N_{\mathrm{n}}\rangle = N, \qquad \langle N_{\mathrm{p}}\rangle = Z, \tag{9}$$

$$\langle J_x\rangle = \omega \mathscr{I}_{\mathrm{c}} = \sqrt{I(I+1)} \tag{10}$$

where $\mathscr{I}_{\mathrm{c}}$ is a core moment of inertia.

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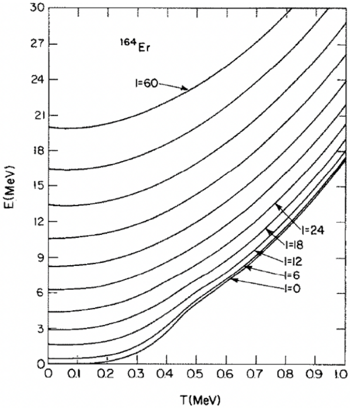

Fig. 2. The energy of the nucleus ^{164}Er as a function of the temperature for different angular momenta.

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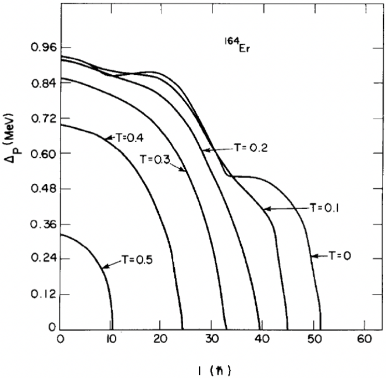

Fig. 4. The gap parameter for the protons in the nucleus ^{164}Er as a function of the angular momentum for different temperatures (in units of MeV). For all temperatures $T \geq 0.6$ MeV the gap vanishes.

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Homeworks

Homework 2: Compute the energy of one- and two- quasiparticle states.

$$\langle\Phi_0|\beta_k H_0 \beta_k^\dagger|\Phi_0\rangle = ? \tag{33}$$

$$\langle\Phi_0|\beta_l\beta_k H_0 \beta_k^\dagger\beta_l^\dagger|\Phi_0\rangle = ? \tag{34}$$

where the Hamiltonian is approximated as

$$H = E_0 + \sum_k E_k \beta_k^+ \beta_k.$$

家庭作业选做题: compute the expectation value of particle number operators for the quasiparticle vacuum and one-quasiparticle states.

$$\langle\Phi_0|\hat{N}|\Phi_0\rangle = ? \tag{35}$$

$$\langle\Phi_0|\beta_k\hat{N}\beta_k^\dagger|\Phi_0\rangle = ? \tag{36}$$

where the particle-number operator is defined as

$$\hat{N} = \sum_k c_k^\dagger c_k$$

Hint: express the particle-number operator in terms of quasiparticle operators and then use the commutation relations among quasiparticle operators and the following relation

$$\beta_k|\Phi_0\rangle = 0.$$