Basic Issues in Theories of Large Amplitude Collective Motion

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- Adiabatic self-consistent collective coordinate (ASCC) method
- GCM/GOA vs ASCC

INT workshop: Quantitative Large Amplitude
Shape Dynamics: fission and heavy ion fusion
INT, Seattle, USA, October 30th, 2013

Brief introduction

- Theories of large amplitude collective motion, associated with TDHF(B)

Adiabatic theories of LACM

- Baranger-Veneroni, 1972-1978

$$\rho(t) = e^{i\chi(t)}\rho_0 e^{-i\chi(t)}$$

  - Expansion with respect to χ

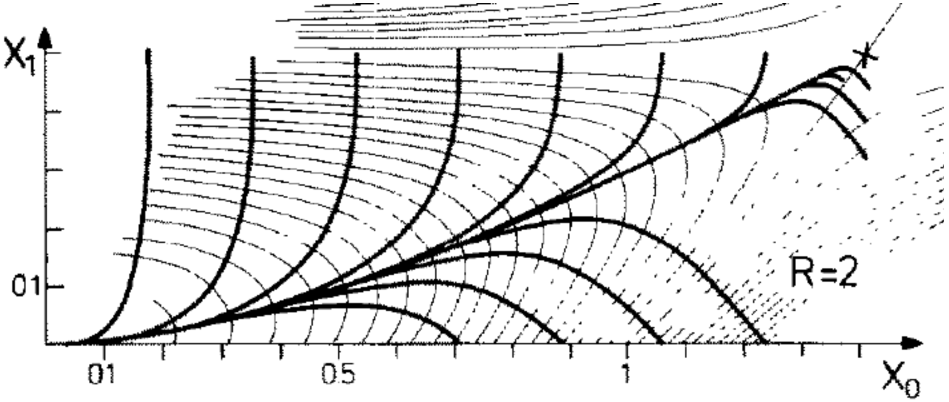
- Villars, 1975-1977
  - Eq. for the collective subspace (zero-th and first-order w.r.t. momenta)

$$\delta\left\langle \Phi(q) \middle| H - \frac{\partial V}{\partial q} Q(q) \middle| \Phi(q) \right\rangle = 0$$

$$\delta\left\langle \Phi(q) \middle| [H, Q(q)] + iM(q)^{-1} \frac{\partial}{\partial q} \middle| \Phi(q) \right\rangle = 0$$

Goeke, Reinhard, Rowe, NPA359 (1981) 408

  - Non-uniqueness problem "Validity condition" (Reinhard, 1978-)



Approaches to Non-uniqueness Problem

(1) Yamamura-Kuriyama-Iida, 1984

Requirement of "analyticity"

(ex) Moya de Guerra-Villars, 1978)

Therefore, *in principle*, we can determine a unique collective path in the ATDHF. The higher-order in *p* can be systematically treated.

In practice, it is only applicable to simple models.

(2) Rowe, Mukhejee-Pal, 1981

Requirement of "Point transf." and equations up to $O(p^2)$

There is no systematic way to go beyond the second order in *p*.

In practice, the method is applicable to realistic models as well.

Non-adiabatic theories of LACM

- Rowe-Bassermann, Marumori, Holzwarth-Yukawa, 1974-
  - Local Harmonic Approach (LHA)
  - Curvature problem
  - Correspondence between, Q,P ↔ Infinitesimal generator, is not guaranteed.

$$\delta\left\langle \Phi(q)\right| H - \frac{\partial V}{\partial q} Q(q) \left| \Phi(q) \right\rangle = 0$$

$$\delta\left\langle \Phi(q)\right| [H, Q(q)] + iM(q)^{-1} P(q) \left| \Phi(q) \right\rangle = 0$$

$$\delta\left\langle \Phi(q)\right| [H, P(q)] - iC(q) Q(q) \left| \Phi(q) \right\rangle = 0$$

- Marumori et al, 1980-
  - Self-consistent collective coordinate (SCC) method
  - The problems of LHA are solved.
  - The SCC equation is solved by the expansion with respect to (q,p).

$$\delta\left\langle \Phi(q,p)\right| \hat{H} - \frac{\partial H}{\partial q}\hat{Q} - \frac{\partial H}{\partial p}\hat{P} \left| \Phi(q) \right\rangle = 0$$

$$H \equiv \left\langle \Phi(q,p)\right| \hat{H} \left| \Phi(q,p) \right\rangle$$

  - “Adiabatic” approx. → LACM (Matsuo, TN, Matsuyanagi, 2000)

Adiabatic Self-consistent Collective Coordinate (ASCC) method

- ASCC: Theory to define a collective submanifold with canonical coordinates. Equations expanded up to 2nd order in collective momenta
  - Collective potential & collective masses
  - leads to the following equations

Constrained mean-field eq.

$$\text{(CMF)}\quad \delta\langle\phi(q)|\hat{H}-(\partial V/\partial q)\hat{Q}(q)|\phi(q)\rangle=0$$

$$\text{(LHE)}\quad \delta\langle\phi(q)|\left[\hat{H}(q),i\hat{Q}(q)\right]-B(q)\hat{P}(q)|\phi(q)\rangle=0$$

Local harmonic eq.

$$\delta\langle\phi(q)|\left[\hat{H}-(\partial V/\partial q)\hat{Q}(q),\hat{P}(q)/i\right]-C(q)\hat{Q}(q)$$

$$-\frac{1}{2B(q)}\left[\left[\hat{H},(\partial V/\partial q)\hat{Q}(q)\right],\hat{Q}(q)\right]|\phi(q)\rangle=0$$

Constrained mean-field calculation

- CMF equation

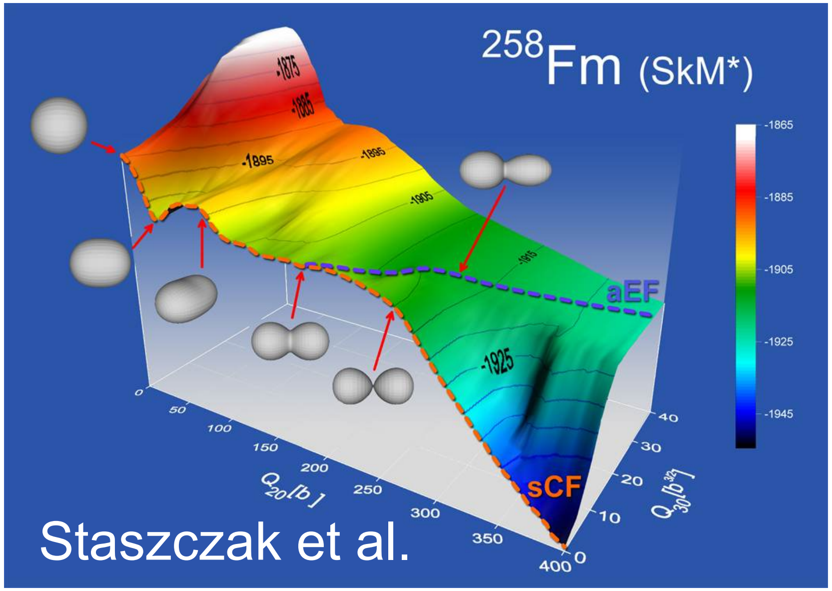
$$\delta\langle\beta|\left(\hat{H}-\lambda\,\hat{Q}\,\right)|\beta\rangle=0,\quad \langle\beta|\hat{Q}\,|\beta\rangle=\beta$$

- Potential energy surface

$$V(\beta)=\langle\beta|\hat{H}|\beta\rangle$$

- Deformed (non-equilibrium) MF states
  - Slater determinants

$$\{|\beta\rangle\}$$



Staszczak et al.

- Next step: Dynamics

GCM & GOA

- Construction of the Hilbert space
  - $\langle \delta\beta | \left(\hat{H} - \lambda \hat{Q} \right) | \beta \rangle = 0$ ➔ Slater determinants $\{|\beta\rangle\}$
- HW eq. to a collective Hamiltonian
  - Generalized eigenvalue problem

$$\int H(\beta,\beta') f(\beta') d\beta' = E \int I(\beta,\beta') f(\beta') d\beta'$$

$$H(\beta,\beta') = \langle \beta | \hat{H} | \beta' \rangle, \quad I(\beta,\beta') = \langle \beta | \beta' \rangle$$

  - Gaussian overlap approx.

$$H(\beta,\beta') \to H_{\mathrm{GOA}}(\beta,\beta') \quad I(\beta,\beta') \to I_{\mathrm{GOA}}(\beta,\beta')$$

$$H_{\mathrm{coll}}(\beta, \partial/\partial\beta)\Psi(\beta) = E\Psi(\beta)$$

  - H_{coll} is constructed from $\hat{H}$, with GOA mass
  - Zero-point energy

$$V(\beta) = \langle \beta | \hat{H} | \beta \rangle + \Delta V(\beta)$$

ASCC method

- ASCC based on the TDVP
  - $\delta\langle\beta|\left(\hat{H}-\lambda\hat{Q}\right)|\beta\rangle=0$ ➔ $V\left(q\right)=H\left(q,p=0\right)=\left\langle\Psi(q)\middle|H\middle|\Psi(q)\right\rangle$
  - $\hat{Q}$ is determined by the local harmonic eq. (LHE)
  - LHE = RPA at the potential minimum
  - LHE (RPA / TV) Mass obtained with $\hat{H}-\lambda\hat{Q}$
  - No zero-point energy $\Delta V\left(q\right)=0$
- Some (non-trivial?) remarks
  - $\hat{Q}$ is not merely the constraint operator
    - LHE Hamiltonian is the one in a moving frame: $\hat{H}-\lambda\hat{Q}$
    - $\hat{Q}(q)=Q_0(q)+\sum_\alpha Q_\alpha^{20}(q)\left(a^+a^+\right)_\alpha+Q_\alpha^{02}(q)\left(aa\right)_\alpha+\boxed{\sum_\mu Q_\mu^{11}(q)\left(a^+a\right)_\mu}$

Trivial example (translation)

- TDHF eq.

$$i\frac{\partial}{\partial t}\rho(t)=\left[h[\rho],\rho(t)\right]$$

- Transformed TDHF $\tilde{\rho}(t)=e^{i\vec{v}t\cdot\vec{p}}\rho(t)e^{-i\vec{v}t\cdot\vec{p}}$

$$\boxed{i\frac{\partial}{\partial t}\tilde{\rho}(t)=\left[h[\tilde{\rho}]-\vec{v}\cdot\vec{p},\tilde{\rho}(t)\right]}$$

  - Quasi-stationary solution in the moving frame

$$\left[h[\tilde{\rho}]-\vec{v}\cdot\vec{p},\tilde{\rho}\right]=0$$

  - Due to Galilean symmetry

$$\tilde{\rho}=e^{im\vec{v}\cdot\vec{r}}\rho_0 e^{-im\vec{v}\cdot\vec{r}} \qquad \mathrm{Tr}\left[\vec{p}\tilde{\rho}\right]=Am\vec{v}$$

  - Intrinsic motion is described by

Equation of collective motion

Marumori et al., PTP 64, 1294 (1980)

- TDHF (TDVP) eq.

$$\delta\left\langle \Psi(t)\right| i\frac{\partial}{\partial t} - H \left|\Psi(t)\right\rangle = 0$$

- Collective variables (q,p)

$$\delta\left\langle \Psi\left(q(t),p(t)\right)\right| i\frac{\partial}{\partial t} - H \left|\Psi\left(q(t),p(t)\right)\right\rangle = 0$$

  - Quasi-stationary states in a moving frame

$$\delta\left\langle \Psi\left(q,p\right)\right| \hat{H} - i\dot{q}\frac{\partial}{\partial q} - i\dot{p}\frac{\partial}{\partial p}\left|\Psi\left(q,p\right)\right\rangle = 0$$

- Basic eq. of the SCC method $\quad \dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}$

$$\delta\left\langle \Psi\left(q,p\right)\right| \hat{H} - \frac{\partial H}{\partial p}\hat{P} - \frac{\partial H}{\partial q}\hat{Q}\left|\Psi\left(q,p\right)\right\rangle = 0 \qquad \left\langle \Psi\left(q,p\right)\right|\left[\hat{Q},\hat{P}\right]\left|\Psi\left(q,p\right)\right\rangle = i$$

Determined by LHE

  - Translational case

$$\delta\left\langle \Psi\left(q,p\right)\right| \hat{H} - \vec{v}\cdot\vec{P}\left|\Psi\left(q,p\right)\right\rangle = 0 \qquad \dot{\vec{R}} = \vec{v}, \quad \dot{\vec{P}} = 0$$

TDHF(B) → Classical Hamilton's form

Blaizot, Ripka, "Quantum Theory of Finite Systems" (1986)
Yamamura, Kuriyama, Prog. Theor. Phys. Suppl. 93 (1987)

The TDHF(B) equation can be described by the classical form.

For instance, using the Thouless form

$$\left|z\right\rangle = \exp\left(\frac{1}{2} z_{ph} c_p^+ c_h\right)\left|\Phi_0\right\rangle$$

The TDHF(B) equation becomes in a form

$$i\dot{z} = 2(1+zz^+)\frac{\partial H}{\partial z^+}(1+z^+z)$$

$$i\dot{z}^+ = -2(1+z^+z)\frac{\partial H}{\partial z}(1+zz^+)$$

$$H(z,z^+) = \frac{\left\langle z\right|H\left|z\right\rangle}{\left\langle z|z\right\rangle} = H\left(\xi,\pi\right)$$

The Holstein-Primakoff-type mapping $\left(\xi + i\pi\right)_{ph}\Big/\sqrt{2} = \left[z(1+z^+z)^{1/2}\right]_{ph}$

$$\dot{\xi}^{ph} = \frac{\partial H}{\partial \pi_{ph}}$$

$$\dot{\pi}_{ph} = -\frac{\partial H}{\partial \xi^{ph}}$$

Harmonic approximation in TDHF

Small fluctuation around the HF state

$$\langle \xi,\pi | H | \xi,\pi \rangle = \langle \Phi_0 | H | \Phi_0 \rangle + \frac{1}{2} \left\langle \left(c_p^+ c_h , c_h^+ c_p \right) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} c_h^+ c_p \\ c_p^+ c_h \end{pmatrix} \right\rangle$$

In terms of classical variables $(\xi^\alpha , \pi_\alpha)$ ph index $\alpha = (ph)$

$$\langle \xi,\pi | H | \xi,\pi \rangle = E_0 + \frac{1}{2} \left(\rho_{ph}, \rho_{hp} \right) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \rho_{hp} \\ \rho_{ph} \end{pmatrix}, \quad \rho_\alpha \approx \frac{1}{\sqrt{2}} \left(\xi^\alpha + i\pi_\alpha \right)$$

$$= E_0 + \frac{1}{2} B^{\alpha\beta} \pi_\alpha \pi_\beta + \frac{1}{2} C_{\alpha\beta} \xi^\alpha \xi^\beta \qquad B^{\alpha\beta} = \left. \frac{\partial H}{\partial \pi_\alpha \partial \pi_\beta} \right|_{\pi=0,\xi=\xi_0}$$

$$= E_0 + \frac{1}{2} \sum_n \left[p_\mu^2 + \omega_n^2 (q^\mu)^2 \right] \qquad C_{\alpha\beta} = \left. \frac{\partial H}{\partial \xi_\alpha \partial \xi_\beta} \right|_{\pi=0,\xi=\xi_0}$$

Linear point transformation $(\xi^\alpha , \pi_\alpha) \rightarrow (q^\mu , p_\mu)$ $H(\xi^\alpha , \pi_\alpha) \rightarrow \bar{H}(q^\mu , p_\mu)$

$$q^\mu = \sqrt{\frac{1}{\omega_\mu}} \sum_\alpha \left(X^\mu + Y^\mu \right)_\alpha \xi^\alpha , \quad p_\mu = \sqrt{\omega_\mu} \sum_\alpha \left(X^\mu - Y^\mu \right)_\alpha \pi_\alpha$$

$$\delta^{\mu\nu} = \frac{\partial q^\mu}{\partial \xi^\alpha} (A-B)^{\alpha\beta} \frac{\partial q^\nu}{\partial \xi^\beta} , \quad \omega_\mu^2 \delta^{\mu\nu} = \frac{\partial \xi^\alpha}{\partial q^\mu} (A+B)_{\alpha\beta} \frac{\partial \xi^\beta}{\partial q^\nu}$$

Harmonic approximation at non-equilibriums

Second derivatives

$$\left.\frac{\partial^2 H}{\partial\xi^\alpha\partial\xi^\beta}\right|_\Sigma = \left.\frac{\partial^2 \bar{H}}{\partial\left(q^c\right)^2}\frac{\partial q^c}{\partial\xi^\alpha}\frac{\partial q^c}{\partial\xi^\beta}\right|_\Sigma + \left.\frac{\partial \bar{H}}{\partial q^c}\frac{\partial^2 q^c}{\partial\xi^\alpha\partial\xi^\beta}\right|_\Sigma$$

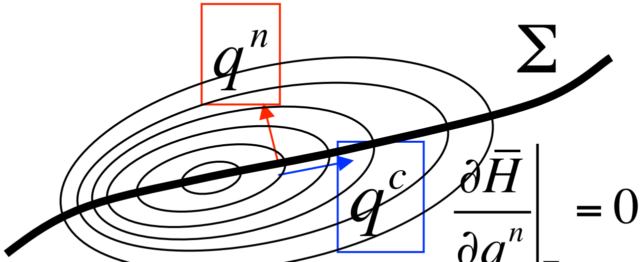
Curvature

$$\left.C_{\alpha\beta}\right|_\Sigma = \left.\frac{\partial^2 H}{\partial\xi^\alpha\partial\xi^\beta}\right|_\Sigma - \left.\frac{\partial \bar{H}}{\partial q^c}\frac{\partial^2 q^c}{\partial\xi^\alpha\partial\xi^\beta}\right|_\Sigma$$

Mass

$$\left.B^{\alpha\beta}\right|_\Sigma = \left.\frac{\partial^2 H}{\partial\pi_\alpha\partial\pi_\beta}\right|_\Sigma - \left.\frac{\partial \bar{H}}{\partial q^c}\frac{\partial^2 q^c}{\partial\pi_\alpha\partial\pi_\beta}\right|_\Sigma$$

Second derivative are NOT tensors.



$$\left.\frac{\partial \bar{H}}{\partial q^n}\right|_\Sigma = 0$$

$$\Sigma : \left(q^c, q^n = 0; p_c = p_n = 0\right)$$

Metric tensor $K_{\alpha\beta} = \sum_\mu \frac{\partial q^\mu}{\partial\xi^\alpha}\frac{\partial q^\mu}{\partial\xi^\beta}$

$$\Gamma^\gamma_{\alpha\beta} \equiv \frac{1}{2}K^{\gamma\delta}\left(K_{\delta\alpha,\beta} + K_{\delta\beta,\alpha} - K_{\alpha\beta,\delta}\right) = g^\gamma_{,\mu} f^\mu_{,\alpha\beta}$$

Affine connection

$$C_{\alpha\beta} = \nabla_{\alpha\beta} H \equiv \frac{\partial^2 H}{\partial\xi^\alpha\partial\xi^\beta} - \Gamma^\gamma_{\alpha\beta}\frac{\partial H}{\partial\xi^\gamma}$$

With this metric, the *collective* space is assumed to be “flat”.

Separation of Nambu-Goldstone modes

TN, Walet, DoDang, PRC61 (1999) 014302

TN, PTEP 2012 (2012) 01A207

Cyclic variable (sym. op.) $\langle \Psi(t) | S | \Psi(t) \rangle = q^s \left(\xi(t), \pi(t) \right)$ or $p_s \left(\xi(t), \pi(t) \right)$

(1) Symmetry operator *S* = momentum

(2) Symmetry operator *S* = coordinate

$$\left[\hat{S}, \hat{H} \right] = 0 \Rightarrow \begin{cases} \{ p_s, H \}_{\mathrm{PB}} = 0 \quad \Rightarrow \quad \dfrac{\partial p_s}{\partial \pi_\alpha} \dfrac{\partial H}{\partial \xi^\alpha} = 0 \quad \Rightarrow \quad C_{\alpha\beta} \dfrac{\partial \xi^\alpha}{\partial q^s} = 0 \\ \{ q^s, H \}_{\mathrm{PB}} = 0 \Rightarrow \dfrac{\partial q^s}{\partial \xi^\alpha} \dfrac{\partial^2 H}{\partial \pi_\alpha \partial \pi_\beta} - \dfrac{\partial^2 q^s}{\partial \pi_\alpha \partial \pi_\beta} \dfrac{\partial H}{\partial \xi^\alpha} = 0 \Rightarrow B^{\alpha\beta} \dfrac{\partial q^s}{\partial \xi^\alpha} = 0 \end{cases}$$

$$\therefore \; B^{\alpha\gamma} C_{\gamma\beta} \frac{\partial q^s}{\partial \xi^\alpha} = B^{\alpha\gamma} C_{\gamma\beta} \frac{\partial \xi^\beta}{\partial q^s} = 0$$

The Nambu-Goldstone modes become zero modes and are separated from the other modes.

Local harmonic eq. in ASCC

Hinohara et al, PTP 117 (2007) 451

TN, Walet, DoDang, PRC61 (1999) 014302

Local Harmonic equation determines the normal modes:

$$B^{\alpha\gamma}C_{\gamma\beta}\frac{\partial\xi^{\beta}}{\partial q^{c}}=\omega^{2}\frac{\partial\xi^{\alpha}}{\partial q^{c}} \qquad B^{\alpha\gamma}C_{\gamma\beta}\frac{\partial q^{c}}{\partial\xi^{\alpha}}=\omega^{2}\frac{\partial q^{c}}{\partial\xi^{\beta}}$$

(1) Invariant property under the transformation:

$$q^{c}\Rightarrow q^{c}+cq^{s},\ p^{s}\Rightarrow p^{s}+cp^{c}$$

$$\frac{\partial\bar{V}}{\partial q^{s}}\Rightarrow\frac{\partial\bar{V}}{\partial q^{s}}-c\frac{\partial\bar{V}}{\partial q^{c}}$$

Requires a “gauge” fixing of “*c*”.

(2) Strong canonicity condition (*prescription*)

Problem

$[\hat{Q}(q),\hat{S}]=0$ to determine $\dfrac{\partial^{2}q}{\partial\xi^{\alpha}\partial\xi^{\beta}}$ and $\dfrac{\partial^{2}q}{\partial\pi_{\alpha}\partial\pi_{\beta}}$

These quantities correspond to $a^{+}a$-part (pp-, hh-part) of $\hat{Q}$ and $\hat{S}$

Adiabatic SCC (Symplectic LHE) — Applications to simple models —

- More realistic applications have been done with the P+Q Hamiltonian.
  - Hinohara et al., PTP **119**, 59 (2008); PRC **80**, 044301 (2009); PRC **82**, 064313 (2010); PRC **85**, 024323 (2012)
  - Sato et al., NPA **849**, 53 (2911), PRC 86, **86,** 024316 (2012)

Applications to O(4) models

Model Hamiltonian

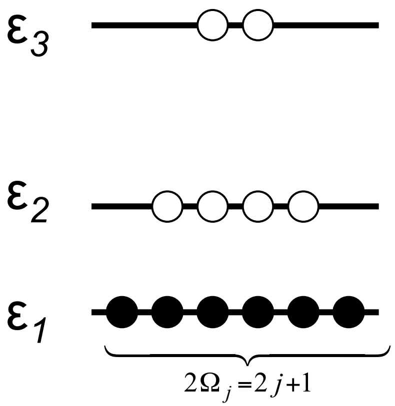
Source of T-odd mean fields

Monopole + “Quadrupole” pairing + “Quadrupole” int.

$$H = h_0 - \frac{1}{2} G_0 \left(P_0^+ P_0 + P_0 P_0^+ \right) - \frac{1}{2} G_2 \left(P_2^+ P_2 + P_2 P_2^+ \right) - \frac{1}{2} \chi Q^2$$

$$P_0 \equiv \sum_j \sum_{m>0} c_{j-m} c_{jm} , \quad P_2 \equiv \sum_j \sum_{m>0} \sigma_{jm} c_{j-m} c_{jm} , \quad Q \equiv \sum_j d_j \sum_m \sigma_{jm} c_{jm}^+ c_{jm}$$

$$\sigma_{jm} = \begin{cases} 1 & |m| < \Omega_j / 2 \\ -1 & |m| > \Omega_j / 2 \end{cases}$$



Parameters

$$\varepsilon_1 = 0, \varepsilon_2 = 1.0, \varepsilon_3 = 3.5$$

$$d_1 = 2.0, d_2 = 1.0, d_3 = 1.0$$

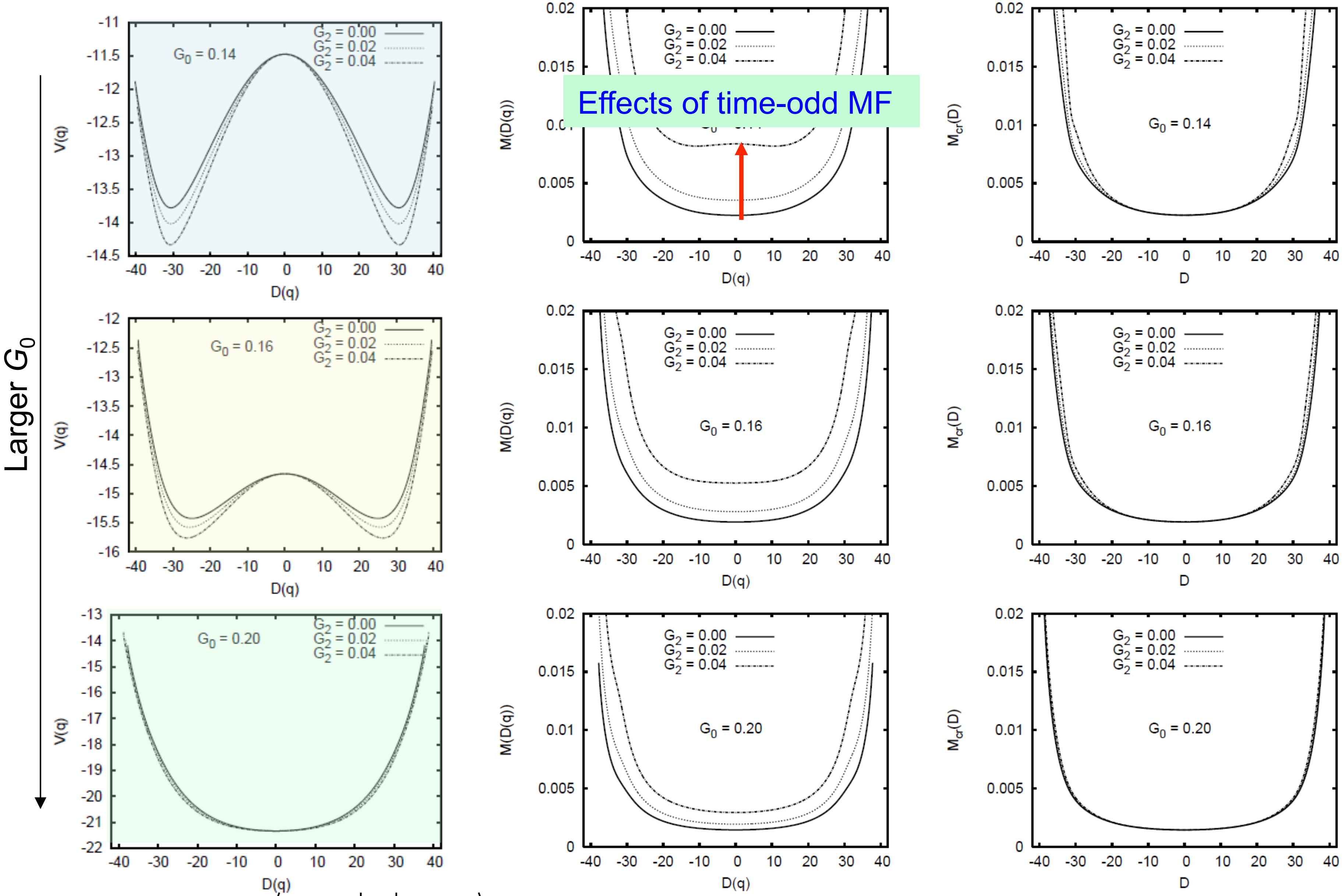
$$\Omega_1 = 14, \Omega_2 = 10, \Omega_3 = 4$$

Hinohara, TN, Matsuo, Matsuyanagi, PTP115 (2006) 567

Potential

Mass: $M=1/B$

Cranking Mass



Larger G_0

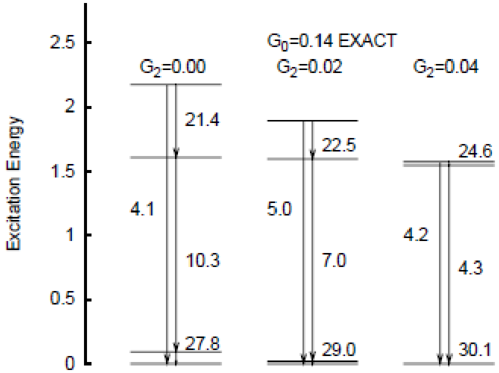
Effects of time-odd MF

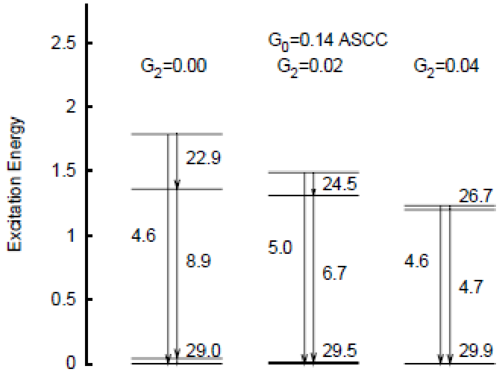
$$D(q) \equiv \langle \phi(q) | Q | \phi(q) \rangle$$

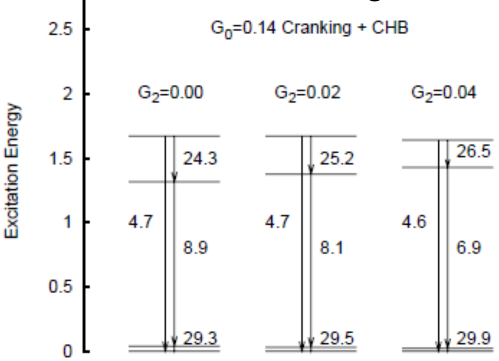
Exact

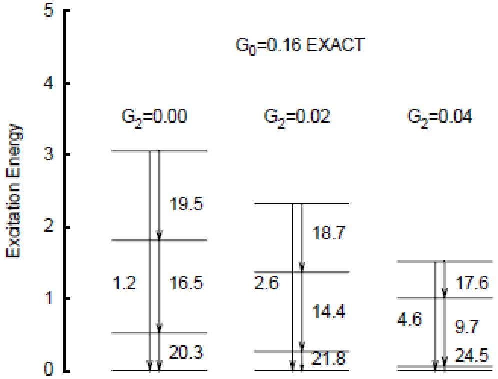
Adiabatic SCC

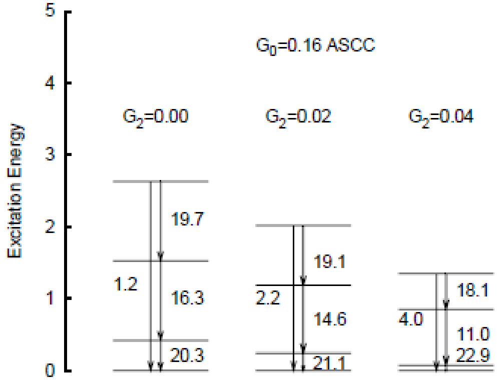
CHB with $M_{cranking}$

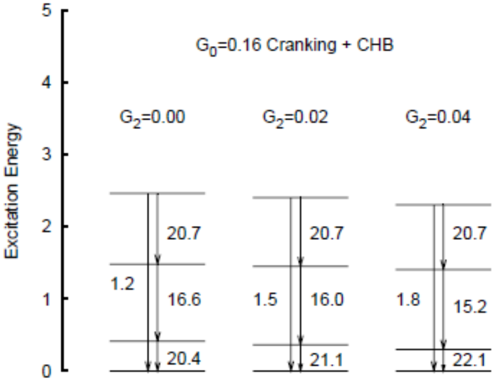


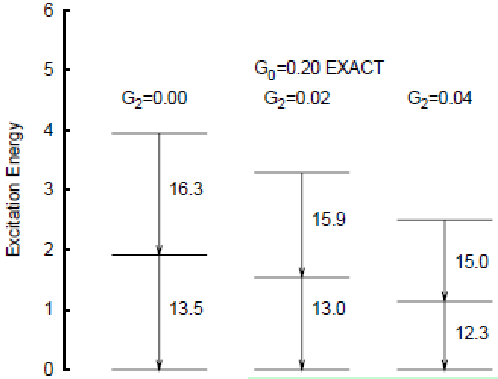


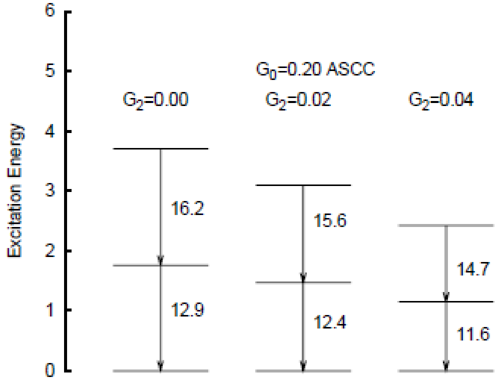


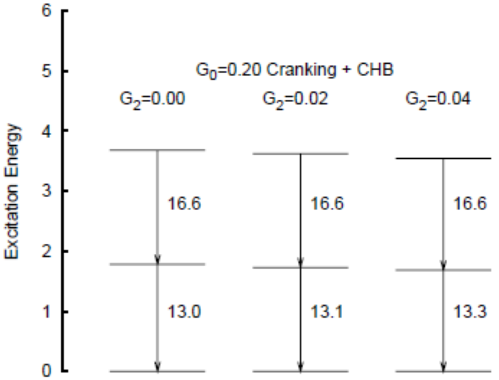












Time-odd effects are neglected in the cranking mass !

Curvature effects

$$\hat{Q}(q) = \sum_{\mu\nu} Q^{A}_{\mu\nu}\left(a^{+}_{\mu}a^{+}_{\nu} + \text{h.c.}\right) + \boxed{\sum_{\mu\nu} Q^{B}_{\mu\nu} a^{+}_{\mu} a_{\nu}}$$

$$\updownarrow$$

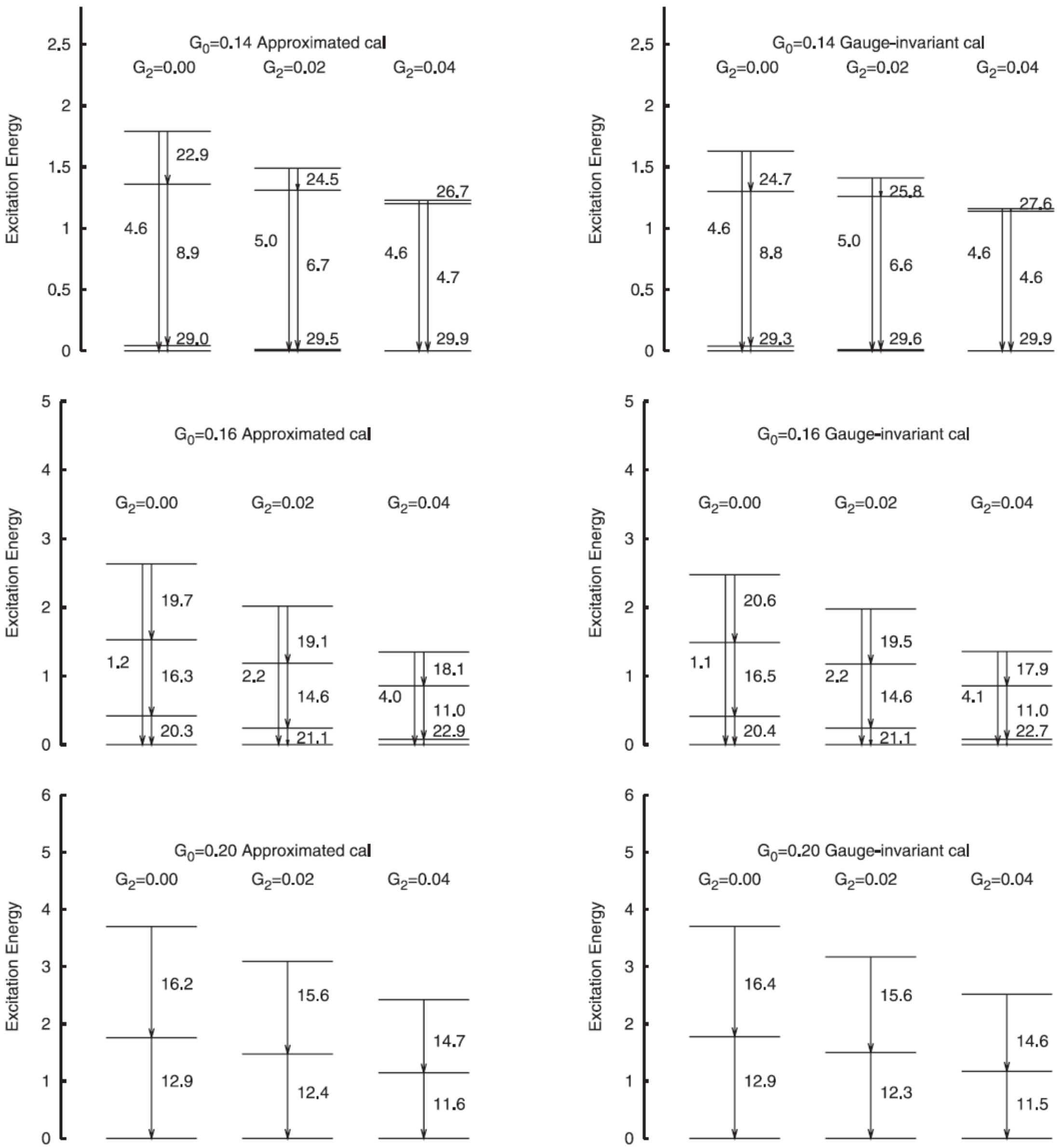
$$\boxed{\frac{\partial q}{\partial \xi^{\alpha} \partial \xi^{\beta}}, \frac{\partial q}{\partial \pi_{\alpha} \partial \pi_{\beta}}}$$

In this model, requiring the gauge invariance, we can determine them.

The curvature effects are weak.

Neglected calc

Full calc



Model of protons and neutrons

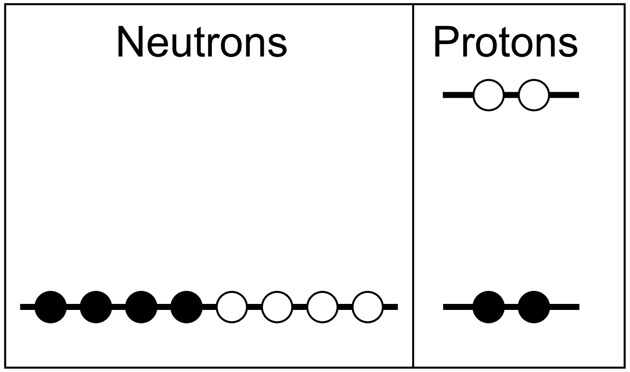
T.N. & Walet, PRC58 (1998) 3397

$$H = H_n + H_p + H_{np} ,$$

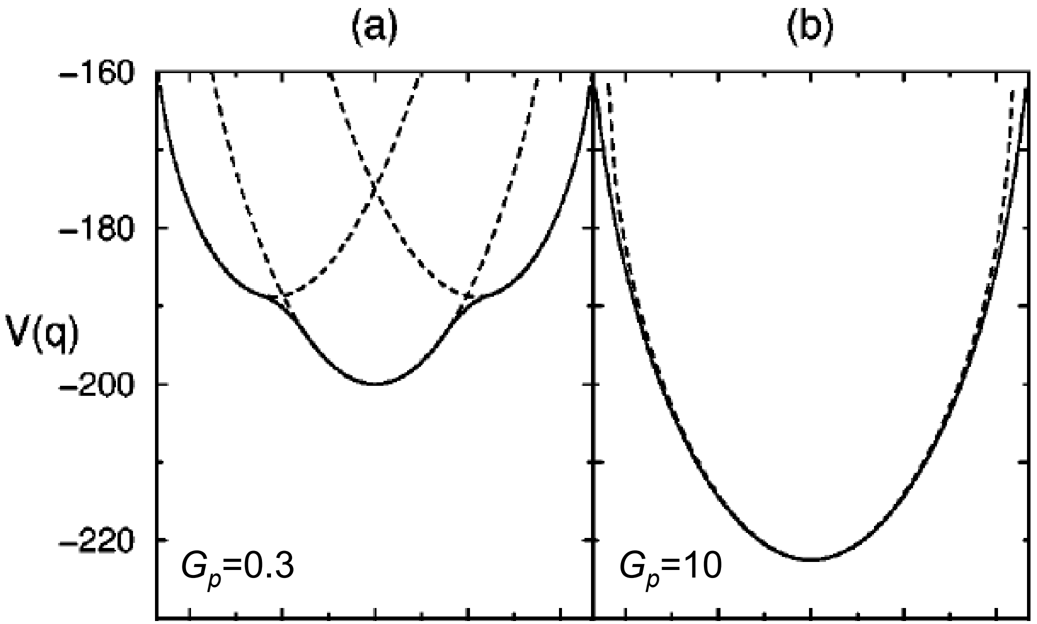
$$H_n = \sum_{i \in n, m_i} \epsilon_i c^\dagger_{j_i m_i} c_{j_i m_i} - G_n P^\dagger_n P_n - \tfrac{1}{2} \kappa Q_n^2 ,$$

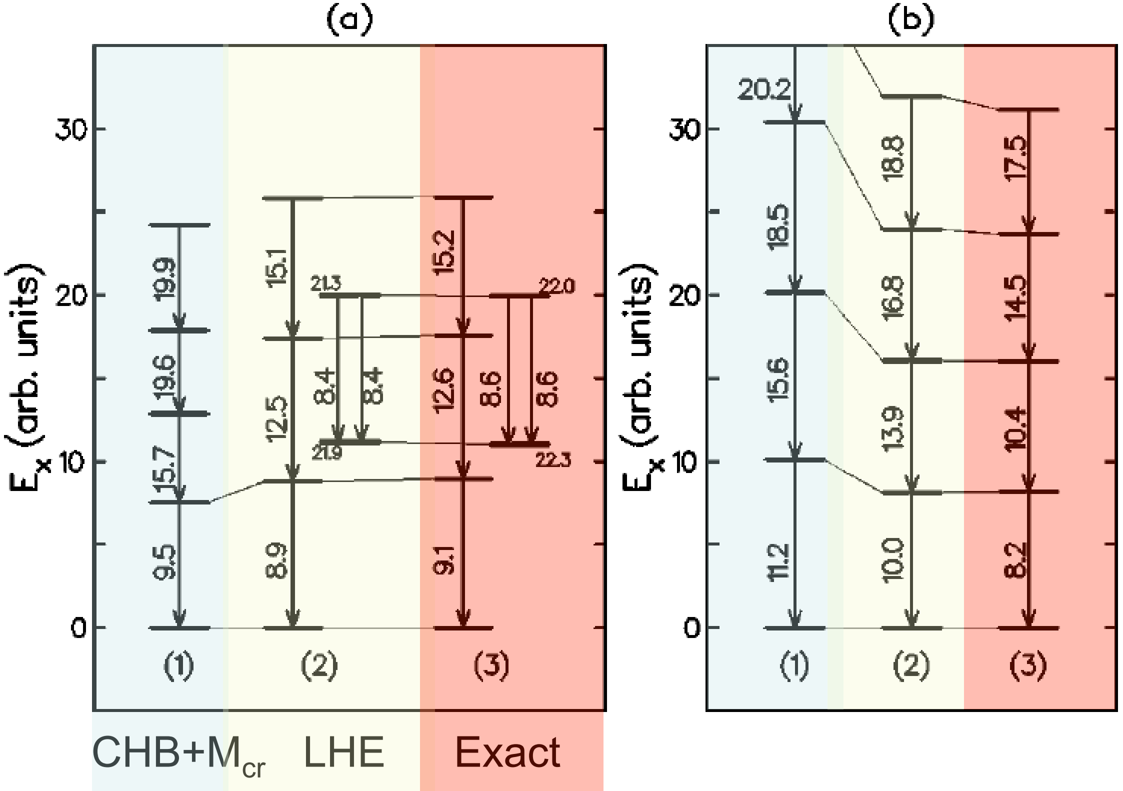
$$H_p = \sum_{i \in p, m_i} \epsilon_i c^\dagger_{j_i m_i} c_{j_i m_i} - G_p P^\dagger_p P_p - \tfrac{1}{2} \kappa Q_p^2 ,$$

$$H_{np} = - \kappa Q_n Q_p ,$$



Upper orbital has a larger quadrupole moment



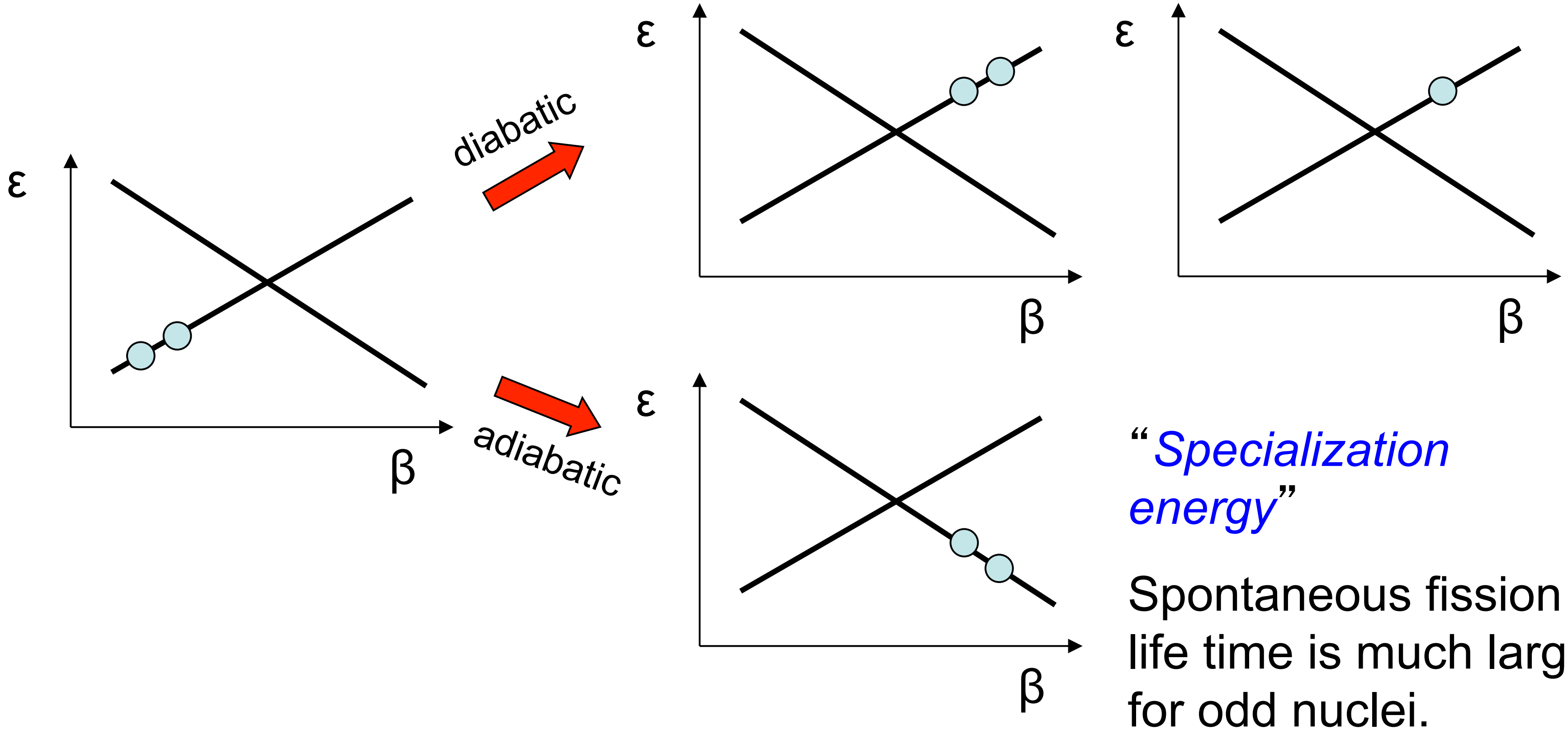


Adiabatic vs Diabatic Dynamics

Review: Nazarewicz, NPA557 (1993) 489c

The problem has been discussed since the paper by Hill and Wheeler (1953)

The pairing interaction plays a key role for configuration changes at level crossings.



"*Specialization energy*"

Spontaneous fission life time is much larger for odd nuclei.

Summary

- Adiabatic Self-consistent Collective Coordinate (ASCC) method to derive a collective submanifold and to determine the collective mass & potential.
- Difference between ASCC & GCM
  - Zero-point energy (=0 and ≠0)
  - Collective mass (RPA and GOA)
  - Hamiltonian ($H\text{-}\lambda Q$ and H)
- Applications to multi-O(4) model
  - ASCC vs Exact
  - ASCC vs GCM vs GOA vs Exact

- Consistent calculation is desired for comparison between these GCM & ASCC (ATDHFB).

Questions

- Can we justify the use of $H - \lambda\hat{Q}$ in GCM/GOA?
- Perhaps, the small-amplitude limit is easy.
  - Small-amplitude HF+GCM/GOA with complex generator coordinates of all ph-degrees of freedom reduces to RPA (Jancovici & Schiff, (1964))
  - Then, how about the HFB+GCM?
  - Does it reduce to QRPA?
  - Where does the effect of $-\lambda\hat{N}$ come from?