Symmetry Breaking and Correlations in Nuclei

I – Spontaneous Symmetry Breaking and Restoration in Finite Systems

Nuclear Many-Body Correlations

short-range

(hard repulsive core of the NN-interaction)

long-range

nuclear resonance modes (giant resonances)

collective correlations

large-amplitude soft modes: (center of mass motion, rotation, low-energy quadrupole vibrations)

...vary smoothly with nucleon number! Can be included implicitly in an effective Energy Density Functional. ...sensitive to shell-effects and strong variations with nucleon number!
Cannot be included in a simple EDF framework.

Spontaneous Symmetry Breaking

Spontaneous Symmetry Breaking (SSB) \Rightarrow the ground state of a QM many-body system has a symmetry that is <u>lower</u> than the symmetry of the underlying Hamiltonian. The system <u>lowers its energy</u> through spontaneous symmetry breaking, resulting in a state of lower symmetry and higher order.

Consider a system whose Lagrangian \mathcal{L} is invariant under some symmetry transformations. For example, \mathcal{L} might be spherically symmetric, i.e. invariant under spatial rotations.

The ground state of the system: 1) unique and invariant under the symmetry transformations of $\mathcal L$

- 2) degenerate and the corresponding eigenstates are not invariant, but transform linearly amongst themselves under the symmetry transformations of \mathcal{L} .
 - ⇒ there is no unique ground state.

If we arbitrarily select one of the degenerate states as the ground state, then the ground state no longer shares the symmetries of $\mathcal{L} \equiv \frac{\text{SPONTANEOUS SYMMETRY BREAKING}}{\text{SPONTANEOUS SYMMETRY BREAKING}}$

The Goldstone model:
$$\mathscr{L}(x) = \left[\partial^{\mu}\phi^{*}(x)\right] \left[\partial_{\mu}\phi(x)\right] - \left.\mu^{2}|\phi(x)|^{2} - \left.\lambda|\phi(x)|^{4}\right]$$

$$\rightarrow$$
 complex scalar field: $\phi(x) = \frac{1}{\sqrt{2}} [\phi_1(x) + i\phi_2(x)]$

$$\rightarrow$$
 relativistic notation: $\frac{\partial \phi}{\partial x^{\mu}} \equiv \partial_{\mu} \phi \equiv \phi_{,\mu} \qquad \frac{\partial \phi}{\partial x_{\mu}} \equiv \partial^{\mu} \phi \equiv \phi_{,\mu}^{\mu}$

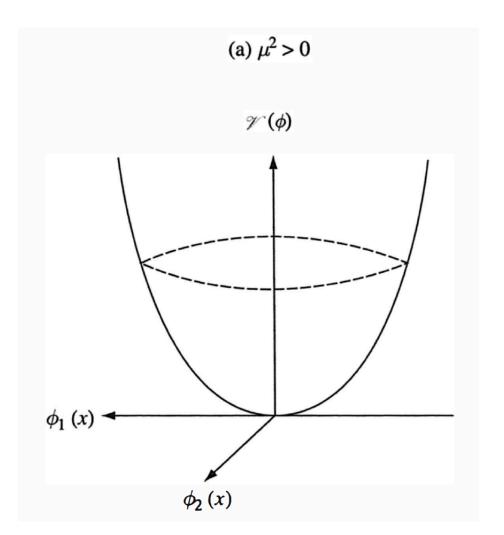
The Lagrangian density is invariant under the global U(1) phase transformations:

$$\phi(x) \to \phi'(x) = \phi(x)e^{i\alpha}, \quad \phi^*(x) \to \phi^{*\prime}(x) = \phi^*(x)e^{-i\alpha}$$

The potential energy density of the field:

$$\mathscr{V}(\phi) = \mu^2 |\phi(x)|^2 + \lambda |\phi(x)|^4$$

For the energy of the field to be bounded from below: $\lambda > 0$. Minimum of the potential ?

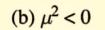


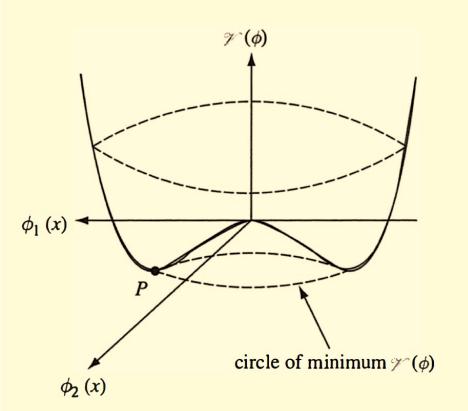
$$\mathscr{V}(\phi) = \mu^2 |\phi(x)|^2 + \lambda |\phi(x)|^4$$

The potential has an absolute minimum for the unique value $\phi(x) = 0 \Rightarrow$ normal modes of oscillation about the stable equilibrium position.

In quantum field theory the state of lowest energy is the vacuum | 0 >. In this case the ground state is unique and the expectation value of the field $\phi(x)$ vanishes:

$$\langle 0|\phi(x)|0\rangle = 0$$





Local maximum for $\phi(x) = 0$ and minimum for:

$$\phi(x) = \phi_0 = \left(\frac{-\mu^2}{2\lambda}\right)^{1/2} e^{i\theta}, \quad 0 \le \theta < 2\pi$$

 \Rightarrow the state of lowest energy is not unique. It is determined by the choice of ϑ , e.g. ϑ =0:

$$\phi_0 = \left(\frac{-\mu^2}{2\lambda}\right)^{1/2} = \frac{1}{\sqrt{2}}v \quad (>0)$$

The symmetry is spontaneously broken because the ground state does not share the symmetry of the Lagrangian and the field $\phi(x)$ does not vanish in the vacuum state:

$$\langle 0|\phi(x)0\rangle = \phi_0$$

 $\phi_0 \rightarrow$ complex order parameter.

 \Rightarrow introduce two real fields $\sigma(x)$ i $\eta(x)$: $\phi(x) = \frac{1}{\sqrt{2}} [\upsilon + \sigma(x) + i\eta(x)]$

In terms of these fields, the Lagrangian density:

$$\mathscr{L}(x) = \frac{1}{2} \left[\partial^{\mu} \sigma(x) \right] \left[\partial_{\mu} \sigma(x) \right] - \frac{1}{2} (2\lambda \upsilon^{2}) \sigma^{2}(x)$$

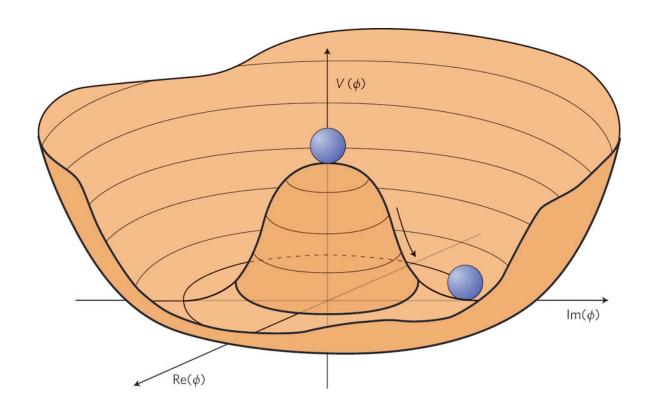
$$+ \frac{1}{2} \left[\partial^{\mu} \eta(x) \right] \left[\partial_{\mu} \eta(x) \right]$$

$$- \lambda \upsilon \sigma(x) \left[\sigma^{2}(x) + \eta^{2}(x) \right] - \frac{1}{4} \lambda \left[\sigma^{2}(x) + \eta^{2}(x) \right]^{2}$$
interaction terms

On quantization, both fields lead to neutral spin-0 particles: the σ boson with the (real positive) mass $(2\lambda v^2)^{1/2}$ and the η boson of mass 0.

 $\sigma(x) \rightarrow$ represents a displacement in the radial plane in which the potential energy density increases quadratically with σ .

 $\eta(x) \rightarrow$ represents a displacement along the valley of minimum potential energy = constant, so that the corresponding quantum excitations: η bosons – are massless.



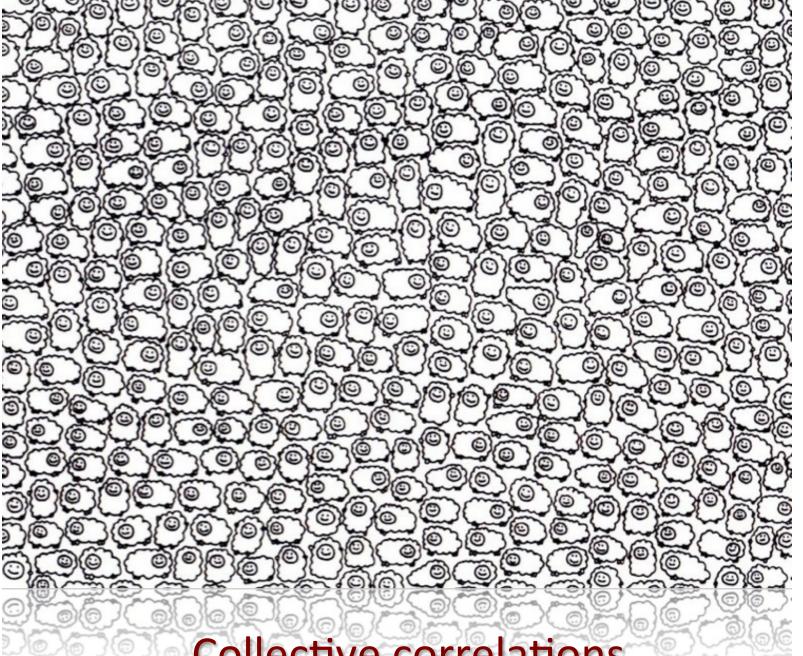
The zero mass of the Goldstone bosons is a consequence of the degeneracy of the vacuum.

SSB in finite systems with a small number of particles

Two-step method:

- 1) symmetry breaking at the mean-field level. The system lowers the energy by including static correlations. The many-body wave function is a single Slater determinant associated with "central mean-field". Examples for nuclei:
- \rightarrow translational invariance of the Hamiltonian \Rightarrow localized solutions
- → rotational invariance ⇒ deformed nucleonic density
- \rightarrow particle number invariance \Rightarrow pairing correlations
- → reflection symmetry ⇒ octupole deformation of the nucleonic density
- 2) Subsequent restoration of the broken symmetry via projection techniques ⇒beyond the mean-field approximation the projected many-body wave function is a linear superposition of Slater determinants and it preserves all the symmetries of the original many-body Hamiltonian ⇒ dynamical correlations additionally lower the energy of the system.

Important! The lower symmetry found at the broken symmetry does not disappear, it becomes *intrinsic* or *hidden*.



Collective correlations

Restoration of Broken Symmetries

A self-consistent mean-field wave function breaks necessarily several symmetries of the nuclear Hamiltonian (translational, rotational).

EXAMPLE: the only translational invariant product wave functions are products of plane waves, but they cannot be used to describe strong correlations between nucleons and their clustering into a finite nucleus.

Symmetry of a Hamiltonian and Broken Symmetry

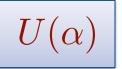
→ symmetry of the Hamiltonian of the system:

$$UHU^+ = H \qquad [H, U] = 0$$

<u>-unitary transformation:</u> preserves the norm of state vectors and the matrix elements of observables.

<u>-symmetry group of H:</u> the eigenvectors of H are classified according to the irreducible representation of the symmetry group.

<u>State of broken symmetry (deformed state):</u> cannot be classified according to an irreducible representation of the symmetry group of the Hamiltonian H.



 \rightarrow set of unitary operators (representing the symmetry group of the Hamiltonan). The parameter α can be discrete or continuous.



$$\langle \Phi \alpha | H | \Phi \alpha \rangle = \langle \Phi | U^{+}(\alpha) H U(\alpha) | \Phi \rangle$$
$$= \langle \Phi | H | \Phi \rangle \quad \forall \alpha$$

 \Rightarrow all deformed states $|\Phi \alpha \rangle$ are DEGENERATE.

 $|\Phi\alpha\rangle = U(\alpha)|\Phi\rangle$

Symmetries of the Hartree-Fock field

 $|\Phi>\rightarrow$ independent-particle state with the associated single-particle density ρ

$$\rho_{ij} = \langle \Phi | a_j^+ a_i | \Phi \rangle \equiv \langle \Phi | \rho | \Phi \rangle$$

→ consider a unitary transformation:

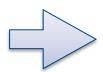
$$|\overline{\Phi}\rangle = U|\Phi\rangle$$



$$\bar{\rho}_{ij} \equiv \langle \overline{\Phi} | a_j^+ a_i | \overline{\Phi} \rangle$$

$$\rightarrow$$
 with: $U^+a_i^+U=\sum_k U_{ik}^*a_k^+$

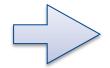
$$U^+a_iU = \sum_k U_{ik}a_k$$



$$\bar{\rho} = U \rho U^+$$

ightarrow in the HF approximation: $E[
ho] = \langle \Phi | H | \Phi
angle$

$$ightarrow$$
 if $UHU^+=H$



$$E[\bar{\rho}] = E[\rho]$$

$$E[\bar{\rho}] = E[\rho] \quad \Box$$

$$h[\bar{\rho}] = Uh[\rho]U^+$$

transformation of the Hartree-Fock hamiltonian

1) the density matrix ρ is invariant under the transformation U:

$$\bar{\rho} = \rho \implies h[\bar{\rho}] = h[\rho]$$

U represents a *self-consistent symmetry* of the HF hamiltonian.

$$\bar{\rho} \neq \rho \qquad [h[\rho], U] \neq 0$$

U represents a **broken symmetry** of the HF hamiltonian.

Example: translational symmetry is always broken by the HF potential of a bound finite system.

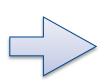
Symmetries in the presence of pairing fields

In the Hartree-Fock-Bogoliubov (HFB) approximation the quasiparticle vacuum is characterized by the generalized density matrix:

$$\mathcal{R} = \left(egin{array}{ccc}
ho & \kappa \ -\kappa^* & 1\!\!1 -
ho^* \end{array}
ight)$$

→ unitary transformation:

$$|\overline{\Phi}\rangle = U|\Phi\rangle$$



$$\bar{\rho}_{ij} = \langle \overline{\Phi} | a_j^+ a_i | \overline{\Phi} \rangle = (U \rho U^+)_{ij}$$

$$\bar{\kappa}_{ij} = \langle \overline{\Phi} | a_j^- a_i | \overline{\Phi} \rangle = (U \kappa \tilde{U})_{ij}$$

$$\bar{\mathcal{R}} = \mathcal{U}\mathcal{R}\mathcal{U}^+ \qquad \mathcal{U} = \begin{pmatrix} U & 0 \\ 0 & U^+ \end{pmatrix}$$

If U represents a symmetry of the Hamiltonian $H \Rightarrow$

$$E[\bar{\mathcal{R}}] = E[\mathcal{R}]$$

$$\mathcal{H}[ar{\mathcal{R}}] = \mathcal{U}\mathcal{H}[\mathcal{R}]\mathcal{U}^+$$
 transformation of the HFB Hamiltonian

1) self-consistent symmetry of the HFB Hamiltonian

$$[\mathcal{R}, \mathcal{U}] = 0$$

$$\bar{\mathcal{R}} = \mathcal{R}$$

$$[\mathcal{R}, \mathcal{U}] = 0$$
 $\bar{\mathcal{R}} = \mathcal{R}$ $\mathcal{U}\mathcal{H}\mathcal{U}^+ = \mathcal{H}$

2) broken symmetry

$$[\mathcal{R}, \mathcal{U}] \neq 0$$

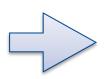
$$ar{\mathcal{R}}
eq \mathcal{R}$$

$$[\mathcal{R}, \mathcal{U}] \neq 0$$
 $\bar{\mathcal{R}} \neq \mathcal{R}$ $\mathcal{U}\mathcal{H}\mathcal{U}^+ \neq \mathcal{H}$

The pairing field breaks the invariance with respect to the transformation induced by the operator:

$$U = e^{iN\phi}$$

$$N = \sum_{i} a_i^{+} a_i$$



$$ar{\mathcal{R}} = \mathcal{U}\mathcal{R}\mathcal{U}^+ = \left(egin{array}{ccc}
ho & \kappa e^{2i\phi} \ -\kappa^* e^{-2i\phi} & 1\!\!\!1 -
ho^* \end{array}
ight)$$

Broken symmetries in finite systems

In *finite systems* broken symmetries arise only as a result of approximations (variational principle applied to a restricted set of trial wave functions).

A **broken symmetry** implies a **degeneracy** of the solutions of variational equations.

$$|\Phi\alpha\rangle \equiv U(\alpha)|\Phi\rangle$$

SYMMETRY RESTORATION → the new wave function is a linear superposition of the degenerate deformed states.

$$|\psi\rangle = \int d\alpha f(\alpha) |\Phi\alpha\rangle$$

The *minimization of the energy* with respect to the expansion coefficients $f(\alpha)$ is equivalent to the *projection* of states of good symmetry from the deformed state $|\Phi\rangle$. The resulting states can be classified according to the *irreps* of the symmetry group.

EXAMPLE: *parity* - discrete broken symmetry

 $|\Phi>$ a normalized state that is not an eigenstate of the **parity operator** Π . [H, Π]=0 implies that the linearly independent states $|\Phi>$ and $\Pi|\Phi>$ are degenerate.

$$\Rightarrow$$
 new trial function:
$$|\psi(\lambda)\rangle = |\Phi\rangle + \lambda \Pi |\Phi\rangle$$

$$\Rightarrow \text{parameter to be evaluated by minimizing}$$
 the energy expectation value

$$E(\lambda) = \frac{\langle \Psi(\lambda) | H | \Psi(\lambda) \rangle}{\langle \Psi(\lambda) | \Psi(\lambda) \rangle} = \langle H \rangle \frac{1 + \lambda^2 + 2\lambda \langle H\Pi \rangle / \langle H \rangle}{1 + \lambda^2 + 2\lambda \langle \Pi \rangle}$$

$$\frac{dE(\lambda)}{d\lambda} = 0 \implies \left[\langle H\Pi \rangle - \langle H \rangle \langle \Pi \rangle \right] (1 - \lambda^2) = 0$$

If $|\Phi>$ is neither an eigenstate of the Hamiltonian H, nor of the parity operator:

$$\langle H\Pi \rangle \neq \langle H \rangle \langle \Pi \rangle \implies \lambda = \pm 1$$

→ parity eigenstates:

$$|\Psi_{\pm}\rangle = \frac{1}{\sqrt{2}}(1\pm\Pi)|\Phi\rangle \implies \Pi|\Psi_{\pm}\rangle = \pm|\Psi_{\pm}\rangle$$

The same states are obtained by simply acting with the projection operators:

$$P_{\pm} = \frac{1}{\sqrt{2}} (1 \pm \Pi)$$

on the deformed state $|\Phi\rangle$. The degeneracy of the deformed states $|\Phi\rangle$ and $\Pi|\Phi\rangle$ has been removed:

$$E_{+} - E_{-} = 2 \frac{\langle H\Pi \rangle - \langle H \rangle \langle \Pi \rangle}{1 - \langle \Pi \rangle^{2}}$$

Non-conservation of particle number

 $| \Phi \rangle$ a normalized state, not an eigenstate of the **particle number operator N**.

$$[H,N] = 0 \qquad \Longrightarrow \qquad e^{-i\alpha N} |\Phi\rangle \quad \alpha \in [0,2\pi]$$
 degenerate states!

→ new function:

$$|\Psi\rangle = \int_0^{2\pi} \frac{d\alpha}{2\pi} f(\alpha) e^{-i\alpha \hat{N}} |\Phi\rangle \equiv \int_0^{2\pi} \frac{d\alpha}{2\pi} f(\alpha) |\Phi\alpha\rangle$$

def.
$$\hat{N}=N-ar{n}, \qquad |\Phi \alpha \rangle \equiv e^{-i\alpha \hat{N}} |\Phi \rangle$$

The projection on states with good particle number is equivalent to the requirement that the energy: $\langle \Psi | H | \Psi \rangle$

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

is stationary with respect to variations of $f^*(\alpha)$ and $f(\alpha)$. $= \frac{\int_0^{2\pi} d\alpha \int_0^{2\pi} d\alpha' f^*(\alpha) \langle \Phi \alpha | H | \Phi \alpha' \rangle f(\alpha')}{\int_0^{2\pi} d\alpha \int_0^{2\pi} d\alpha' f^*(\alpha) \langle \Phi \alpha | \Phi \alpha' \rangle f(\alpha')}$



$$\int_0^{2\pi} \frac{d\alpha'}{2\pi} \langle \Phi | e^{i\hat{N}(\alpha - \alpha')} (H - E) | \Phi \rangle f(\alpha') = 0$$

Hill-Wheeler equation

the solutions are eigenstates of the particle number operator!

Fourier transform:

$$f(\alpha) = \sum_{n=0}^{\infty} f_n e^{i(n-\bar{n})\alpha} \implies f_n = \int_0^{2\pi} \frac{d\alpha}{2\pi} e^{-i(n-\bar{n})\alpha} f(\alpha)$$

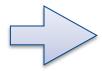


HW equation:
$$\sum_{n=0}^{\infty} f_n \langle \Phi | (H-E) P_n | \Phi \rangle e^{i(n-\bar{n})\alpha} = 0$$

where:

$$P_n \equiv \int_0^{2\pi} rac{dlpha}{2\pi} e^{-i(N-n)lpha}$$
 $ightarrow$ operator projecting onto states with particle number n.

The Hill-Wheeler equation is valid for all angles α :



$$f_n \langle \Phi | (H - E) P_n | \Phi \rangle = 0$$

nonvanishing coefficients exist only if the energy E equals:

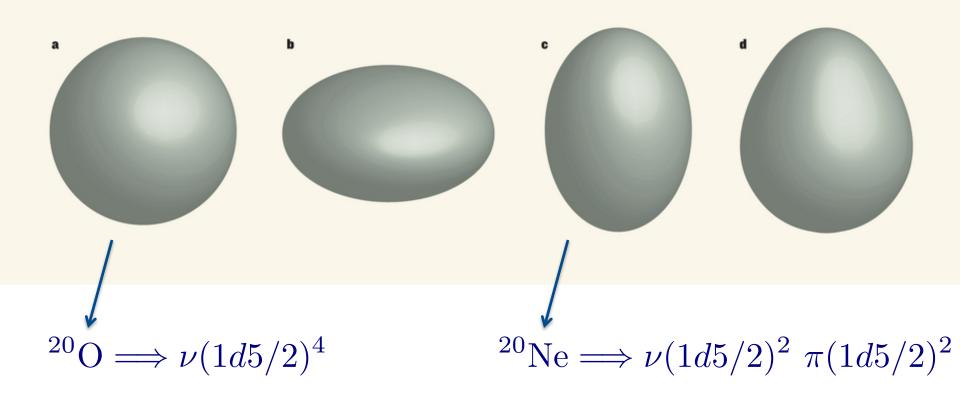
$$E_n = \frac{\langle \Phi | HP_n | \Phi \rangle}{\langle \Phi | P_n | \Psi \rangle}$$

The solution of the HW equation is the projected state:

$$|\Psi\rangle = f_n |\Psi_n\rangle, \qquad |\Psi_n\rangle \equiv P_n |\Phi\rangle$$

 \Rightarrow f_n is a normalization constant.

Nuclear deformation



Deformation-driving part of the effective interaction \rightarrow T=0 $Q_p \cdot Q_n$ force

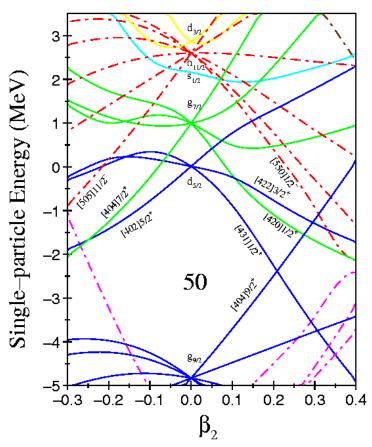
 \rightarrow deformation results from the coupling of nuclear surface oscillations to the motion of individual (valence) nucleons. The particle-vibration coupling leads to the *nuclear* Jahn-Teller effect \Rightarrow the lowest-energy intrinsic state is not an eigenstate characterized by the symmetry group of the total Hamiltonian.

The nuclear Jahn-Teller effect

$$\{ec{Q}\}\equiv\{Q_j\}$$
 SLOW (collective) coordinates $\{ec{x}\}\equiv\{x_j\}$ FAST (noncollective) coordinates $H=T_{ec{Q}}+T_{ec{x}}+V(ec{Q},ec{x})$

⇒ at a given point in the collective space one solves the eigenproblem for the non-collective Hamiltonian:

$$[T_{\vec{x}} + V(\vec{Q}, \vec{x})]\psi_n(\vec{x}; \vec{Q}) = E_n(\vec{Q})\psi_n(\vec{x}; \vec{Q})$$



The total wave function:

$$\Psi = \sum_{n} \psi_{n}(\vec{x}; \vec{Q}) \chi_{n}(\vec{Q})$$

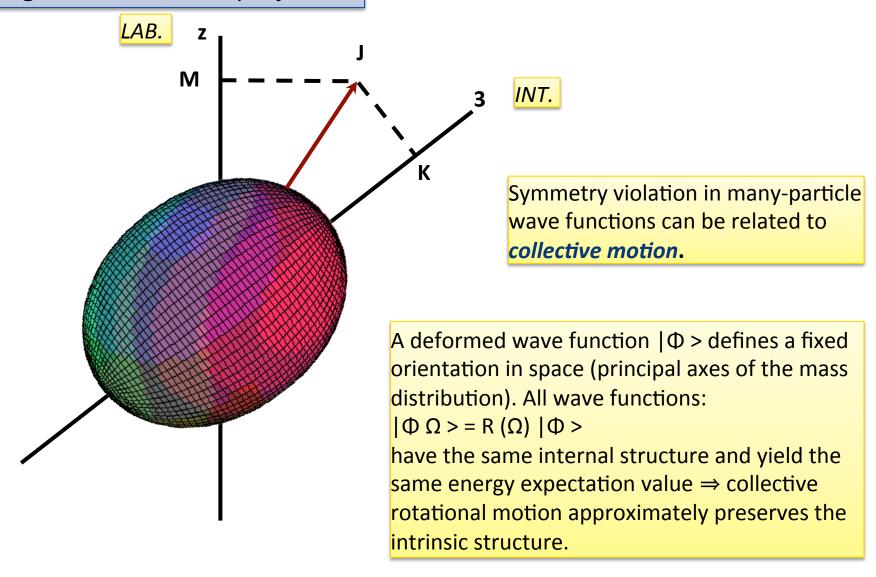
collective wave function that corresponds to the effective potential!

$$\sum_{m} [\delta_{mn} T_{\vec{Q}} + V_{mn}(\vec{Q})] \chi_m(\vec{Q}) = E_n \chi_n(\vec{Q})$$

The effective collective potential $V_{mn}(\mathbf{Q})$ contains the coupling term between different single-particle states:

$$\sum_{m} < n|T_{\vec{Q}}|m > \chi_m(\vec{Q})$$

Angular momentum projection



Angular momentum operators in the laboratory and intrinsic frames

INT.
$$\hat{e}_a$$
 $(a=1,2,3)$: $\hat{e}_a \cdot \hat{e}_b = \delta_{ab}$, $\hat{e}_a \times \hat{e}_b = \epsilon_{abc}\hat{e}_c$

LAB.
$$\hat{u}_i$$
 $(i=x,y,z)$: $\hat{e}_a = \tilde{\mathcal{R}}_{ai}(\Omega)\hat{u}_i, \quad \Omega = \{\alpha,\beta,\gamma\}$

Euler angles

The Euler angles are dynamical variables which specify the orientation of the intrinsic frame.

Def. intrinsic angular momentum operators:

$$I_a = \hat{e}_a \cdot \vec{J}$$

$$[I_a, J_i] = 0 \quad \forall a, i$$
$$[I_a, I_b] = -i\epsilon_{abc}I_c$$
$$\vec{I}^2 = \sum_a I_a^2 = \sum_i J_i^2 = \vec{J}^2$$

$$ec{I}^{\ 2}=ec{J}^{\ 2},I_3,J_z$$

set of commuting operators, can be diagonalized simultaneously.

$$\vec{I}^{2}|IKM\rangle = I(I+1)|IKM\rangle$$
 $I_{3}|IKM\rangle = K|IKM\rangle - I \le K \le I$
 $J_{z}|IKM\rangle = M|IKM\rangle - I \le M \le I$

$$\sum_{IKM} |IKM\rangle\langle IKM| = 1, \qquad \langle IKM|I'K'M'\rangle = \delta_{II'}\delta_{KK'}\delta_{MM'}$$

The states | IKM > can be represented by the wave functions < Ω | IKM >, which depend on the Euler angles $\Omega = \{\alpha, \beta, \gamma\}$. With the definition of the state $|\Omega>$:

$$|\Omega\rangle = \mathcal{R}(\Omega)|\Omega = 0\rangle$$

$$\langle \Omega | IKM \rangle = \langle \Omega = 0 | \mathcal{R}^{+}(\Omega) | IKM \rangle$$
$$= \sum_{I'K'M'} \langle \Omega = 0 | I'K'M' \rangle \langle I'K'M' | \mathcal{R}^{+}(\Omega) | IKM \rangle$$

The rotation does not change the intrinsic angular momenta => K=K' and I=I'. If the Euler angles are chosen in such a way that the INT and LAB frames coincide for Ω =0:

$$\langle \Omega = 0 | IKM \rangle = c_I \delta_{KM} \qquad c_I = \sqrt{(2I+1)/8\pi^2}$$

$$\langle \Omega | IKM \rangle = \sqrt{(2I+1)/8\pi^2} D_{MK}^I(\Omega)$$
$$= \sqrt{(2I+1)/8\pi^2} e^{i\alpha M} d_{MK}^I(\beta) e^{i\gamma K}$$

$$\langle IKM|I'K'M'\rangle = \frac{2I+1}{8\pi^2} \int d\Omega D_{M'K'}^{I'}(\Omega) D_{MK}^{I^*}(\Omega)$$
$$= \delta_{II'}\delta_{KK'}\delta_{MM'}$$

Variational principle and angular momentum projection

Deformed state $|\Phi>$, not an eigenstate of $J^{'2},\ J_3$

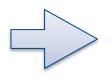
$$\mathcal{R}(\alpha, \beta, \gamma) = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z}$$

$$[H,\mathcal{R}]=0 \implies |\Phi\Omega
angle = \mathcal{R}(\Omega)|\Phi
angle \,\,\,$$
 degenerate states

$$\Rightarrow \text{ new trial function: } |\Psi\rangle = \int d\Omega f(\Omega) |\Phi\Omega\rangle \equiv \int d\Omega f(\Omega) \mathcal{R}(\Omega) |\Phi\rangle$$

The weight function $f(\Omega)$ is determined by requiring that the energy expectation:

$$E=rac{\langle\Psi|H|\Psi
angle}{\langle\Psi|\Psi
angle}$$
 is stationary with respect to variations of f* and f.



Hill-Wheeler equation

$$\int d\Omega' \langle \Phi \Omega | H - E | \Phi \Omega' \rangle f(\Omega') = 0$$

The solutions of the HW equation are eigenstates of the operators $ec{J}^{2}$, $ec{J}_{3}$

$$f(\Omega) = \sum_{IMK} \frac{2I+1}{8\pi^2} f_{MK}^I D_{MK}^I(\Omega) \Rightarrow f_{MK}^I = \int d\Omega f(\Omega) D_{MK}^{I^*}(\Omega)$$

$$|\Psi\rangle = \sum_{IMK} f_{MK}^I P_{MK}^I |\Phi\rangle$$

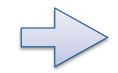
$$P_{MK}^{I} = \frac{2I+1}{8\pi^2} \int d\Omega D_{MK}^{I}(\Omega) \mathcal{R}(\Omega)$$

$$\left(P_{MK}^I\right)^+ = P_{KM}^I$$

$$(P_{MK}^{I})^{+} = P_{KM}^{I} \qquad (P_{MK}^{I})^{+} P_{M'K'}^{I'} = \delta_{II'} \delta_{MM'} P_{KK'}^{I}$$

not quite a projector!

with:
$$[H, P_{MK}^I] = 0$$



$$\sum_{K'} \langle \Phi | (H - E) P_{KK'}^I | \Phi \rangle f_{MK'}^I = 0$$

 \Rightarrow eigenvalues determined by the equation:

$$\det \left[\langle \Phi | (H - E) P_{KK'}^I | \Phi \rangle \right] = 0$$

a) the HW equation is equivalent to the diagonalization of the hamiltonian in the basis $P^I_{MK}|\Phi
angle$

b) H does not connect states with I≠I', and the eigenvalues do not depend on M

$$\Rightarrow$$
 eigenstates:
$$\left| \Psi_{IM} \right\rangle = \sum_{K} f^{I}_{MK} P^{I}_{MK} |\Phi\rangle$$

In cases when the wave function $|\Phi\rangle$ has axial symmetry \Rightarrow K=0 and the coefficients are determined by the normalization of $|\Psi\rangle$. In general the Hamiltonian has to be minimized with respect to the coefficients f.

Projection before and after variation

How do we determine the deformed (symmetry-violating) intrinsic function $|\Phi\rangle$?

i) Variation before the projection (VBP)

 $|\Phi>$ is determined by the variational principle:

$$\delta \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0$$

The deformed solution is a superposition of eigenstates of the corresponding symmetry operator (for example, angular momentum). The wave function:

$$|\Psi_I\rangle = P^I|\Phi\rangle$$

is no longer a product wave function, but a complicated superposition of Slater determinants. It contains many more correlations than the function $|\Phi\rangle$.

This method violates the variational principle, because we do not vary the projected wave function. It does not allow for changes in the self-consistent mean-field for different values of I (within a rotational band).

ii) Variation after projection (VAP)

$$\delta \frac{\langle \Psi_I | H | \Psi_I \rangle}{\langle \Phi_I | \Psi_I \rangle} = \delta \frac{\langle \Phi | P^I H P^I | \Phi \rangle}{\langle \Phi | P^I P^I | \Phi \rangle} = 0$$

 \Rightarrow minimize the expectation value of the projected energy P^IHP^I within the set of product wave functions $|\Phi>$.

This method corresponds to a double variation, using the ansatz:

$$|\Psi\rangle = \int d\Omega f(\Omega) \mathcal{R}(\Omega) |\Phi\rangle$$

and varying the energy with respect to both the weight function $f(\Omega)$ and the generating function $|\Phi\rangle$.

Much more complicated than VBP!