6 BEYOND THE HARTREE-FOCK APPROXIMATION

6.1 SYMMETRY BREAKING

Symmetries

In nuclear physics $[\hat{X}, H] = 0$ for

$$\{\hat{X}\} = \{\underbrace{\hat{N}, \hat{Z}}_{\text{neutron and proton number}}, \underbrace{\hat{\vec{P}}}_{\text{linear momentum}}, \underbrace{\hat{J}^2, \hat{J}_z}_{\text{total angular momentum and z-projection}}, \underbrace{\hat{\Pi}}_{\text{parity}}, \underbrace{\hat{T}^2}_{\text{time reversal operator}}\}$$

The solutions $|\Psi_i^x\rangle$ of the many-body Schrödinger equation

$$H|\Psi_i^x\rangle = E_i |\Psi_i^x\rangle$$

are labelled by quantum numbers $\{x\}$:

- $N, Z \in \mathbb{N}$
- $\vec{P} \in \mathbb{R}^3$
- $2J \in \mathbb{N}$ and $2M \in \mathbb{Z}$ such that $-J \leq M \leq J$
- $\Pi = \pm 1$
- $T^2 = (-1)^N (-1)^Z$

The nuclear part of H, in addition, nearly commutes with the isospin operators $\hat{T}^2, \hat{T}_z$.

In which space do we vary $|\phi\rangle$ (or $\{\varphi_\alpha\}$ or $\rho_{\alpha\beta}$) when minimising $E[\rho]$?

The natural way is to perform the variation such that $|\phi\rangle$ carries the same quantum numbers $\{x\}$ of $|\Psi_0^+\rangle$.

However, this might be too constrained for a relatively simple wave function like a Slater determinant!

Example:

$$\hat{\vec{P}}\,|\phi\rangle = \vec{P}\,|\phi\rangle$$

$$\Rightarrow \varphi(\vec{r}) = \varphi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$$

$$\Rightarrow \rho(\vec{r}) = \rho \qquad \text{constant density}$$

$\downarrow$

Misses the correlations that induce spatial localisation of the internal motion

→ usually broken in nuclear structure calculations

→ similar situation holds for other symmetries

Spontaneous symmetry breaking

Expand the horizon: the variation of $|\phi\rangle$ can be performed allowing for (spontaneous) symmetry breaking.

Let $|\phi\rangle$ span different irreducible representations (IRREPs) of a symmetry group, e.g. $SO(3)$

$$|\Phi\rangle = \sum_{J=0,2,4,\dots} \sum_{M\leq|J|} C_{JM} |\Theta^{JM}\rangle$$

For an even-even nucleus, the ground state is characterised by $J=0$. Here one chooses to consider a linear combination of $J=0$ and higher (even) values of J.

By doing this:

- Certain (long-range) correlations are included in $|\Phi\rangle$. As a consequence, the corresponding energy E^{HF} will be generally lower than for a symmetry-conserving variation.

- However, $|\Phi\rangle$ may not carry good quantum numbers. One can see this as describing a wave packet rather than the ground state. It might be problematic to compute certain quantities, e.g. those relying on selection rules (e.g. $BE(2)$).

- Symmetries have to be eventually restored: projected HF. This typically brings additional correlation energy

- Note that the shell model follows an approach orthogonal to this and expand

$$|\Psi_0^x\rangle = \sum_k C_{0k} |\Phi_k^x\rangle$$

symmetry-conserving excited Slater determinants

Physical content of symmetry breaking

Symmetry	Group	Casimir	Correlations	Type of nuclei	Excitation pattern
Translation	$T(3)$	$\hat{\vec{P}}$	spatial localisation	All	Surface vibrations
Rotations in real space	$SO(3)$	$\hat{J}^2$	angular localisation	Doubly open-shell	Rotational bands
Rotations in gauge space	$U(1)$	$\hat{N}, \hat{Z}$	pairing (superfluidity)	Singly and doubly open-shell	Energy gap

- Symmetries can be enforced or relaxed (in the variation of $|\Phi\rangle$) depending on the nucleus
- Enforcing symmetries allows to exploit them in the calculations
  - → work with an effective basis
  - → reduced dimensionality of the problem and gain in CPU costs

6.2 HARTREE-FOCK-BOGOLYUBOV APPROXIMATION

Bogolyubov states

Consider creation operators $b^+_\alpha |0\rangle = |\alpha\rangle$ with $\{b_\alpha, b^+_\beta\} = \delta_{\alpha\beta}$

Slater determinant

- $|\phi\rangle \equiv \prod_{i=1}^{A} a_i^+ |0\rangle$

with

$$a^+_\mu = \sum_\alpha U_{\alpha\mu} b^+_\alpha$$

unitary transformation

$\Downarrow$

- Vacuum state

$$\begin{cases} a^+_\mu |\phi\rangle = 0 & \text{for } \mu \in [1, A] \\ a_\mu |\phi\rangle = 0 & \text{for } \mu \in [A, \infty] \end{cases}$$

- symmetry-conserving

$$\hat{A}|\phi\rangle = A|\phi\rangle$$

Bogolyubov state

- $|\phi\rangle \equiv \prod_\mu \beta_\mu |0\rangle$

with

$$\beta_\mu \equiv \sum_\alpha \left[U^*_{\alpha\mu} b_\alpha + V^*_{\alpha\mu} b^+_\alpha \right]$$

quasiparticle operators

unitary transformation

$$\begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix}$$

$\Downarrow$

- Vacuum state

$$\beta_\mu |\phi\rangle = 0 \quad \forall \mu$$

- symmetry-breaking

$$\hat{A}|\phi\rangle \neq A|\phi\rangle$$

Density matrices

In addition to the (hermitian) normal density matrix

$$\rho_{\alpha\beta} \equiv \langle \phi | b_\beta^+ b_\alpha | \phi \rangle = \rho_{\beta\alpha}^*$$

an (antisymmetric) anomalous density matrix appears

$$\kappa_{\alpha\beta} \equiv \langle \phi | b_\beta b_\alpha | \phi \rangle = -\kappa_{\beta\alpha}$$

encodes the symmetry breaking

If $\kappa \neq 0 \Rightarrow \rho^2 \neq \rho$ and one needs to introduce a generalised density matrix

$$R = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$

that is now idempotent $R^2 = R$.

HFB energy

The variational space is enlarged to the full Fock space $\mathcal{F}$, while keeping a simple product trial-state

$$|\phi\rangle \equiv \prod_\mu \beta_\mu |0\rangle$$

where β_μ mix b_α and b_α^+ but still fullfil standard anticommutation relations.

Wick's theorem with respect to $|\Phi\rangle$ applied to H gives

$$E^{HFB} = \sum_{\alpha\beta} t_{\alpha\beta}\, \rho_{\beta\alpha} + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, \rho_{\gamma\alpha}\, \rho_{\delta\beta} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, \kappa^*_{\alpha\beta}\, \kappa_{\gamma\delta}$$

$$= E[\rho, \kappa, \kappa^*]$$

<u>Equations of motion</u>

- In the minimisation procedure, independent variables are

$$\rho_{ij},\ \rho^*_{ij},\ \kappa_{ij},\ \kappa^*_{ij} \qquad \text{for } j \leq i$$

- The constraint $\rho^2 = \rho$ is generalised to $R^2 = R$
- One needs to further constrain $\langle\phi|\hat{A}|\phi\rangle = A$ since a free variation would lead to

$$A \to \infty$$
$$E^{HFB} \to -\infty$$

$\downarrow$

Hence set $\delta\left[E[\rho,\kappa,\kappa^*] - \lambda\, \mathrm{Tr}\{\rho\} - \mathrm{Tr}\{\Lambda(R^2 - R)\}\right] = 0$

this is how a matrix of Lagrange parameters

under variations δR and get

$$\mathcal{H}\begin{pmatrix} U \\ V \end{pmatrix}_\mu \equiv \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}\begin{pmatrix} U \\ V \end{pmatrix}_\mu = E_\mu \begin{pmatrix} U \\ V \end{pmatrix}_\mu$$

where

$$h_{\alpha\gamma} \equiv \frac{\delta E[\rho, \kappa, \kappa^*]}{\delta \rho_{\gamma\alpha}} = t_{\alpha\gamma} + \sum_{\beta\delta} \bar{V}_{\alpha\beta\gamma\delta}\, \rho_{\delta\beta}$$

Hartree-Fock field

$$\Delta_{\alpha\gamma} \equiv \frac{\delta E[\rho, \kappa, \kappa^*]}{\delta \kappa^*_{\alpha\gamma}} = \frac{1}{2}\sum_{\beta\delta} \bar{V}_{\alpha\gamma\beta\delta}\, \kappa_{\beta\delta}$$

Bogolyubov field (or pairing field)

- As for HF, this is not a standard eigenvalue problem since

$$\mathcal{H} = \mathcal{H}[\rho, \kappa, \kappa^*] = \mathcal{H}[U, V]$$

6.3 BEYOND THE MEAN FIELD APPROXIMATION

Correlations beyond HF

(See end of chapter 5)

Correlations beyond HFB

Using Wick's theorem with respect to $|\phi\rangle$ in HFB quasi-particle basis

$$H = \underbrace{E^{HFB} + \sum_\alpha E_\alpha \beta^+_\alpha \beta_\alpha}_{H_0'} + \underbrace{:V_2:}_{H_1'}$$

HFB approximation consist in taking $H^{HFB} = H_0'$ and neglecting H_1'

Then $\quad H^{HFB}|\phi\rangle = E^{HFB}|\phi\rangle$

However H^{HFB} displays other eigenstates depicted as two-quasiparticle excitations on top of $|\phi\rangle$

$$H^{HFB}|\phi^{\alpha\beta\dots}\rangle = E^{\alpha\beta\dots}|\phi^{\alpha\beta\dots}\rangle$$

with
$$\begin{cases} |\phi^{\alpha\beta\dots}\rangle = \beta^+_\alpha \beta^+_\beta \dots |\phi\rangle \\ E^{\alpha\beta\dots} = E^{HFB} + E_\alpha + E_\beta + \dots \end{cases}$$

The exact ground-state energy will be

$$E_0 = E^{HFB} + \Delta E_0^{HFB}$$

correlation energy due to effects of H_1'

Brillouin's theorem states that $\langle\phi|H_1'|\phi^{\alpha\beta}\rangle = 0$

however H_1' couples $|\phi\rangle$ to $|\phi^{\alpha\beta\gamma\delta}\rangle$, $|\phi^{\alpha\beta\gamma\delta\zeta\varepsilon}\rangle$, ...

i.e.

$$\langle\phi|H_1'|\phi^{\alpha\beta\gamma\delta}\rangle \neq 0$$

$\downarrow$

Correlation expansion methods

Express exact wave function as

$$|\Psi\rangle = W|\phi\rangle$$

$|\phi\rangle$ — reference state (HF or HFB)

W — wave operator (includes corrections on top of a reference state)

E.g. for HFB reference state

$$|\Psi\rangle = |\phi\rangle + |\phi^{\alpha\beta}\rangle + |\phi^{\alpha\beta\gamma\delta}\rangle + \dots$$

Total energy is

$$E_0 = \langle\Psi|H|\Psi\rangle = \underbrace{\langle\phi|H_0'|\phi\rangle}_{E^{HFB}} + \underbrace{\langle\phi|H_1'|\phi^{\alpha\beta}\rangle + \dots}_{\Delta E_0^{HFB}}$$

ΔE_0^{HFB} — scope of many-body techniques