Resonating mean-field theoretical approach to shape coexistence in nuclei

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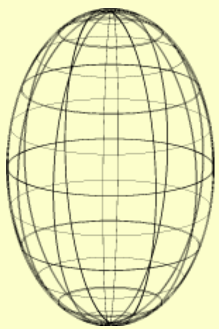
Introduction

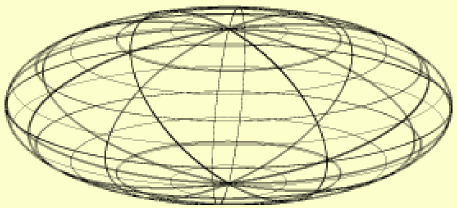
(Prolate-Oblate) Shape Coexistence

There exist multi stable shapes in the same energy region



prolate

($\gamma = 0°$)



oblate

($\gamma = 60°$)

Explanation of shape coexistence in nuclei
by the usual mean-field(MF) theory

Each stable shapes ⟺ Differrent MF solutions

It can't describe the correlation between the multi energy minima in the same energy region

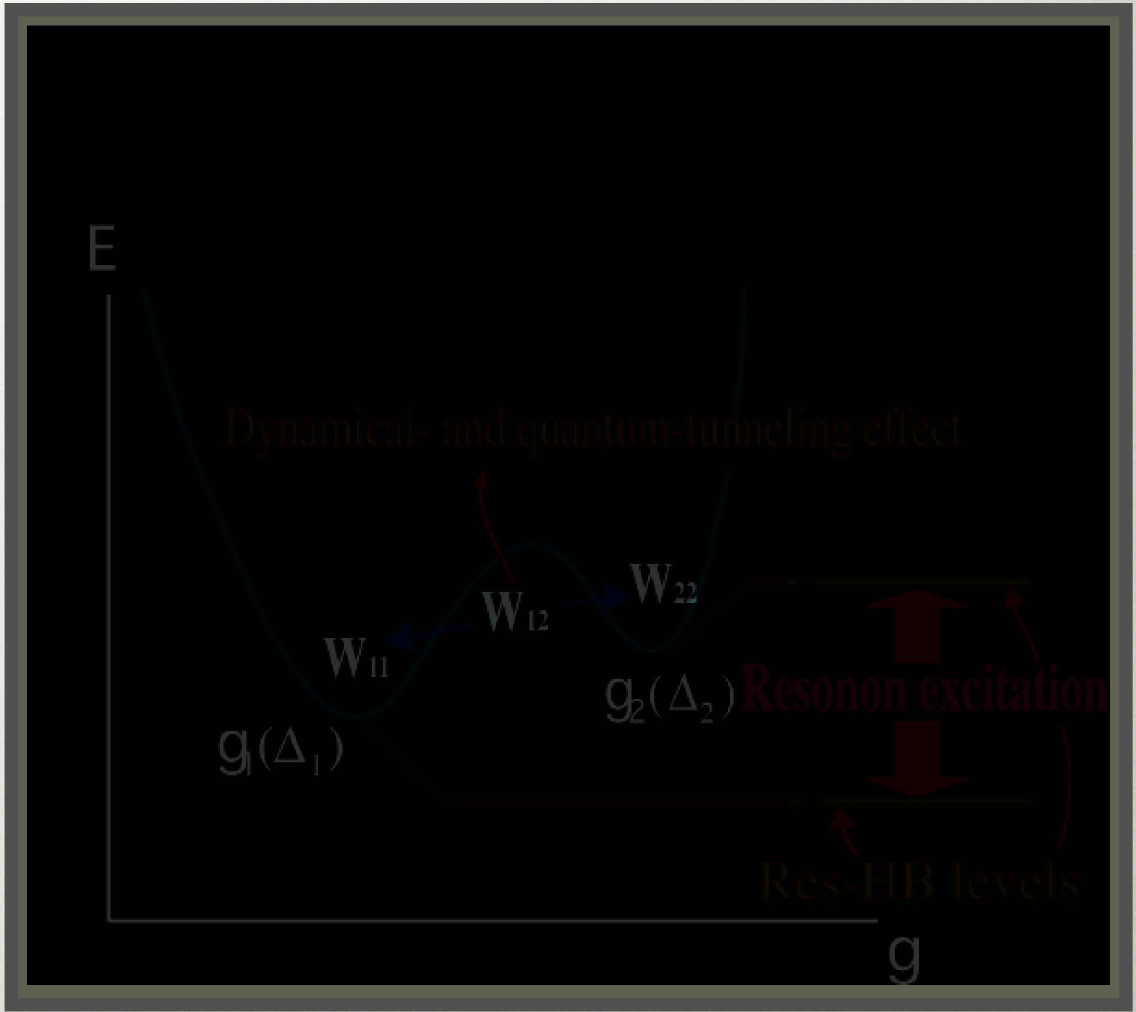
$$\langle prolate | oblate \rangle = \ ?$$

The resonating Hartree-Bogoliubov (Res-HB) theory

takes into account the quantum- and dynamical tunneling effects between different correlation states

$$\boxed{|\Psi\rangle = \sum_s |g_s\rangle c_s}$$

- $c_s \cdots$ mixing coefficient
- The $|g_r\rangle$'s are non-orthogonal and represent different correlation states



Normalization condition

$$\langle\Psi|\Psi\rangle = 1$$

The Res-HB CI (configuration interaction) equation

$$\sum_s \{H[W_{rs}] - E\} \cdot [\det z_{rs}]^{\frac{1}{2}} c_s = 0$$

The Res-HB eigenvalue equation

$$\left.\begin{aligned}
&[\mathcal{F}_r u_r]_i = \epsilon_{ri} u_{ri}, \quad \epsilon_{ri} = \widetilde{\epsilon}_{ri} - 2\{H[W_{rr}] - E\}|c_r|^2 \\
&\mathcal{F}_r \equiv \mathcal{F}[W_{rr}]|c_r|^2 + \textstyle\sum_s'(\mathcal{K}_{rs} c_r^* c_s + \mathcal{K}_{rs}^\dagger c_r c_s^*) = \mathcal{F}_r^\dagger
\end{aligned}\right\}$$

☆ Orbital concept is still surviving in the Res-HB state !?

The former application

S. Nishiyama and H. Fukutome, J.Phys. G: Nucl. Part. Phys. **18** (1992) 317.

A solution of the Res-HB eigenvalue eq. is not converged !

The Res-HB gap equation

Model

- 3-j orbital model

orbital energy [MeV]	e_a= 4.8 (3.0)	e_b= 3.0 (1.0)	e_c= 3.0 (2.0)
principal quantum num.	n_a= 1 (0)	n_b= 0 (0)	n_c= 1 (1)
angular momentum	l_a= 3 (5)	l_b= 4 (4)	l_c= 2 (2)
spin	j_a= 7 / 2 (11 / 2)	j_b= 7 / 2 (7 / 2)	j_c= 3 / 2 (3 / 2)

- Interaction strength of pair. int. : g=1.0 (1.0)
- Interaction strength of quad. int. : X=0.44 (0.44)
- Particle number : PN=18 (22)
- Harmonic oscillator parameter : A=9.0 (11.0)

Case I

Case II

- Introduce a chemical potential for particle num. conservation
- (Pairing interaction) + (Quadrupole interaction) model

Pairing int. plus Quadrupole int. model (P+QQ model)

(Baranger & Kumar Nucl.Phys.**62**(1965)113)

Parameters … $\beta, \ \gamma, \ \Delta, \ \lambda$

Two-step diagonalization

(1) Diagonalization of QQ force in the Hartree frame

(2) Diagonalization of Pairing interaction term

… Gap equation & Particle-number conservation

$$\longrightarrow \quad \Delta, \ \lambda$$

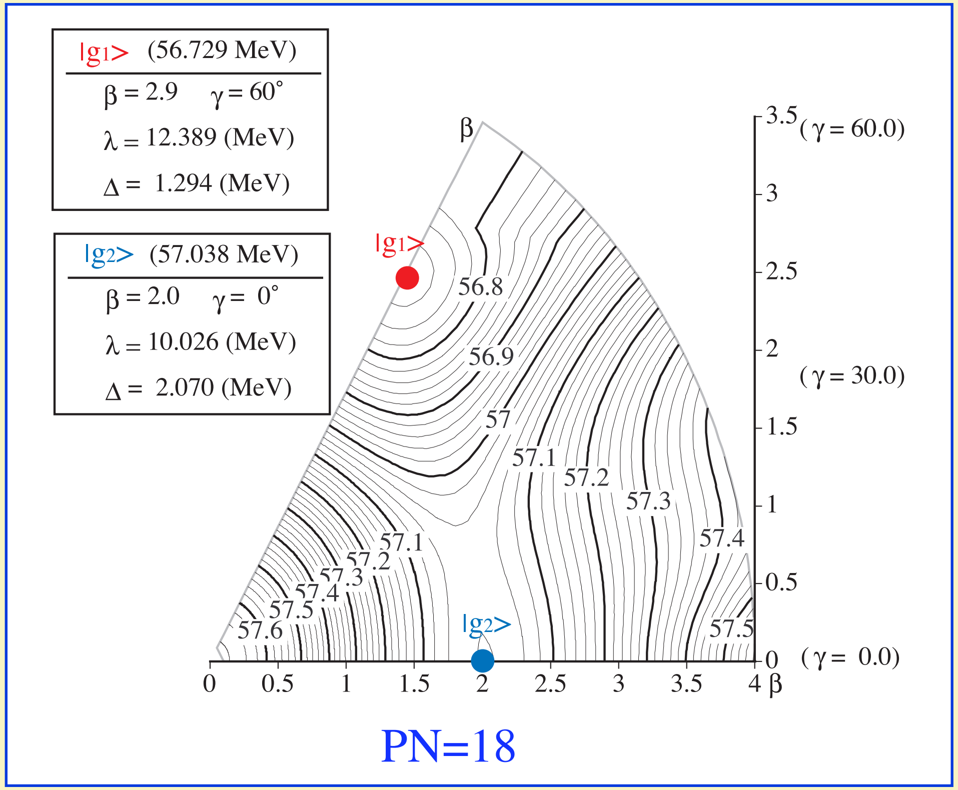
Variation of the MF energy

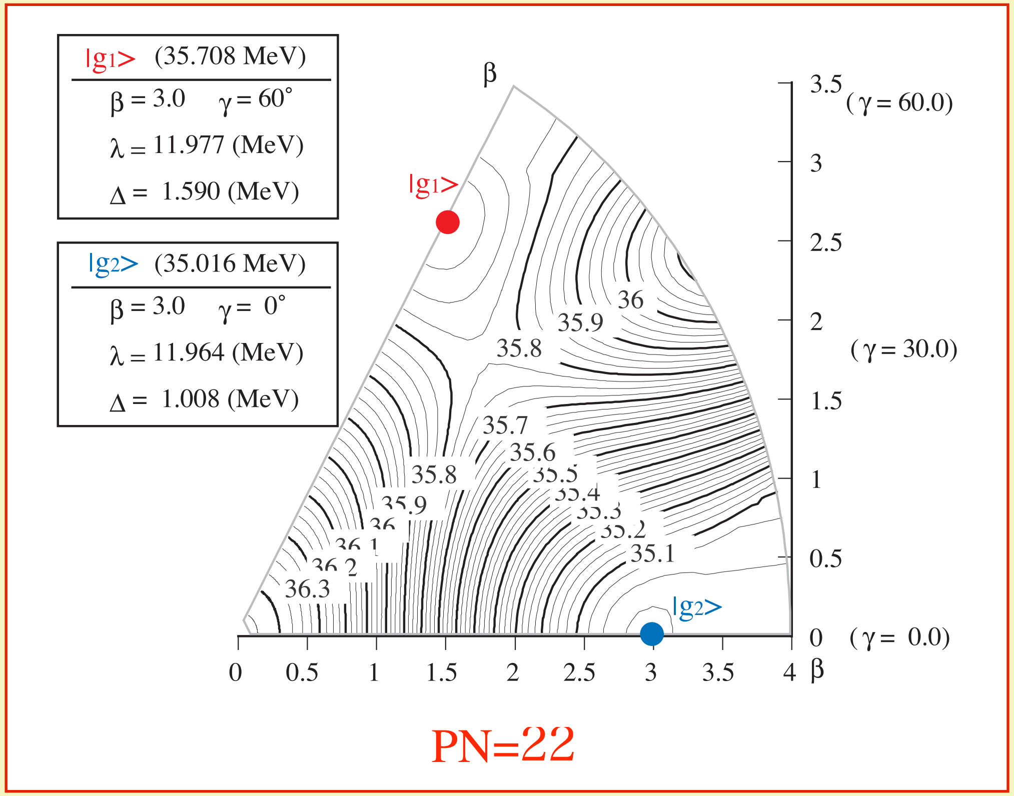
with respect to deformation parameters

$$\frac{\partial E}{\partial \beta} = 0, \qquad \frac{\partial E}{\partial \gamma} = 0 \quad \longrightarrow \quad \beta, \ \gamma$$

Choice of the superposed HB wavefunctions

Usual HB solutions





Superposition of two HB wave functions :

$$|\Psi\rangle = c_1|g_1(\beta_1, \gamma_1, \Delta_1, \lambda)\rangle + c_2|g_2(\beta_2, \gamma_2, \Delta_2, \lambda)\rangle$$

★ $(\beta_1, \gamma_1, \beta_2, \gamma_2)$ ⟵ Usual HB solutions

The P+QQ model in the Res-HB theory

SCF Hartree potential

$$\Gamma_{k,\alpha\beta} \equiv \sum_\mu \langle \alpha | \hat{Q}_\mu | \beta \rangle \Gamma_{k,\mu} \qquad (k=1,2)$$

$$\Gamma_{k,0} = \beta_k \cos\gamma_k, \quad \Gamma_{k,2'} = \beta_k \sin\gamma_k$$

Hartree approx.

$$F_{kk,\alpha\beta} = (\varepsilon_\alpha - \lambda)\delta_{\alpha\beta} + \Gamma_{k,\alpha\beta}$$

$$F_{kk,\alpha\beta} w^*_{k,\beta i} = e_{k,i} w^*_{k,\alpha i}$$

BCS quantities

$$E_{k,i} = \left(e^2_{k,i} + \Delta^2_k\right)^{\frac{1}{2}}$$

$$V_{k,i} = \frac{1}{2}\left(1 - \frac{e_{i,k}}{E_{i,k}}\right) = 1 - U^2_{i,k}$$

Interstate density matrix

$$W_{rs} = \begin{bmatrix} R_{rs} & K_{rs} \\ -K^*_{sr} & 1 - R^*_{sr} \end{bmatrix}$$

$$\Delta_{rs} = \frac{1}{2} g s_\delta K_{rs,\delta\bar{\delta}} \qquad (r,s=1,2)$$

$$\Gamma_{rs} = \sum_\mu \Gamma_{rs,\mu}, \quad \Gamma_{rs,\mu} = \chi \sum_{\alpha\beta} \langle \alpha | \hat{Q}_\mu | \beta \rangle R_{rs,\beta\alpha}$$

$$\Gamma_{rs,0} = \beta_{rs} \cos\gamma_{rs}, \quad \Gamma_{rs,2'} = \beta_{rs} \sin\gamma_{rs}$$

Hamiltonian matrix elements

$$H[W_{11}] = \sum_{\alpha}(e_a - \lambda)R_{11,\alpha\alpha} - \frac{1}{g}|\Delta_{11}|^2 - \frac{1}{2\chi}\beta_{11}^2$$

$$H[W_{22}] = \sum_{\alpha}(e_a - \lambda)R_{22,\alpha\alpha} - \frac{1}{g}|\Delta_{22}|^2 - \frac{1}{2\chi}\beta_{22}^2$$

$$H[W_{12}] = \sum_{\alpha}(e_a - \lambda)R_{12,\alpha\alpha} - \frac{1}{g}\Delta_{12}\Delta_{21} - \frac{1}{2\chi}\beta_{12}^2 = H[W_{21}]$$

$$E = \begin{bmatrix} E_{\mathrm{gr}}^{\mathrm{Res}} \\ \\ E_{\mathrm{ex}}^{\mathrm{Res}} \end{bmatrix} = \frac{1}{2(1 - \det z_{12})}\left\{H[W_{11}] + H[W_{22}] - 2H[W_{12}]\cdot \det z_{12} \mp E_{\mathrm{dis}}^{\frac{1}{2}}\right\}$$

$$E_{\mathrm{dis}} \equiv (H[W_{11}] - H[W_{22}])^2 + 4\,(H[W_{11}] - H[W_{12}]) \times (H[W_{22}] - H[W_{12}])\cdot \det z_{12}$$

Res-HB theoretical gap equations

$$\frac{\partial}{\partial \Delta_1} E_{\rm gr}^{\rm Res}(\Delta_1, \Delta_2) = 0, \qquad \frac{\partial}{\partial \Delta_2} E_{\rm gr}^{\rm Res}(\Delta_1, \Delta_2) = 0$$

$$\xrightarrow{|c_r|^2 \to 1}$$ HB gap eq.

Particle-number conservation conditions

$$\mathcal{N} - PN = 0 \qquad \text{where} \quad \mathcal{N} = \langle \Psi | \hat{N} | \Psi \rangle$$

for the Res-HB field

$$\sum_{i=1}^{N} V_{r,i}^* V_{r,i} - PN = 0 \quad (r = 1, 2)$$

for the each superposed HB field

Energy gap

$$
\begin{aligned}
\Delta^{\mathrm{Res}}_{\mathrm{gr(ex)}} &= \frac{1}{2} g \langle \Psi_{\mathrm{gr(ex)}} | \sum_{\alpha} s_\alpha c_{\bar{\alpha}} c_\alpha | \Psi_{\mathrm{gr(ex)}} \rangle \\
&= \Delta_{11} |c_{1,\mathrm{gr(ex)}}|^2 + \Delta_{22} |c_{2,\mathrm{gr(ex)}}|^2 \\
&+ \Delta_{12} c^*_{1,\mathrm{gr(ex)}} c_{2,\mathrm{gr(ex)}} [\det z_{12}]^{\frac{1}{2}} + \Delta_{21} c_{1,\mathrm{gr(ex)}} c^*_{2,\mathrm{gr(ex)}} [\det z^*_{12}]^{\frac{1}{2}}
\end{aligned}
$$

Deformation parameters

$$
\begin{aligned}
\Gamma^{\mathrm{Res}}_{\mathrm{gr(ex)},0} &= \Gamma_{11,0} |c_{1,\mathrm{gr(ex)}}|^2 + \Gamma_{22,0} |c_{2,\mathrm{gr(ex)}}|^2 \\
&+ \Gamma_{12,0} \left(c^*_{1,\mathrm{gr(ex)}} c_{2,\mathrm{gr(ex)}} [\det z_{12}]^{\frac{1}{2}} + c_{1,\mathrm{gr(ex)}} c^*_{2,\mathrm{gr(ex)}} [\det z^*_{12}]^{\frac{1}{2}} \right)
\end{aligned}
$$

$$
\begin{aligned}
\Gamma^{\mathrm{Res}}_{\mathrm{gr(ex)},2'} &= \Gamma_{11,2'} |c_{1,\mathrm{gr(ex)}}|^2 + \Gamma_{22,2'} |c_{2,\mathrm{gr(ex)}}|^2 \\
&+ \Gamma_{12,2'} \left(c^*_{1,\mathrm{gr(ex)}} c_{2,\mathrm{gr(ex)}} [\det z_{12}]^{\frac{1}{2}} + c_{1,\mathrm{gr(ex)}} c^*_{2,\mathrm{gr(ex)}} [\det z^*_{12}]^{\frac{1}{2}} \right)
\end{aligned}
$$

$$
\boxed{\Gamma^{\mathrm{Res}}_{\mathrm{gr(ex)},0} = \beta^{\mathrm{Res}}_{\mathrm{gr(ex)}} \cos \gamma^{\mathrm{Res}}_{\mathrm{gr(ex)}}, \qquad \Gamma^{\mathrm{Res}}_{\mathrm{gr(ex)},2'} = \beta^{\mathrm{Res}}_{\mathrm{gr(ex)}} \sin \gamma^{\mathrm{Res}}_{\mathrm{gr(ex)}}}
$$

Numerical results for case I (PN=18)

(energy in MeV)

		HB	Res-HB gr.	Res-HB ex.
Input	β_1	2.9	2.9	
	β_2	2.0	2.0	
	γ_1	60°	60°	
	γ_2	0°	0°	
	Δ_1	1.29	0.37	
	Δ_2	2.07	0.64	
	λ	12.340, 10.026	0.000	
Output	$H[W_{11}]$ (E_{HB})	56.729	56.784	
	$H[W_{22}]$ (E_{HB})	57.038	57.397	
	$H[W_{12}]\cdot[\det z_{12}]^{1/2}$		-6.364	
	C_1		0.723	0.691
	C_2		0.690	-0.724
	$[\det z_{12}]^{1/2}$		1.370E-3	
	E_{Res}		50.650	63.549
	$\mathcal{N}$	18.000	18.000	18.000
	β_{Res}		2.381	2.508
	γ_{Res}		35.404°	33.801°
	Δ_{Res}		0.297	0.182

Numerical results for case II (PN=22) (energy in MeV)

		HB	Res-HB gr.	Res-HB ex.
Input	β_1	3.0	3.0	
	β_2	3.0	3.0	
	γ_1	60°	60°	
	γ_2	0°	0°	
	Δ_1	1.59	0.16	
	Δ_2	1.01	0.43	
	λ	11.978, 11.964	-0.005	
Output	$H[W_{11}]$ (E_{HB})	35.708	35.865	
	$H[W_{22}]$ (E_{HB})	35.017	35.135	
	$H[W_{12}]\cdot[\det z_{12}]^{1/2}$		-2.585	
	C_1		0.655	0.755
	C_2		0.755	-0.655
	$[\det z_{12}]^{1/2}$		2.233E-4	
	E_{Res}		33.653	39.000
	$\mathcal{N}$	22.000	22.000	22.000
	β_{Res}		2.778	2.865
	γ_{Res}		26.780°	36.371°
	Δ_{Res}		0.221	0.037

Discussion

Interstate deformation parameters

$$\Delta'_{rs} \equiv \Delta_{rs} \cdot [\det z_{rs}]^{\frac{1}{4}}, \quad \beta'_{rs} \equiv \beta_{rs} \cdot [\det z_{rs}]^{\frac{1}{4}}$$

$$E^{\mathrm{Res}} = \sum_{r,s} \langle g_r | H | g_s \rangle c_r^* c_s$$

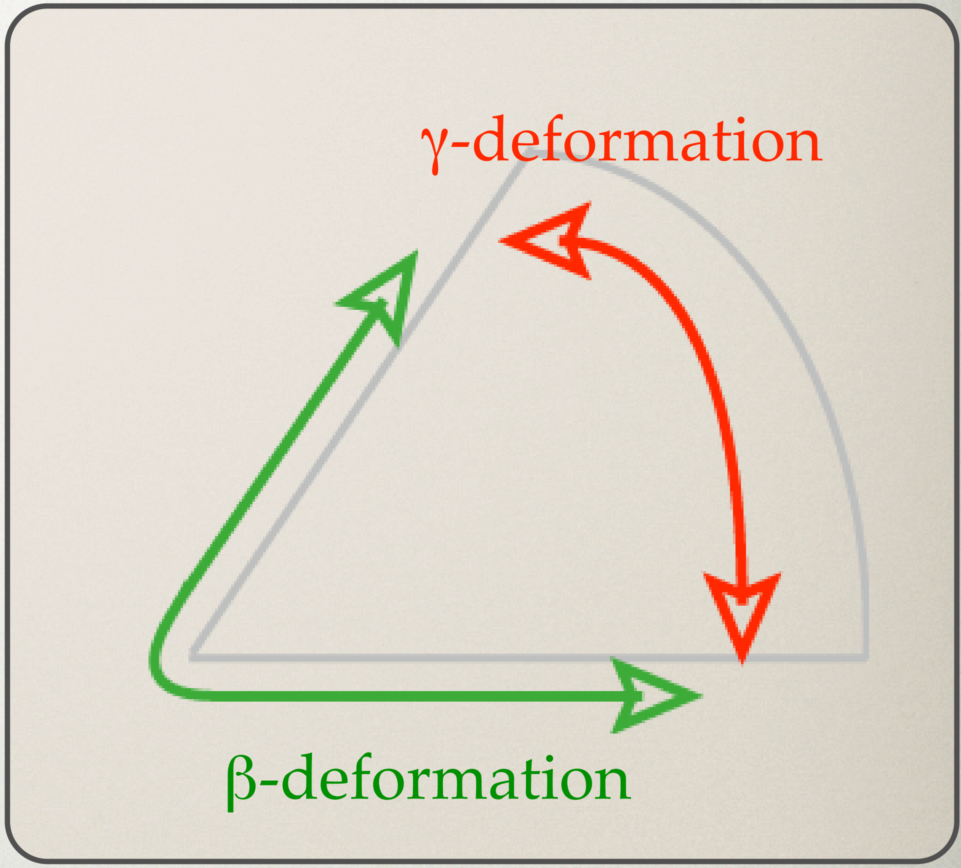
$$\begin{aligned} \langle g_r | H | g_s \rangle &= H[W_{rs}] \cdot [\det z_{rs}]^{\frac{1}{2}} \\ &= \{\sum_{\alpha} (e_\alpha - \lambda) R_{rs,\alpha\alpha}\} \cdot [\det z_{rs}]^{\frac{1}{2}} - \frac{1}{g} |\Delta'_{rs}|^2 - \frac{1}{2\chi} {\beta'}^2_{rs} \end{aligned}$$

Case I (PN=18)

β'_{11}	3.16	γ'_{11}	60.0°	Δ'_{11}	0.44
β'_{12}	2.30	γ'_{12}	55.5°	Δ'_{12}	-4.80
β'_{22}	2.44	γ'_{22}	0.8°	Δ'_{21}	-0.88
				Δ'_{22}	-0.92

Case II (PN=22)

β'_{11}	3.41	γ'_{11}	60.0°	Δ'_{11}	0.19
β'_{12}	1.22	γ'_{12}	55.6°	Δ'_{12}	-6.14
β'_{22}	3.08	γ'_{22}	0.0°	Δ'_{21}	-0.14
				Δ'_{22}	-0.45



Summary

- ❒ Superposition of two HB wave functions
  by using the parameters of the HB solutions
- ❒ The Res-HB theoretical gap equations
- ❒ The HB theoretical picture holds in the Res-MF field
- ❒ The ground state is shifted to lower state than the HB one
- ❒ A new definition of interstate deformation parameters

SO(2N) coherent state representation of a fermion system

- SO(2N) Lie algebra which is constructed by pair operators;

$$E^{\alpha}_{\beta} = c^{\dagger}_{\alpha} c_{\beta} - \tfrac{1}{2}\delta_{\alpha\beta}, \; E_{\alpha\beta} = c_{\alpha} c_{\beta}, \; E^{\alpha\beta} = c^{\dagger}_{\alpha} c^{\dagger}_{\beta}$$

$$E^{\alpha\dagger}_{\beta} = E^{\beta}_{\alpha}, \qquad E^{\alpha\beta} = -E^{\dagger}_{\alpha\beta}$$

- SO(2N) Bogoliubov transformation

$$U(g)(c, \, c^{\dagger})U^{\dagger}(g) = (c, \, c^{\dagger})g,$$

$$g \equiv \left[\begin{array}{cc} a & b^* \\ b & a^* \end{array} \right], \qquad g^{\dagger} g = g g^{\dagger} = 1$$

- State vector

$$|\Psi\rangle = 2^{N-1} \int U(g) |0\rangle \langle 0| U^\dagger(g) |\Psi\rangle \, dg = 2^{N-1} \int |g\rangle \, \Psi(g) dg$$

- Overlap integral

$$\langle g|g'\rangle = \langle 0| U^\dagger(g) U(g') |0\rangle = \langle 0| U(g^\dagger g') |0\rangle$$

Schrödinger equation in coherent state representation

$$\int \{\langle g| H |g'\rangle - E \langle g|g'\rangle\} \Psi(g') dg' = 0$$

$$\langle g| H |g'\rangle = \langle 0| U^\dagger(g) H U(g') |0\rangle$$

The interstate density matrix and the Schrödinger equation

2N×N isometric matrix

$$u = \begin{bmatrix} b \\ a \end{bmatrix}, \qquad u^\dagger u = 1$$

Overlap integral

$$\left.\begin{aligned} &\langle g|g'\rangle = \left[\det\left(a^\dagger a' + b^\dagger b'\right)\right]^{\frac{1}{2}} = [\det z]^{\frac{1}{2}} \\ &z \equiv u^\dagger u', \;\; z = (z_{ij}) \end{aligned}\right\}$$

Interstate density matrix

$$W(g,g') = u' z^{-1} u^\dagger = \begin{bmatrix} R(g,g') & K(g,g') \\ -K^*(g,g') & 1 - R^*(g,g') \end{bmatrix}$$

$$R(g,g') = b' z^{-1} b^\dagger, \quad K(g,g') = b' z^{-1} a^\dagger$$

Hamiltonian of the system

$$\left.\begin{aligned} H &= h_{\alpha\beta}\left(E^{\alpha}_{\beta} + \tfrac{1}{2}\delta_{\alpha\beta}\right) + \tfrac{1}{4}\,[\alpha\beta|\gamma\delta]\,E^{\alpha\gamma}E_{\delta\beta} \\ [\alpha\beta|\gamma\delta] &= -\,[\alpha\delta|\gamma\beta] = [\gamma\delta|\alpha\beta] = [\beta\alpha|\delta\gamma]^{*} \end{aligned}\right\}$$

Hamiltonian matrix element

$$\langle g|\,H\,|g'\rangle = H[W(g,g')]\cdot[\det z]^{\frac{1}{2}}$$

$$\begin{aligned} H[W(g,g')] &= h_{\alpha\beta}R_{\beta\alpha}(g,g') \\ &\quad + \frac{1}{2}\,[\alpha\beta|\gamma\delta]\left\{R_{\beta\alpha}(g,g')R_{\delta\gamma}(g,g') - \frac{1}{2}K^{*}_{\alpha\gamma}(g',g)K_{\delta\beta}(g,g')\right\} \end{aligned}$$

The explicit expression of the integral Schrödinger equation

$$\int\{H[W(g,g')] - E\}\cdot[\det z]^{\frac{1}{2}}\,\Psi(g')dg' = 0$$

Resonating Hartree-Bogoliubov approximation

The state $|\Psi\rangle$ is approximated as

$$|\Psi\rangle = \sum_s |g_s\rangle\, c_s$$

- c_s ··· mixing coefficient
- The $|g_r\rangle$'s are non-orthogonal and represent different correlation states

The matrix z and the HB interstate density matrix

$$z_{rs} = u_r^\dagger u_s, \qquad W_{rs} = u_s z_{rs}^{-1} u_r^\dagger$$

Normalization condition

$$\langle\Psi|\Psi\rangle = \sum_{rs} \langle g_r|g_s\rangle\, c_r^* c_s = \sum_{rs} [\det z_{rs}]^{\frac{1}{2}}\, c_r^* c_s = 1$$

Expectation value of the Hamiltonian

$$\langle\Psi|\, H\, |\Psi\rangle = \sum_{rs} \langle g_r|\, H\, |g_s\rangle\, c_r^* c_s = \sum_{rs} H[W_{rs}][\det z_{rs}]^{\frac{1}{2}}\, c_r^* c_s$$

Lagrangian

$$L = \langle\Psi| H |\Psi\rangle - E \langle\Psi|\Psi\rangle = \sum_{rs} \{H[W_{rs}] - E\} [\det z_{rs}]^{\frac{1}{2}} c_r^* c_s$$

The Res-HB CI(configuration interaction) equation

$$\sum_s \{H[W_{rs}] - E\} \cdot [\det z_{rs}]^{\frac{1}{2}} c_s = 0$$

The Res-HB equation

$$\left.\begin{array}{l} \sum_s \mathcal{K}_{rs} c_r^* c_s = 0 \\ \mathcal{K}_{rs} \equiv \{(1 - W_{rs})\mathcal{F}[W_{rs}] + H[W_{rs}] - E\} \cdot W_{rs} \cdot [\det z_{rs}]^{\frac{1}{2}} \end{array}\right\}$$

Interstate Fock operator

$$\mathcal{F}[W_{rs}] \equiv \left[\begin{array}{cc} F(g_r, g_s) & D(g_r, g_s) \\ -D^*(g_r, g_s) & -F^*(g_r, g_s) \end{array} \right]$$

$$\left.\begin{array}{l} F_{\alpha\beta}(g_r, g_s) \equiv \dfrac{\delta H[W(g_r, g_s)]}{\delta R_{\beta\alpha}(g_r, g_s)} = h_{\alpha\beta} + [\alpha\beta|\gamma\delta]\, R_{\delta\gamma}(g_r, g_s), \\ D_{\alpha\beta}(g_r, g_s) \equiv \dfrac{\delta H[W(g_r, g_s)]}{\delta K^*_{\beta\alpha}(g_s, g_r)} = -\dfrac{1}{2} [\alpha\gamma|\beta\delta]\, K_{\delta\gamma}(g_r, g_s). \end{array}\right\}$$

The Res-HB eigenvalue equation

$$\left.\begin{aligned} [\mathcal{F}_r u_r]_i = \epsilon_{ri} u_{ri}, \quad \epsilon_{ri} = \widetilde{\epsilon}_{ri} - 2\{H[W_{rr}] - E\}|c_r|^2 \\ \mathcal{F}_r \equiv \mathcal{F}[W_{rr}]|c_r|^2 + {\sum}'_s (\mathcal{K}_{rs} c_r^* c_s + \mathcal{K}_{rs}^\dagger c_r c_s^*) = \mathcal{F}_r^\dagger \end{aligned}\right\}$$

where $\widetilde{\epsilon}_r = (\delta_{ij}\widetilde{\epsilon}_{ri})$ is given by ;

$$u_r^\dagger \mathcal{F}_r u_r + 2\{H[W_{rr}] - E\}|c_r|^2 = u_r^\dagger \mathcal{F}[W_{rr}]|c_r|^2 u_r = \widetilde{\epsilon}_r$$

$$\widetilde{\epsilon}_r = \begin{bmatrix} \widetilde{\epsilon}_{r1} & & & & & \\ & \ddots & & & 0 & \\ & & \widetilde{\epsilon}_{rN} & & & \\ & & & -\widetilde{\epsilon}_{r1} & & \\ & 0 & & & \ddots & \\ & & & & & -\widetilde{\epsilon}_{rN} \end{bmatrix}$$

☆ Orbital concept is still surviving in the Res-HB state !?

☆ The eigenvalues $\widetilde{\epsilon}_{ri}$ tend to the usual HB orbital energies in the limit $|c_r|^2 \to 1$