Sum rule and Giant Resonances

Sum rule and giant resonances

Giant resonances are typical collective modes of excitation at high energy, and exhaust major portion of the sum rule

Isoscalar (T=0)	Monopole (0^+)	$f_\lambda(r)Y_{\lambda\mu}$
	Quadrupole (2^+)	
	Octupole (3^-)	
Isovector (T=1)	Monopole (0^+)	$\tau_i f_\lambda(r)Y_{\lambda\mu}$
	Dipole (1^-)	
	Quadrupole (2^+)	
	Gamow-Teller (1^+)	$\tau_i \sigma_j f_0(r)$
	Spin-monopole (1^+)	$\tau_i f_0(r)\left(\vec{\sigma} \times Y_1\right)_{I\mu}$
	Spin-dipole (0^-, 1^-, 2^-)	

Sum rule

$$m_1 = \sum_n E_n \left| \langle n | F | 0 \rangle \right|^2 \quad \Rightarrow \quad \text{(Energy - weighted) Sum Rule}$$

$$m_p = \sum_n E_n^p \left| \langle n | F | 0 \rangle \right|^2$$

Odd-*p* moments can be expressed by the ground-state expectation value.

$$m_1 = \sum_n E_n \left| \langle n | F | 0 \rangle \right|^2 = \frac{1}{2} \langle 0 | [F,[H,F]] | 0 \rangle$$

$$m_p = \sum_n E_n^p \left| \langle n | F | 0 \rangle \right|^2 = \frac{1}{2} \langle 0 | [[F,H],[H,[H,F]]] | 0 \rangle$$

If $\hat{F} = \sum_i f(\vec{r}_i)$ and the Hamiltonian does not have momentum dependence,

$$m_1 = \frac{1}{2m} \langle 0 | \sum_{i=1}^{A} (\nabla f)_i^2 | 0 \rangle$$

$$m_3 = \frac{1}{2} \left(\frac{2}{m} \right)^2 \frac{\partial^2}{\partial \eta^2} E(\eta) \Big|_{\eta = 0}, \quad E(\eta) = \langle 0 | e^{-\eta G} H e^{\eta G} | 0 \rangle, \quad G = -\frac{m}{2} [H,F]$$

Physical meaning of sum rule

Nucles under an impulse external field

$$V(t) = F\delta(t) = \delta(t)\sum_{i=1}^{A} f(\vec{r}_i)$$

Nucleons *i* change its momentum by $\Delta\vec{p}_i = -\nabla_i f(\vec{r}_i)$

The nucleon at t<0 has zero velocity expectation value, then this field creates the velocity field:

$$\vec{v}(\vec{r}) = -\frac{\nabla f(\vec{r})}{m}$$

Energy transferred to nucleon i is $\Delta\varepsilon_i = \frac{\left|\nabla_i f(\vec{r}_i)\right|^2}{2m}$

Thus, the energy weighted sum rule has the following physical meaning.

$$\sum_n E_n \left|\langle n|F|0\rangle\right|^2 = \frac{1}{2m}\langle 0|\sum_{i=1}^{A}(\nabla f)_i^2|0\rangle$$

The energy absorbed by nucleus:

(Exc. energy) x (probability)

The energy transferred to nucleons in the nucleus

Meaing of m_3

$$m_3 = \frac{1}{2}\left(\frac{2}{m}\right)^2 \frac{\partial^2}{\partial \eta^2} E(\eta)\Big|_{\eta=0}$$

$$E(\eta) = \left\langle 0 \left| e^{-\eta G} H e^{\eta G} \right| 0 \right\rangle, \quad G = -\frac{m}{2}[H, F]$$

If $f(\vec{r}) = r^\lambda Y_{\lambda\mu}(\hat{r})$ and the Hamiltonian does not have momentum dependence,

$$G = -\frac{m}{2}[H, F] = \frac{1}{2}\sum_i \left(\nabla r^\lambda Y_{\lambda\mu}(\hat{r})\right)_i \cdot \nabla_i$$

The state $e^{\eta G}\left|0\right\rangle$ introduces the velocity field $\vec{v}(\vec{r}) \sim \nabla r^\lambda Y_{\lambda\mu}(\hat{r})$

Its energy curvature with respect to the “deformation” is directly related to m_3.

*E*1 sum rule

Isovector dipole operator

"E1 recoil charge"

$$\hat{F} = e\sum_{i=1}^{A} (\tau_z)_i \left(z_i - R_z\right) = \sum_{i=1}^{N} \frac{Ze}{A} z_i - \sum_{i=N+1}^{N+Z} \frac{Ne}{A} z_i$$

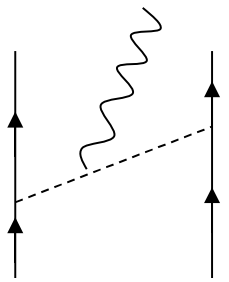
Assuming the ground state has I=0,

$$m_1 = \frac{NZ}{2Am}(1+\kappa)$$

The interaction usually contains the isospin-dependent terms.

$$\kappa > 0$$

This includes effects of meson exchange current.



$\kappa = 0 \Rightarrow$ Thomas-Reiche-Kuhn (TRK) sum rule

Isoscalar giant resonance

$$\hat{F} = \sum_i f(\vec{r}_i) \qquad f(\vec{r}) = r^\lambda Y_{\lambda 0}(\hat{r})$$

The previous formulae lead to

$$m_1 = \frac{1}{2m}\frac{\lambda(2\lambda+1)}{4\pi}\left\langle 0\left|\sum_{i=1}^{A} r_i^{2\lambda-2}\right|0\right\rangle, \quad m_3 = \frac{1}{2}\left(\frac{2}{m}\right)^2 \frac{\partial^2}{\partial\eta^2} E(\eta)\Big|_{\eta=0}$$

$$E(\eta) = \left\langle 0\left|e^{-\eta G} H e^{\eta G}\right|0\right\rangle, \quad G = \frac{1}{2}\sum_{i=1}^{A}\left((\nabla r^\lambda Y_{\lambda 0})\cdot\nabla\right)_i$$

For instance, for the quadrupole operator,

$$m_3 = \frac{1}{2}\left(\frac{2}{m}\right)^2 \frac{5}{16\pi}\cdot 8\langle T\rangle$$

<*T*>: Kinetic energy expectation value

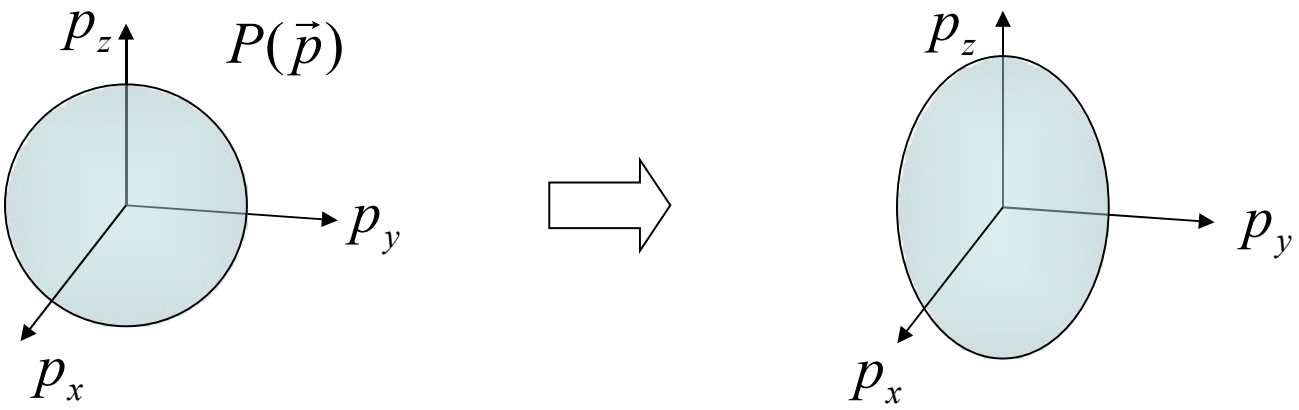
Giant quadrupole resonance energy

$$\omega_{2^+}^2 \sim \frac{m_3}{m_1} = \frac{4\langle T\rangle}{mA\langle r^2\rangle} \approx 2\omega_0, \quad \left(\because \langle T\rangle \approx m\omega_0^2 A\langle r^2\rangle/2\right)$$

Fermi Liquid Properties

$$m_3 \propto \frac{1}{2}\frac{\partial^2}{\partial \eta^2} E(\eta)\Big|_{\eta=0} \propto \langle T \rangle$$

The density change of the ISGQR is a surface type, however, the restoring force for ISGQR originates from the kinetic energy.



The vibration leads to a deformation in the momentum distribution

This is different from low-lying surface vibrations and different from the classical (incompressible) liquid model.

Four-current sum rule

Suzuki, Rowe, NPA286 (1977) 307.

Suzuki, Prog. Theor. Phys. 64 (1980) 1627.

$$\sum_n \langle 0|\vec{j}(\vec{r})|n\rangle\langle n|\rho(\vec{r}')|0\rangle = -\frac{i}{2m}\rho_0(\vec{r})\nabla\,\delta(\vec{r}-\vec{r}')$$

Using the continuity equation $\nabla\cdot\vec{j}(\vec{r}) = i[\rho(\vec{r}), H]$

and a property of the density operator $\int \rho(\vec{r}) f(\vec{r}) d\vec{r} = \sum_{i=1}^{A} f(r_i)$

we can obtain the energy-weighted sum rule for the density operator

$$\sum_n E_n \langle 0|\rho(\vec{r})|n\rangle\langle n|F|0\rangle = -\frac{1}{2m}\nabla\cdot\rho_0(\vec{r})\nabla f(\vec{r})$$

The normal m_1 sum rule can be easily derived from this formula.

Taking the photoexcitation operator $f(\vec{r}) = r^\lambda Y_{\lambda 0}(\hat{r})$

$$\sum_n E_n \langle 0|\rho(\vec{r})|n\rangle\langle n|F|0\rangle = -\frac{\lambda}{2m} r^{\lambda-1}\frac{d\rho_0}{dr} Y_{\lambda\mu}(\hat{r})$$

$$\langle 0|\rho(\vec{r})|n\rangle \sim r^{\lambda-1}\frac{d\rho_0}{dr} Y_{\lambda\mu}(\hat{r})$$

Transition density of the Tassie model for the giant resonance

Time-Dependent Density Functional Theory (TDDFT)

Basic ideas of the unified (collective) model

- Nucleons are *independently* moving in a potential that *slowly* changes.
  - Collective motion induces oscillation/rotation of the potential.
  - The fluctuation of the potential changes the nucleonic single-particle motion.

Consistent with the idea of

Time-Dependent Mean-Field Theory

or

Time-Dependent Density-Functional Theory

Time-dependent density-functional theory (TDDFT)

- Basic theorem of DFT (Hohenberg-Kohn)
- Basic theorem of TDDFT (Runge-Gross)
- Perturbative regime: Linear response and random-phase approximation
  - Matrix formulation
  - Green's function method
  - Real-time method
  - Finite amplitude method
- Non-perturbative regime
  - Theories of large-amplitude collective motion

Density Functional Theory

- Quantum Mechanics
  - Many-body wave functions;

$$\Psi\ (\vec{r}_1, \cdots, \vec{r}_N)$$

- Density Functional Theory
  - Density clouds;

$$F[\rho\ (\vec{r})]$$

The many-particle system can be described by a functional of density distribution in the three-dimensional space.

Hohenberg-Kohn Theorem (1)

The first theorem

Hohenberg & Kohn (1964)

Density ρ(r) determines $v(\boldsymbol{r})$,

except for arbitrary choice of zero point.

A system with a one-body potential $v(\vec{r})$

$$H_v \Psi_{gs}^{v} = E_{gs}^{v} \Psi_{gs}^{v}$$

$$H_v = H + \sum_i v(\vec{r}_i)$$

$$= \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} w(\vec{r}_i, \vec{r}_j) + \sum_i v(\vec{r}_i)$$

Existence of one-to-one mapping: $v(\vec{r}) \leftrightarrow \Psi_v^{gs} \leftrightarrow \rho_v(\vec{r})$

Strictly speaking, one-to-one or one-to-none

v-representative

① $v(\vec{r}) \leftrightarrow \Psi_{gs}^{v}$ Here , we assume the non-degenerate g.s.

Reductio ad absurdum: Assuming

different $v(\vec{r})$ and $v'(\vec{r})$ produces the same ground state Ψ_{gs}^{v}

$$(H + V)\Psi_{gs}^{v} = E_{gs}^{v}\Psi_{gs}^{v} \qquad V = \sum_i v(\vec{r}_i)$$

$$-) \quad (H + V')\Psi_{gs}^{v} = E_{gs}^{v'}\Psi_{gs}^{v} \qquad V' = \sum_i v'(\vec{r}_i)$$

$$(V - V')\Psi_{gs}^{v} = (E_{gs}^{v} - E_{gs}^{v'})\Psi_{gs}^{v}$$

V and V' are identical except for constant. → Contradiction

② $\Psi^{v}_{gs} \leftrightarrow \rho_v$

$$(H+V)\Psi^{v}_{gs} = E^{v}_{gs}\Psi^{v}_{gs}$$

$$(H+V')\Psi^{v'}_{gs} = E^{v'}_{gs}\Psi^{v'}_{gs}$$

Again, *reductio ad absurdum*

assuming different states $\Psi^{v}_{gs}, \Psi^{v'}_{gs}$ with $v(\vec{r}), v'(\vec{r})$ produces the same density ρ_v

$$E^{v}_{gs} = \left\langle \Psi^{v}_{gs} \middle| H+V \middle| \Psi^{v}_{gs} \right\rangle$$

$$< \left\langle \Psi^{v'}_{gs} \middle| H+V \middle| \Psi^{v'}_{gs} \right\rangle$$

$$E^{v}_{gs} < E^{v'}_{gs} + \int d\vec{r}\left[v(\vec{r}) - v'(\vec{r})\right]\rho_v(\vec{r})$$

$$H+V = H+V'+(V-V')$$

$$\left\langle \Psi^{v}_{gs} \middle| V \middle| \Psi^{v}_{gs} \right\rangle = \int d\vec{r}\, v(\vec{r})\rho_v(\vec{r})$$

Replacing V ↔ V'

$$E^{v'}_{gs} < E^{v}_{gs} + \int d\vec{r}\left[v'(\vec{r}) - v(\vec{r})\right]\rho_v(\vec{r})$$

$$\therefore\ E^{v}_{gs} + E^{v'}_{gs} < E^{v}_{gs} + E^{v'}_{gs}$$ Contradiction !

Here, we assume that the density ρ_v is v-representative.

For degenerate case, we can prove one-to-one $v(\vec{r}) \leftrightarrow \rho_v(\vec{r})$

Hohenberg-Kohn Theorem (2)

The second theorem

There is a energy density functional and the variational principle determines energy and density of the ground state.

Any physical quantity must be a functional of density.

From theorem (1) $v(\vec{r}) \leftrightarrow \Psi_{gs}^{v} \leftrightarrow \rho_{v}$

➡ Many-body wave function $\Psi\left[\rho\left(\vec{r}\right)\right]$ is a functional of densityρ(**r**).

Energy functional for external potential *v* (***r***)

$$E_v[\rho] \equiv \langle \Psi[\rho] | H + V | \Psi[\rho] \rangle$$

$$E_v[\rho_v] = E_v^{gs} < E_v[\rho]$$

Variational principle holds for v-representative density

$$E_v[\rho] = F_{HK}[\rho] + \int \rho(\vec{r}) v(\vec{r}) d\vec{r}$$

$F_{HK}[\rho]$: v-independent universal functional

The following variation leads to all the ground-state properties.

$$\delta \left\{ F[\rho] + \int \rho(\vec{r}) v(\vec{r}) d\vec{r} - \mu \left(\int \rho(\vec{r}) d\vec{r} - N \right) \right\} = 0$$

In principle, any physical quantity of the ground state should be a functional of density.

Variation with respect to many-body wave functions $\Psi(\vec{r}_1, \cdots, \vec{r}_N)$

↓

Variation with respect to one-body density $\rho(\vec{r})$

↓

Physical quantity $A[\rho(\vec{r})] = \left\langle \Psi[\rho] \middle| \hat{A} \middle| \Psi[\rho] \right\rangle$

v-representative⟶ N-representative

Levy (1979, 1982)

The “N-representative density” means that it has a corresponding many-body wave function.

Ritz’ Variational Principle

$$\mathrm{Min}\left\langle \Psi\left(r_1,..,r_N\right)\middle|H\middle|\Psi\left(r_1,..,r_N\right)\right\rangle \Rightarrow \Psi_{gs}\left(r_1,..,r_N\right)$$

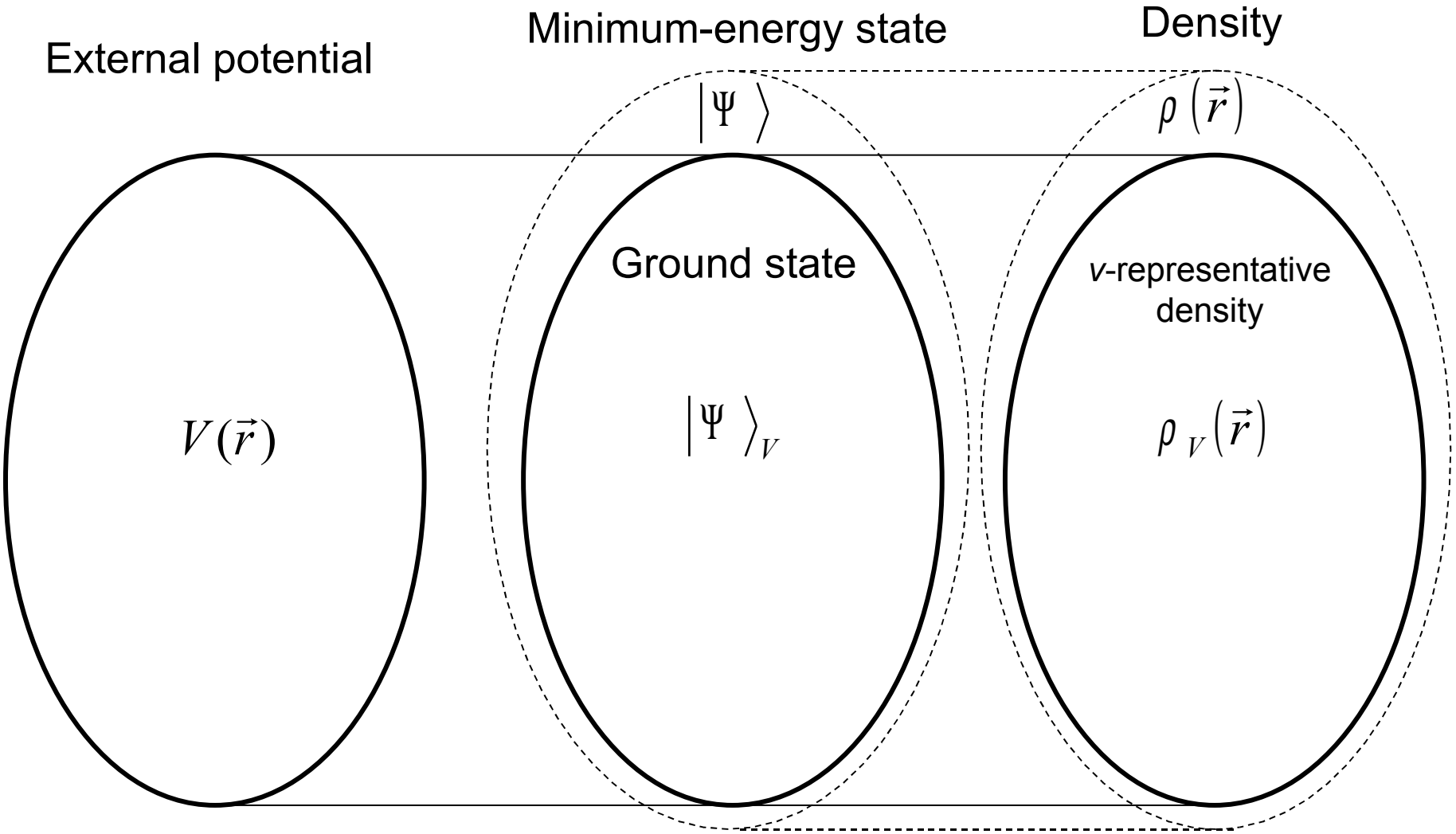
$$H\Psi_{gs}\left(r_1,..,r_N\right) = E_{gs}\Psi_{gs}\left(r_1,..,r_N\right)$$

Decomposed into two steps

$$\mathrm{Min}\left\langle \Psi\middle|H\middle|\Psi\right\rangle = \underset{\rho(\vec{r})}{\mathrm{Min}}\left[\underset{\Psi\to\rho(\vec{r})}{\mathrm{Min}}\left\langle \Psi\middle|H\middle|\Psi\right\rangle\right]$$

$$F\left[\rho\left(\vec{r}\right)\right] \equiv \underset{\Psi\to\rho(\vec{r})}{\mathrm{Min}}\left\langle \Psi\middle|H\middle|\Psi\right\rangle$$

One-to-one Correspondence



Time-dependent “HK” theorem

Runge & Gross (1984)

One-to-one mapping between time-dependent density ρ(***r***,*t*) and time-dependent potential *v*(***r***,*t*)

except for a constant shift of the potential

Condition for the external potential:

Possibility of the Taylor expansion around finite time t_0

$$v(\mathbf{r},t) = \sum_{k=0}^{\infty} \frac{1}{k!} v_k(\mathbf{r}) \left(t - t_0\right)^k$$

The initial state is arbitrary.

This condition allows an impulse potential, but forbids adiabatic switch-on.

Schrödinger equation: $$i\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H(t)\left|\Psi(t)\right\rangle$$

Current density follows the equation

$$i\frac{\partial}{\partial t}\mathbf{j}(\mathbf{r},t) = \left\langle\Psi(t)\right|\left[\hat{\mathbf{j}}(\mathbf{r}), H(t)\right]\left|\Psi(t)\right\rangle \qquad (1)$$

Different potentials, $v(\mathbf{r},t)$, $v'(\mathbf{r},t)$, make time evolution from the same initial state into Ψ(t)、Ψ'(t) $v_k(\mathbf{r}) - v_k'(\mathbf{r}) \neq c \quad \text{for } {}^{\exists}k$

$$\left(\frac{\partial}{\partial t}\right)^{k+1}\left\{\mathbf{j}(\mathbf{r},t) - \mathbf{j}'(\mathbf{r},t)\right\}\Big|_{t=t_0} = -\rho(\mathbf{r},t_0)\nabla w_k(\mathbf{r})$$

$$w_k(\mathbf{r}) = \left(\frac{\partial}{\partial t}\right)^{k}\left\{v(\mathbf{r},t) - v'(\mathbf{r},t)\right\}\Big|_{t=t_0} = v_k(\mathbf{r}) - v'_k(\mathbf{r}) \neq c$$

$$\therefore \quad \mathbf{j}(\mathbf{r},t) \neq \mathbf{j}'(\mathbf{r},t) \xrightarrow{\text{Continuity eq.}} \rho(\mathbf{r},t) \neq \rho'(\mathbf{r},t)$$

at $t > t_0$

Problem 1: Two external potentials are different, when their expansion

$$v(\mathbf{r},t) = \sum_{k=0}^{\infty} \frac{1}{k!} v_k(\mathbf{r})\left(t - t_0\right)^k$$

has different coefficients at the zero-th order

$$v_0(\mathbf{r}) - v_0'(\mathbf{r}) \neq c$$

Using eq. (1), show

$$\frac{\partial}{\partial t}\left\{ \mathbf{j}(\mathbf{r},t) - \mathbf{j}'(\mathbf{r},t)\right\}\Big|_{t=t_0} = -\rho(\mathbf{r},t_0)\nabla w_0(\mathbf{r})$$

$$w_0(\mathbf{r}) = \left\{ v(\mathbf{r},t) - v'(\mathbf{r},t)\right\}\Big|_{t=t_0} = v_0(\mathbf{r}) - v'_0(\mathbf{r}) \neq c$$

Next, if $v_0(\mathbf{r}) - v_0'(\mathbf{r}) = c$, but $v_1(\mathbf{r}) - v_1'(\mathbf{r}) \neq c$,

then, show

$$\left(\frac{\partial}{\partial t}\right)^2 \left\{ \mathbf{j}(\mathbf{r},t) - \mathbf{j}'(\mathbf{r},t)\right\}\Big|_{t=t_0} = -\rho(\mathbf{r},t_0)\nabla w_1(\mathbf{r})$$

Problem 2: Using the continuity equation and the following equation

$$\left(\frac{\partial}{\partial t}\right)^{k+1}\left\{\mathbf{j}(\mathbf{r},t)-\mathbf{j}'(\mathbf{r},t)\right\}\Big|_{t=t_0} = -\rho(\mathbf{r},t_0)\nabla w_k(\mathbf{r})$$

$$w_k(\mathbf{r}) = \left(\frac{\partial}{\partial t}\right)^{k}\left\{v(\mathbf{r},t)-v'(\mathbf{r},t)\right\}\Big|_{t=t_0} = v_k(\mathbf{r})-v'_k(\mathbf{r}) \neq c$$

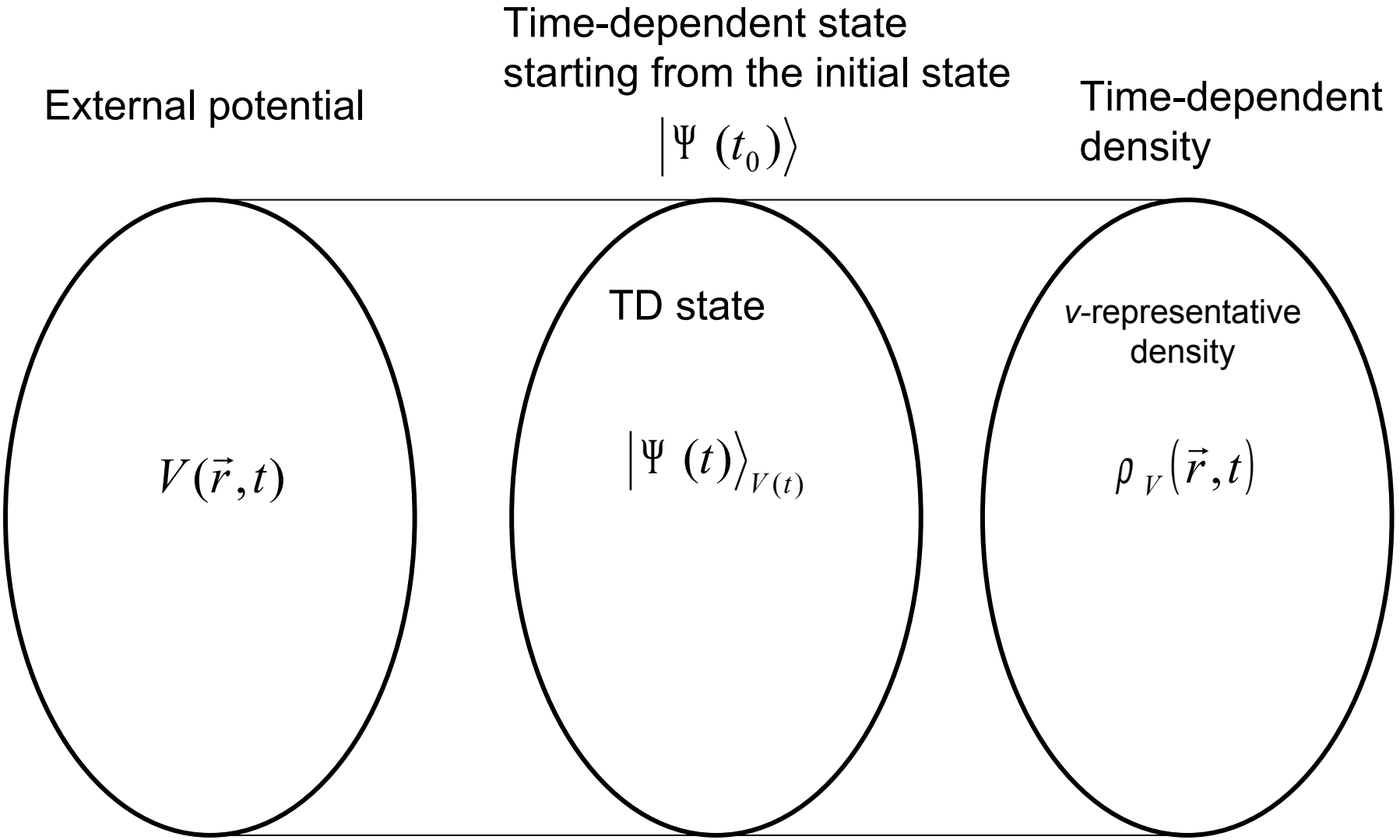
prove that

$$\left(\frac{\partial}{\partial t}\right)^{k+2}\left\{\rho(\mathbf{r},t)-\rho'(\mathbf{r},t)\right\}\Big|_{t=t_0} = \nabla\cdot\left\{\rho(\mathbf{r},t_0)\nabla w_k(\mathbf{r})\right\}$$

Then, show that the right-hand side cannot vanish identically, with

$$\nabla w_k(\mathbf{r}) \neq 0$$

One-to-one Correspondence



The universal density functional exists, and the variational principle determines the time evolution.

From the first theorem, we have ρ(***r***,*t*) ↔Ψ(t). Thus, the variation of the following function determines ρ(***r***,*t*) .

$$S[\rho\,] = \int_{t_0}^{t_1} dt \left\langle \Psi\,[\rho\,](t) \left| i\frac{\partial}{\partial t} - H(t) \right| \Psi\,[\rho\,](t) \right\rangle$$

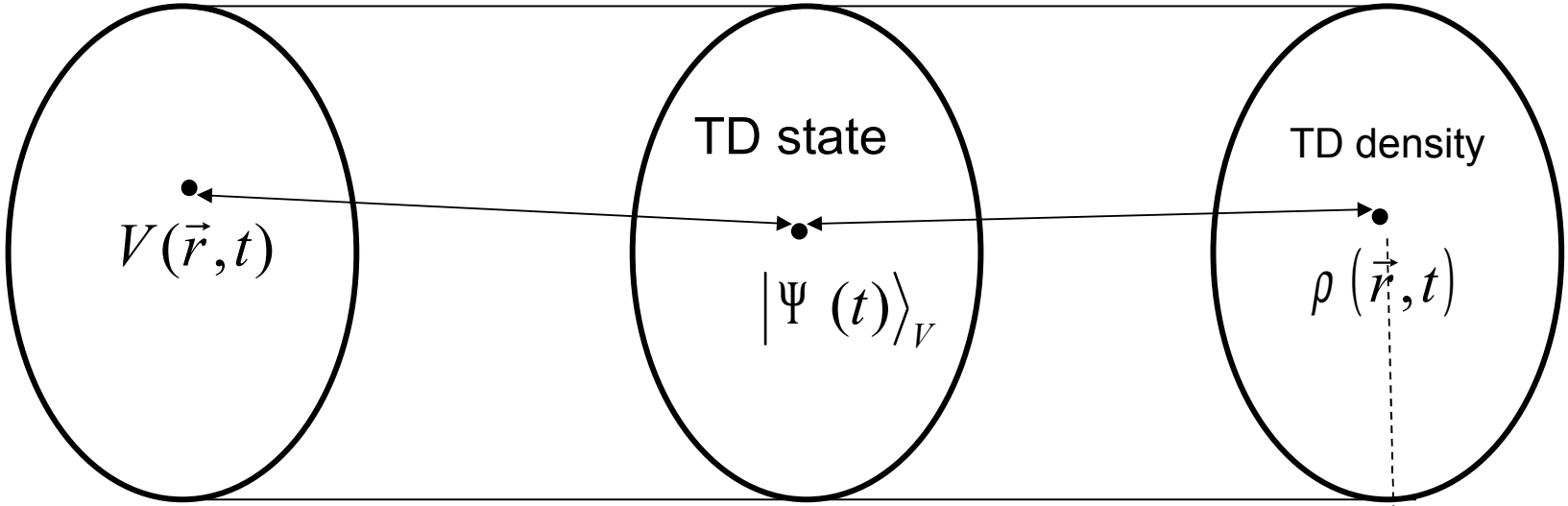
$$S[\rho\,] = \widetilde{S}[\rho\,] - \int_{t_0}^{t_1} dt \int d\mathbf{r}\rho\,(\mathbf{r},t) v(\mathbf{r},t)$$

The universal functional $\widetilde{S}[\rho\,]$ is determined.

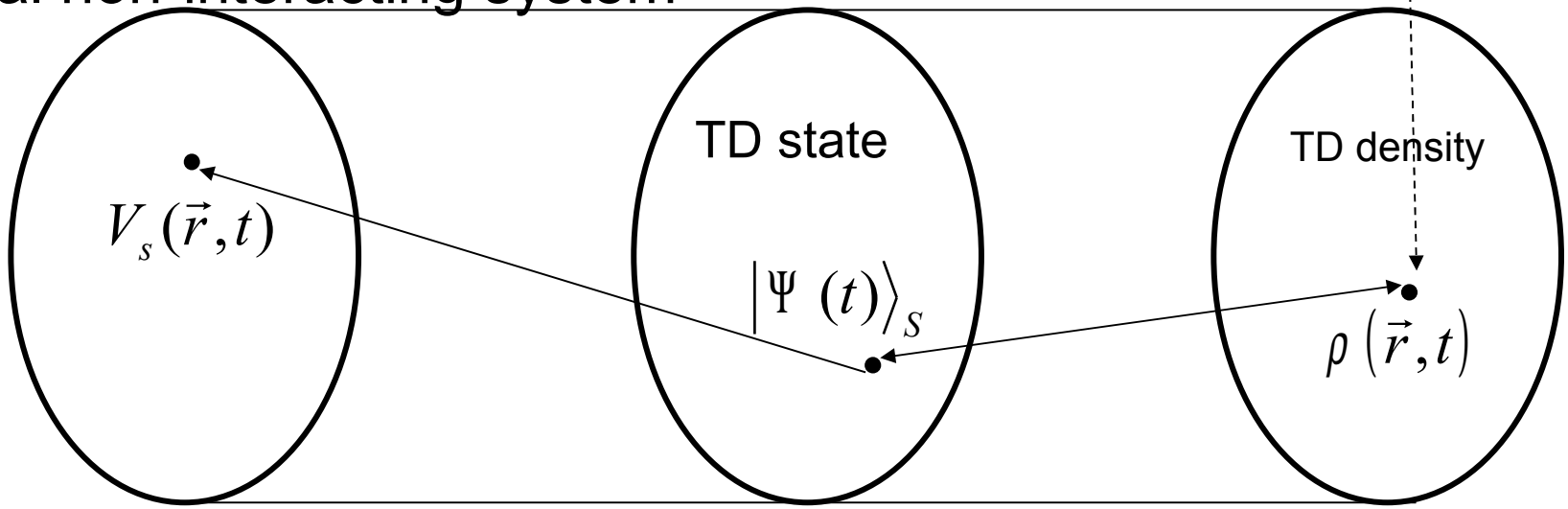
v-representative density is assumed.

TD Kohn-Sham Scheme

Real interacting system



Virtual non-interacting system



Time-dependent KS theory

Assuming non-interacting v-representability $\rho(\vec{r},t) = \sum_{i=1}^{N} |\phi_i(\vec{r},t)|^2$

Time-dependent Kohn-Sham (TDKS) equation

$$i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + v_s[\rho](\mathbf{r},t)\right)\phi_i(\mathbf{r},t)$$

$$v_s[\rho](\mathbf{r},t) = \frac{\delta \bar{S}[\rho]}{\delta\rho(\mathbf{r},t)}$$

$$\bar{S}[\rho] \equiv S[\rho] - \int_{t_0}^{t_1}\left\langle \Phi_D[\rho](t)\left| i\frac{\partial}{\partial t} - T\right|\Phi_D[\rho](t)\right\rangle$$

Solving the TDKS equation, in principle, we can obtain the exact time evolution of many-body systems.

The functional depends on ρ(***r***,*t*) and the initial state Ψ_0.

Time-dependent quantities
→ Information on excited states

$$\left|\Psi\ (0)\right\rangle = \sum_n c_n \left|\Phi\ _n\right\rangle \quad \Rightarrow \quad \left|\Psi\ (t)\right\rangle = \sum_n c_n e^{-iE_n t} \left|\Phi\ _n\right\rangle$$

Energy projection

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left|\Psi\ (t)\right\rangle e^{iEt} dt = \sum_n c_n \left|\Phi\ _n\right\rangle \delta\ (E - E_n)$$

Finite time period $T \sim 1/\Gamma$ → Finite energy resolution

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \left|\Psi\ (t)\right\rangle e^{iEt} e^{-\Gamma |t|/2} dt = \sum_n \frac{c_n}{\pi} \frac{\Gamma/2}{(E - E_n)^2 + (\Gamma/2)^2} \left|\Phi\ _n\right\rangle$$

TDHF(TDDFT) calculation in 3D real space

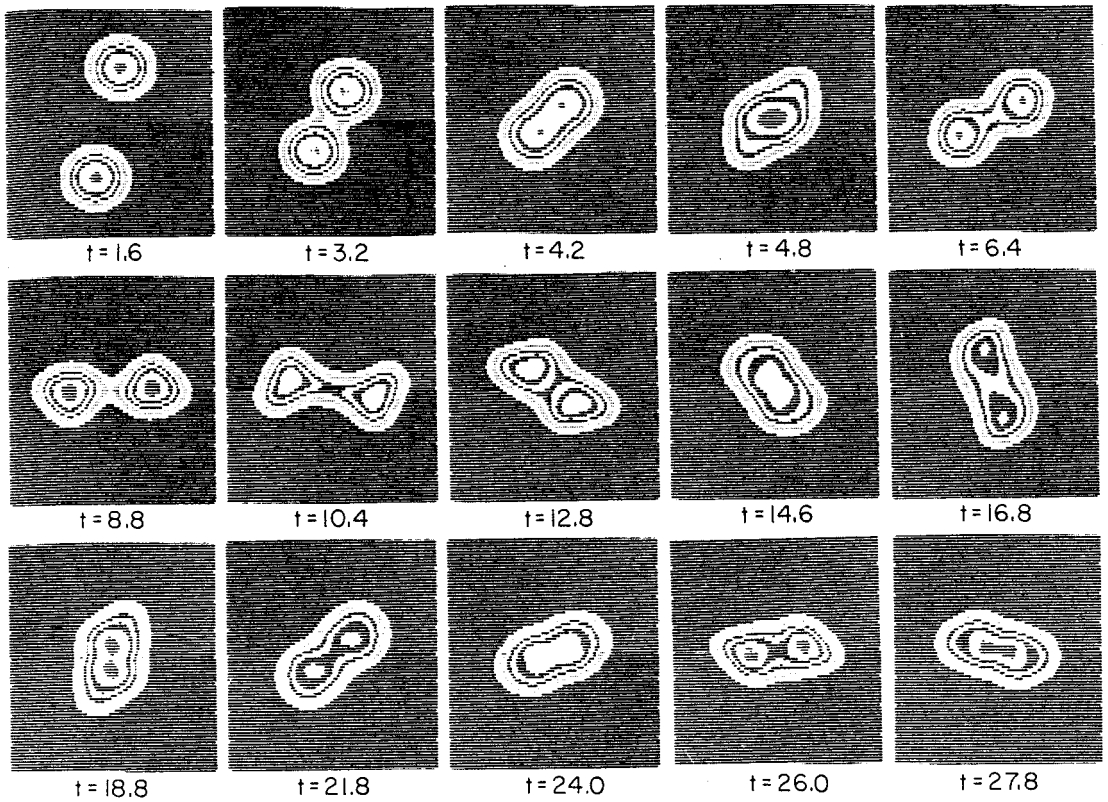


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{lab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

H. Flocard, S.E. Koonin, M.S. Weiss, Phys. Rev. 17(1978)1682.

Small-amplitude limit (Random-phase approximation)

One-body operator under a TD external potential

$$i\frac{\partial}{\partial t}\rho(t) = \left[h_{\mathrm{KS}}[\rho(t)] + V_{\mathrm{ext}}(t), \rho(t)\right]$$

Assuming that the external potential is weak,

$$\rho(t) = \rho_0 + \delta\rho(t) \qquad h(t) = h_0 + \delta h(t) = h_0 + \left.\frac{\delta h}{\delta \rho}\right|_{\rho_0} \cdot \delta\rho(t)$$

$$i\frac{\partial}{\partial t}\delta\rho(t) = \left[h_0, \delta\rho(t)\right] + \left[\delta h(t) + V_{\mathrm{ext}}(t), \rho_0\right]$$

Let us take the external field with a fixed frequency ω,

$$V_{\mathrm{ext}}(t) = V_{\mathrm{ext}}(\omega)e^{-i\omega t} + V_{\mathrm{ext}}^{+}(\omega)e^{+i\omega t}$$

The density and residual field also oscillate with ω,

$$\delta\rho(t) = \delta\rho(\omega)e^{-i\omega t} + \delta\rho^{+}(\omega)e^{+i\omega t}$$

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

The linear response (RPA) equation

$$\omega\,\delta\rho(\omega) = [h_0, \delta\rho(\omega)] + [\delta h(\omega) + V_{\mathrm{ext}}(\omega), \rho_0]$$

Note that all the quantities, except for ρ_0 and h_0, are non-hermitian.

$$\delta\rho(t) = \sum_{i=1}^{A} \left(|\delta\psi_i(t)\rangle\langle\phi_i| + |\phi_i\rangle\langle\delta\psi_i(t)| \right)$$

$$\delta\rho(\omega) = \sum_{i=1}^{A} \left(|X_i(\omega)\rangle\langle\phi_i| + |\phi_i\rangle\langle Y_i(\omega)| \right)$$

This leads to the following equations for X and Y:

$$\omega\,|X_i(\omega)\rangle = (h_0 - \varepsilon_i)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\mathrm{ext}}(\omega)\}|\phi_i\rangle$$

$$\omega\,\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\mathrm{ext}}(\omega)\}\hat{Q}$$

$$\hat{Q} = \sum_{i=1}^{A} \left(1 - |\phi_i\rangle\langle\phi_i|\right)$$

These are often called “RPA equations” in nuclear physics.
X and Y are called “forward” and “backward” amplitudes.

If we start from the TDHF with a “density-independent” Hamiltonian (not from the energy functional), then, there is other ways to formulate the RPA. (see TextBooks)

Matrix formulation

$$\omega \left| X_i(\omega) \right\rangle = \left(h_0 - \varepsilon_i \right) \left| X_i(\omega) \right\rangle + \hat{Q}\{\delta h(\omega) + V_{\text{ext}}(\omega)\} \left| \phi_i \right\rangle$$
$$\omega \left\langle Y_i(\omega) \right| = - \left\langle Y_i(\omega) \right| \left(h_0 - \varepsilon_i \right) - \left\langle \phi_i \right| \{\delta h(\omega) + V_{\text{ext}}(\omega)\} \hat{Q} \qquad (1)$$

$$\hat{Q} = \sum_{i=1}^{A} \left(1 - \left| \phi_i \right\rangle \left\langle \phi_i \right| \right)$$

If we expand the X and Y in *particle orbitals*:

$$\left| X_i(\omega) \right\rangle = \sum_{m > A} \left| \phi_m \right\rangle X_{mi}(\omega), \quad \left| Y_i(\omega) \right\rangle = \sum_{m > A} \left| \phi_m \right\rangle Y^*_{mi}(\omega)$$

Taking overlaps of Eq.(1) with particle orbitals

$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = - \begin{pmatrix} (V_{\text{ext}})_{mi} \\ (V_{\text{ext}})_{im} \end{pmatrix}$$

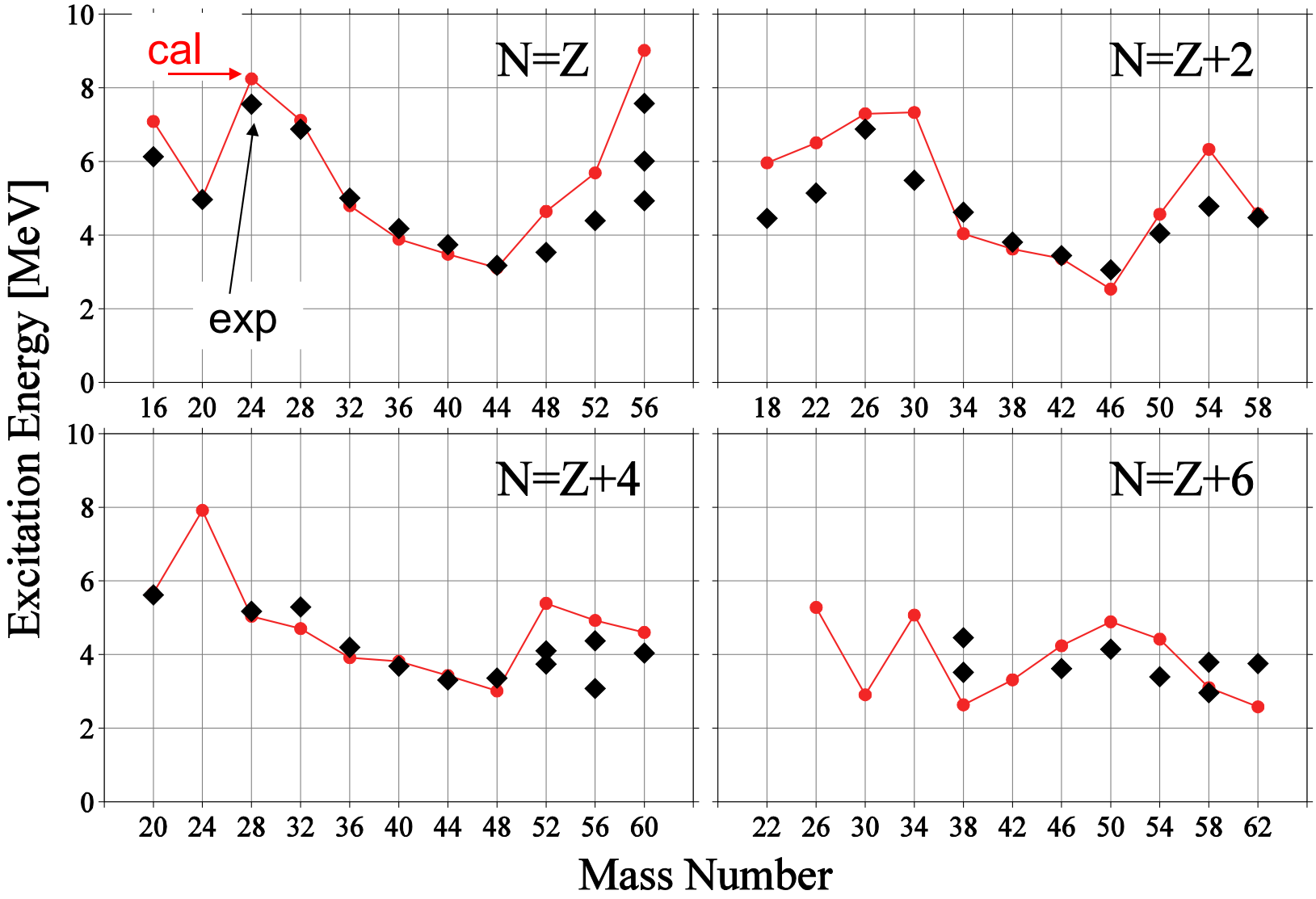
$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{nj}} \right|_{\rho_0} \right| \phi_i \right\rangle$$

$$B_{mi,nj} = \left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{jn}} \right|_{\rho_0} \right| \phi_i \right\rangle$$

In many cases, setting V_{ext}=0 and solve the normal modes of excitations:

→ Diagonalization of the matrix

Lowest negative-parity states (SGII functional)



Green's function method

$$\omega\,\delta\rho(\omega) = [h_0, \delta\rho(\omega)] + [\delta h(\omega) + V_{\text{ext}}(\omega), \rho_0] \qquad (2)$$

Multiply Eq.(2) with $|\phi_i\rangle\langle\phi_i|$ from the right and from the left:

$$\delta\rho(\omega)|\phi_i\rangle\langle\phi_i| = (\omega + \varepsilon_i - h_0)^{-1}[V_{\text{scf}}, \rho_0]|\phi_i\rangle\langle\phi_i| \qquad (3\text{-}1)$$

$$|\phi_i\rangle\langle\phi_i|\delta\rho(\omega) = |\phi_i\rangle\langle\phi_i|[V_{\text{scf}}, \rho_0](\omega - \varepsilon_i + h_0)^{-1} \qquad (3\text{-}2)$$

$$V_{\text{scf}}(\omega) \equiv V_{\text{ext}}(\omega) + \delta h(\omega)$$

Sum up with respect to occupied orbitals *i*, then, add (3-1) and (3-2), using the orthonormalization condition for KS orbitals ($\rho^2=\rho$):

$$\delta\rho(\omega) = \{\rho_0, \delta\rho(\omega)\}$$

$$\delta\rho(\omega) = \sum_i \{G_0(\varepsilon_i + \omega)V_{\text{scf}}|\phi_i\rangle\langle\phi_i| + |\phi_i\rangle\langle\phi_i|V_{\text{scf}}G_0(\varepsilon_i - \omega)\} \qquad G_0(E) \equiv (E - h_0)^{-1}$$

If the V_{scf} is local, we can rewrite this as follows:

$$\delta\rho(\mathbf{r};\omega) = \sum_i \int d\mathbf{r}\{G_0(\mathbf{r},\mathbf{r}';\varepsilon_i + \omega)V_{\text{scf}}(\mathbf{r}')\phi_i(\mathbf{r}')\phi_i^*(\mathbf{r}) + \phi_i(\mathbf{r})\phi_i^*(\mathbf{r}')V_{\text{scf}}(\mathbf{r}')G_0(\mathbf{r}',\mathbf{r}:\varepsilon_i - \omega)\}$$

$$= \int d\mathbf{r}\Pi_0(\mathbf{r},\mathbf{r}';\omega)V_{\text{scf}}(\mathbf{r}';\omega)$$

where the independent-particle response function is defined by

$$\Pi_0(\mathbf{r},\mathbf{r}';\omega) \equiv \sum_i \int d\mathbf{r}\{\phi_i(\mathbf{r})G_0^*(\mathbf{r},\mathbf{r}':\varepsilon_i - \omega^*)\phi_i^*(\mathbf{r}') + \phi_i^*(\mathbf{r})G_0(\mathbf{r},\mathbf{r}';\varepsilon_i + \omega)\phi_i(\mathbf{r}')\}$$

Green's function method (cont.)

An advantage of the Green's function method is that we can treat the continuum exactly. Shlomo and Bertsch, NPA243 (1975) 507.

$$\omega \rightarrow \omega + i\eta$$

$$\Pi_0(\mathbf{r},\mathbf{r}';\omega + i\eta) = \sum_i \int d\mathbf{r}\left\{ \phi_i(\mathbf{r}) G_0^{(+)*}(\mathbf{r},\mathbf{r}':\varepsilon_i - \omega)\phi_i^*(\mathbf{r}') + \phi_i^*(\mathbf{r}) G_0^{(+)}(\mathbf{r},\mathbf{r}';\varepsilon_i + \omega)\phi_i(\mathbf{r}')\right\}$$

$$G_0^{(\pm)}(E) \equiv \left(E \pm i\eta - h_0\right)^{-1}$$

In case h_0 is spherical, the Green's function can be easily obtained by the partial-wave expansion:

$$G_0^{(+)}(E) = 2m\frac{1}{rr'}\sum_{lm}\frac{u_l(r_<)v_l^{(+)}(r_>)}{W[u_l, v_l^{(+)}]} Y_{lm}(\hat{r})Y_{lm}^*(\hat{r}')$$

In case h_0 is deformed, we can construct the Green's function by using the following identity: T.N. and Yabana, JCP114 (2001) 2550; PRC71 (2005) 024301.

$$G_{\mathrm{def}}^{(\pm)}(E) = G_{\mathrm{sph}}^{(\pm)}(E) + G_{\mathrm{sph}}^{(\pm)}(E)\left(h_{\mathrm{def}} - h_{\mathrm{sph}}\right)G_{\mathrm{def}}^{(\pm)}(E)$$

Real-time method

In the RPA calculations (matrix formulation & Green's function method), the most tedious part is the calculation of the residual induced fields:

$$\delta h(\omega) = \left.\frac{\delta h}{\delta \rho}\right|_{\rho_0} \cdot \delta \rho(\omega)$$

In the original time-dependent equations, this effect is included in the self-consistent potential:

$$h[\rho(t)] = h_0 + \delta h(t), \qquad \delta h(t) = \left.\frac{\delta h}{\delta \rho}\right|_{\rho_0} \cdot \delta \rho(t)$$

Therefore, in principle, the RPA can be achieved by solving the TD Kohn-Sham equations, starting from the ground state with a weak perturbation.

$$i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + v_s[\rho](\mathbf{r},t) + V_{\text{ext}}(t)\right)\phi_i(\mathbf{r},t)$$

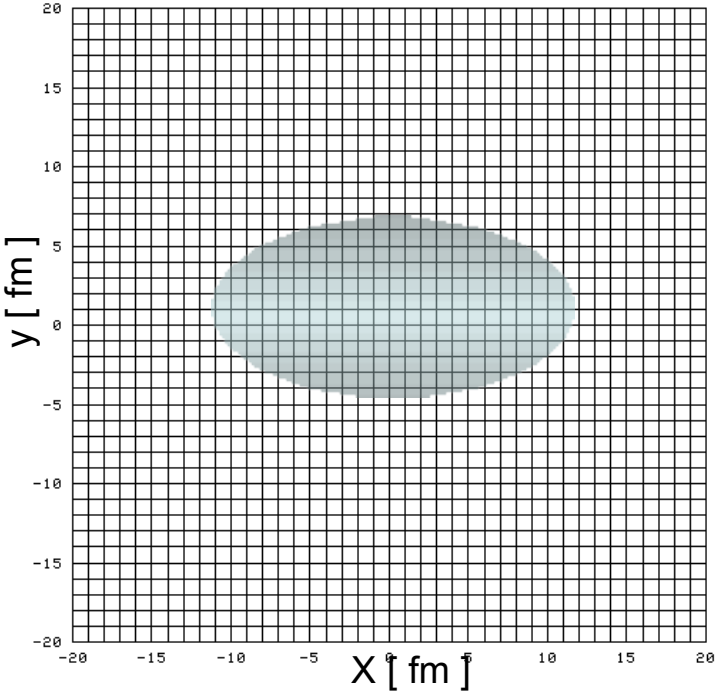
Skyrme TDDFT in real space

Time-dependent Hartree-Fock equation $\quad -i\tilde{\eta}(r)$

$$i\frac{\partial}{\partial t}\psi_i(\mathbf{r}\sigma\tau,t) = \left(h_{\mathrm{Sk}}[\rho,\tau,\mathbf{j},\mathbf{s},\overleftrightarrow{\mathbf{J}}](t) + V_{\mathrm{ext}}(t)\right)\psi_i(\mathbf{r}\sigma\tau,t)$$

3D space is discretized in lattice

Single-particle orbital: $\varphi_i(\mathbf{r},t) = \{\varphi_i(\mathbf{r}_k,t_n)\}_{k=1,\cdots Mr}^{n=1,\cdots Mt}, \quad i = 1,\cdots,N$



N: Number of particles

Mr: Number of mesh points

Mt: Number of time slices

Spatial mesh size is about 1 fm.

Time step is about 0.2 fm/c

Nakatsukasa, Yabana, Phys. Rev. C71 (2005) 024301

Calculation of time evolution

Time evolution is calculated by the finite-order Taylor expansion

$$\psi_i(t+\Delta t) = \exp\left(-i\int_t^{t+\Delta t} h(t')dt'\right)\psi_i(t)$$

$$\approx \sum_n \frac{\left(-i\Delta t\, h(t+\Delta t/2)\right)^n}{n!}\psi_i(t)$$

Violation of the unitarity is negligible if the time step is small enough:

$$\Delta t\, \varepsilon_{\max} << 1$$

$\varepsilon_{\max}$ The maximum (single-particle) eigenenergy in the model space

Real-time calculation of response functions

1. Weak instantaneous external perturbation

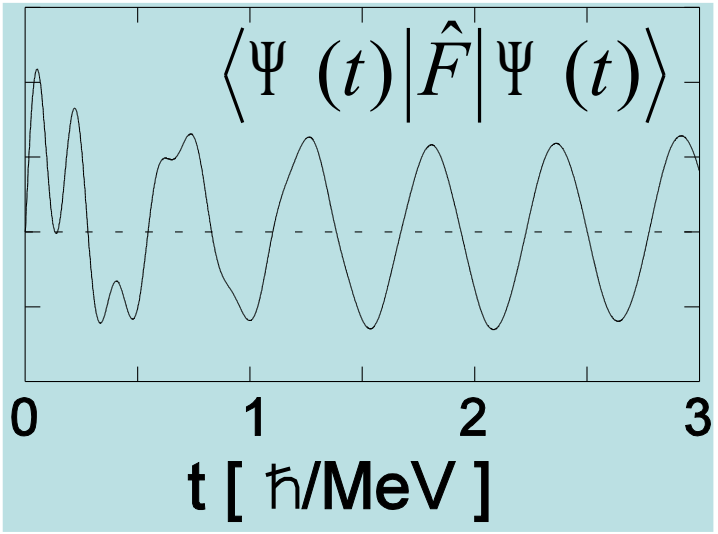
$$V_{\text{ext}}(t) = \eta \hat{F} \delta(t)$$

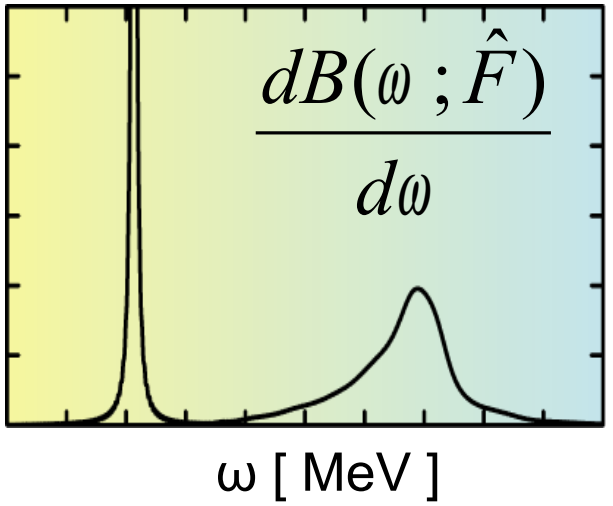
3. Calculate time evolution of

$$\langle \Psi(t) | \hat{F} | \Psi(t) \rangle$$

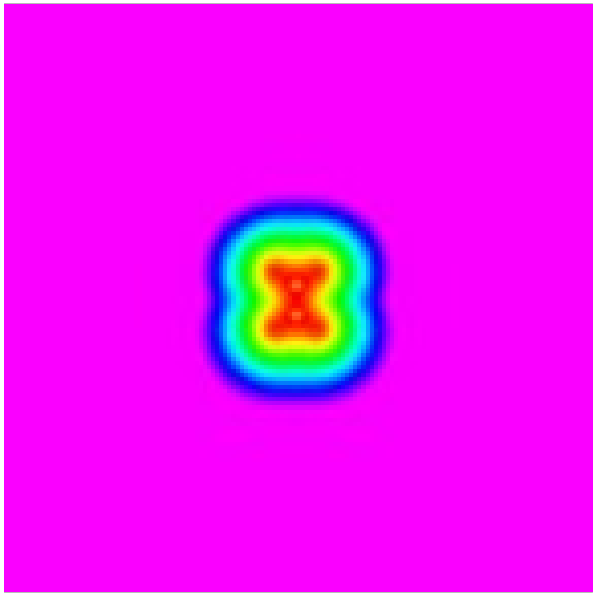
5. Fourier transform to energy domain

$$\frac{dB(\omega;\hat{F})}{d\omega} = -\frac{1}{\pi\eta} \mathrm{Im} \int \langle \Psi(t) | \hat{F} | \Psi(t) \rangle e^{i\omega t} dt$$





Real-time dynamics of electrons in photoabsorption of molecules

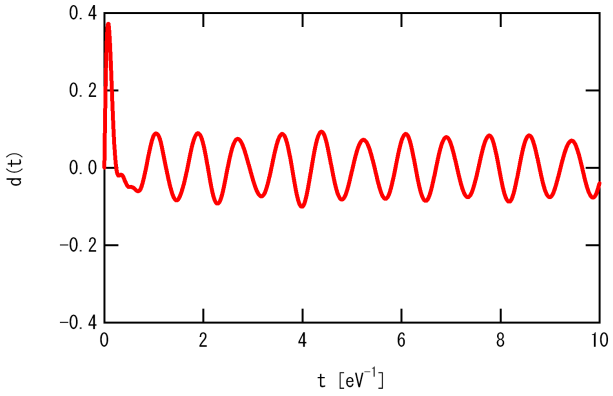


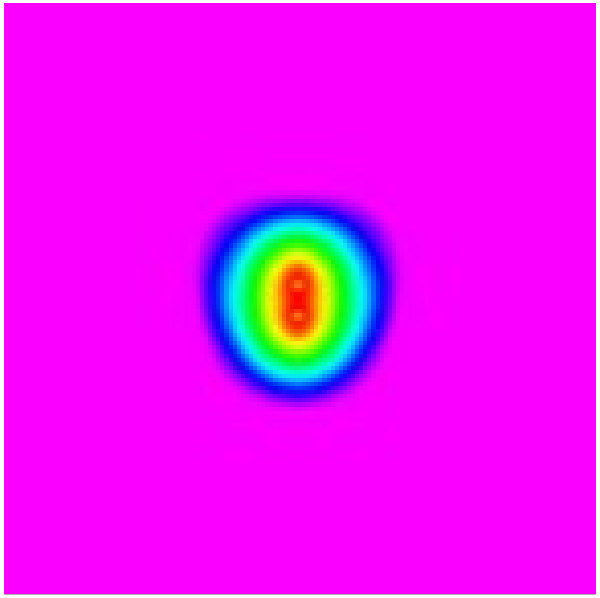
1. External perturbation t=0

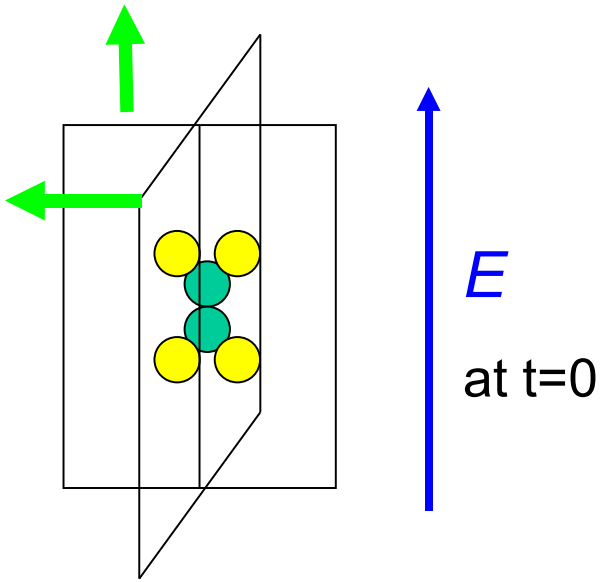
$$V_{ext}(\mathbf{r},t) = -\varepsilon\, r_i \delta(t), \quad i = x, y, z$$

2. Time evolution of dipole moment

$$d_i(t) \propto \int r_i \rho(\mathbf{r},t)$$

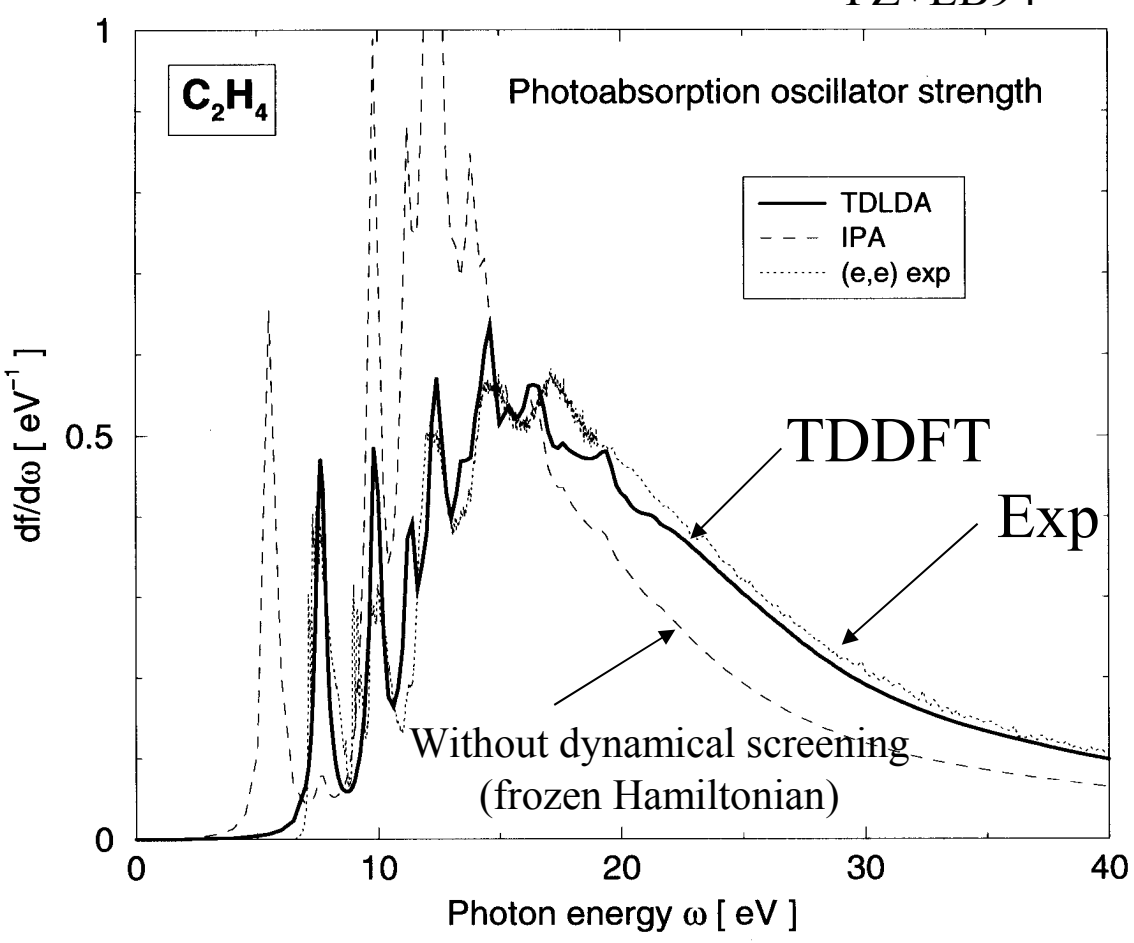






Comparison with measurement (linear optical absorption)

TDDFT accurately describe optical absorption
Dynamical screening effect is significant

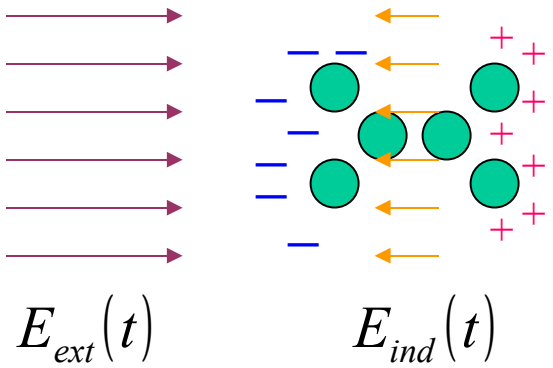


$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t) = h[n(\vec{r},t)]\psi_i(\vec{r},t)$$

with Dynamical screening

without

$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t) = h[n_0(\vec{r})]\psi_i(\vec{r},t)$$

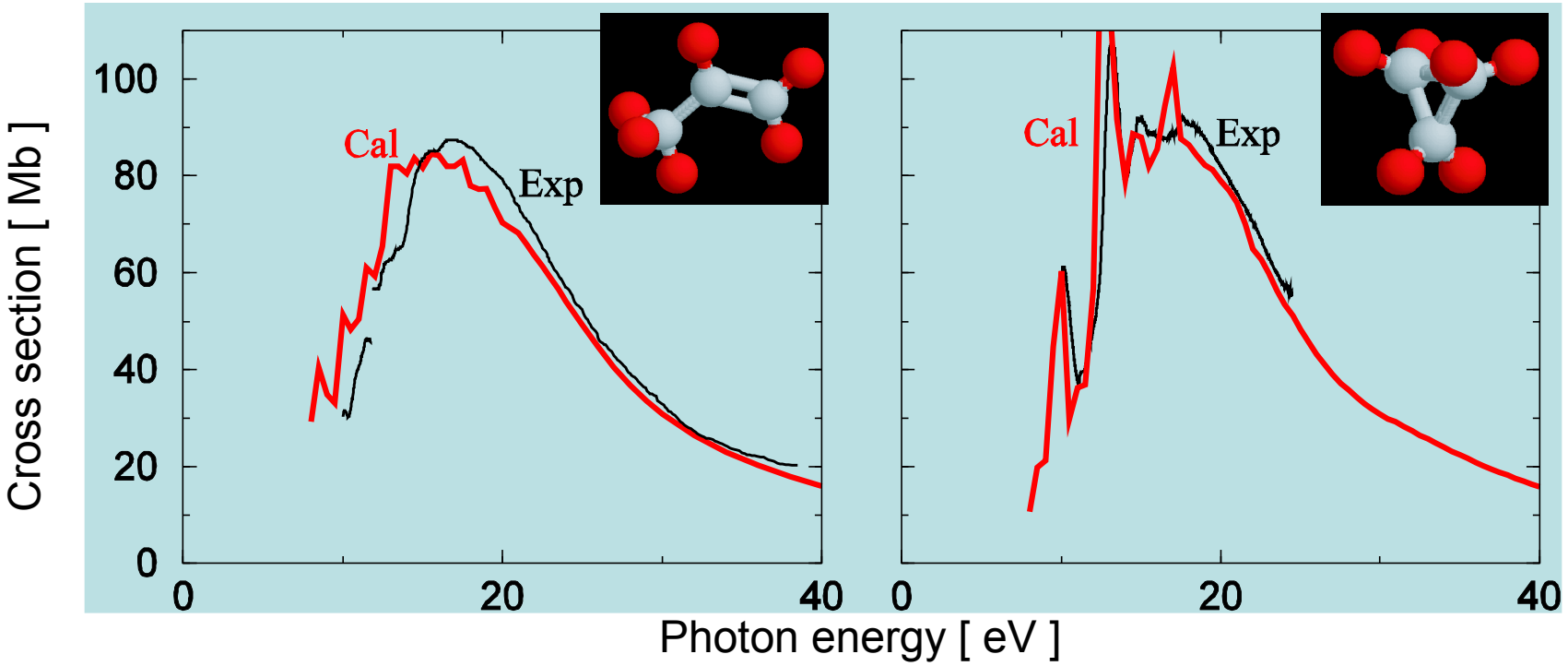


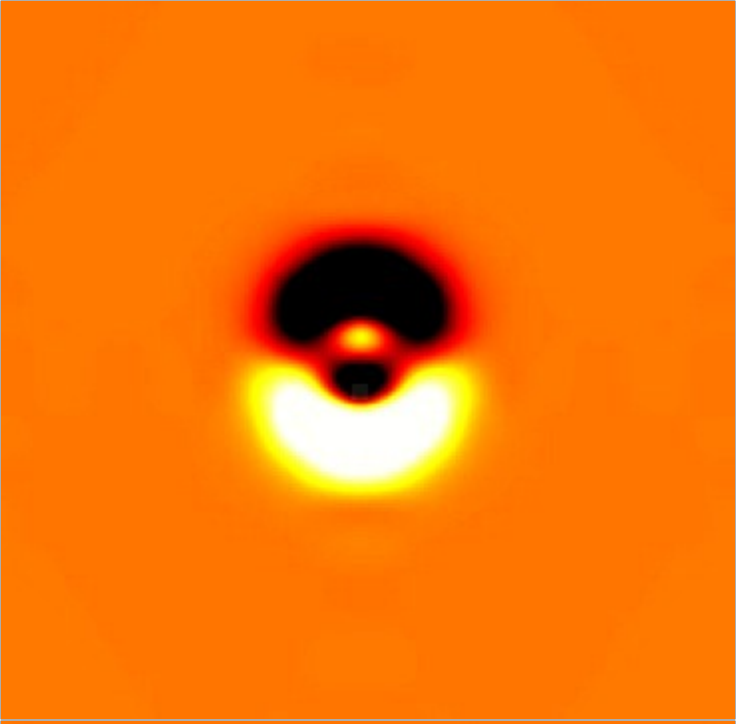
T. Nakatsukasa, K. Yabana, J. Chem. Phys. 114(2001)2550.

Photoabsorption cross section in C_3H_6 isomer molecules

Nakatsukasa & Yabana, Chem. Phys. Lett. 374 (2003) 613.

- TDLDA cal with LB94 in 3D real space
- 33401 lattice points (r < 6 Å)
- Isomer effects can be understood in terms of symmetry and anti-screening effects on bound-to-continuum excitations.





Neutrons

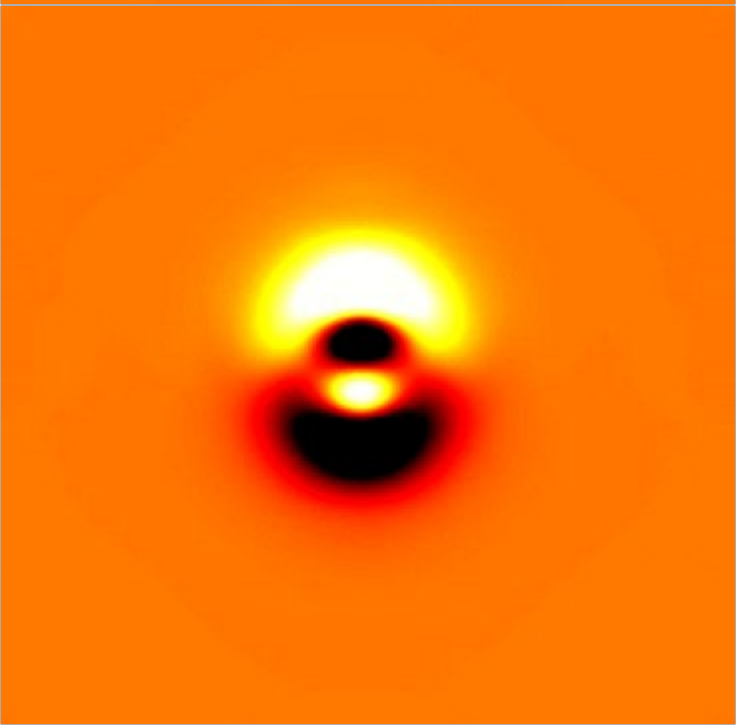
^{16}O

$$\delta\rho_n(t) = \rho_n(t) - (\rho_0)_n$$

Time-dep. transition density

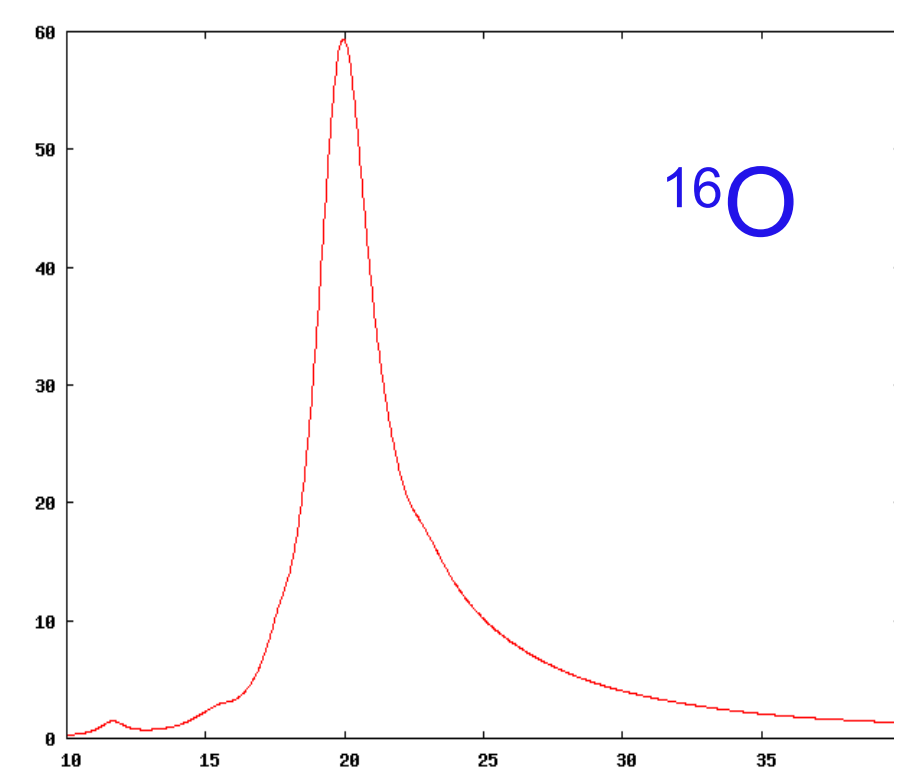
δρ> 0

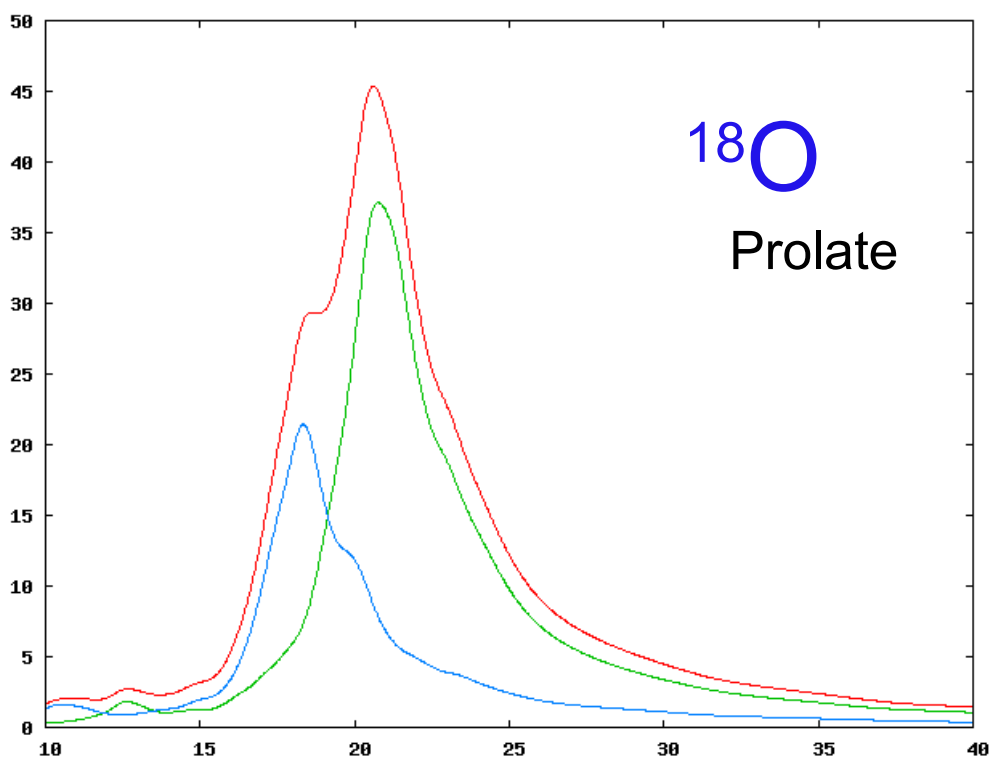
δρ< 0

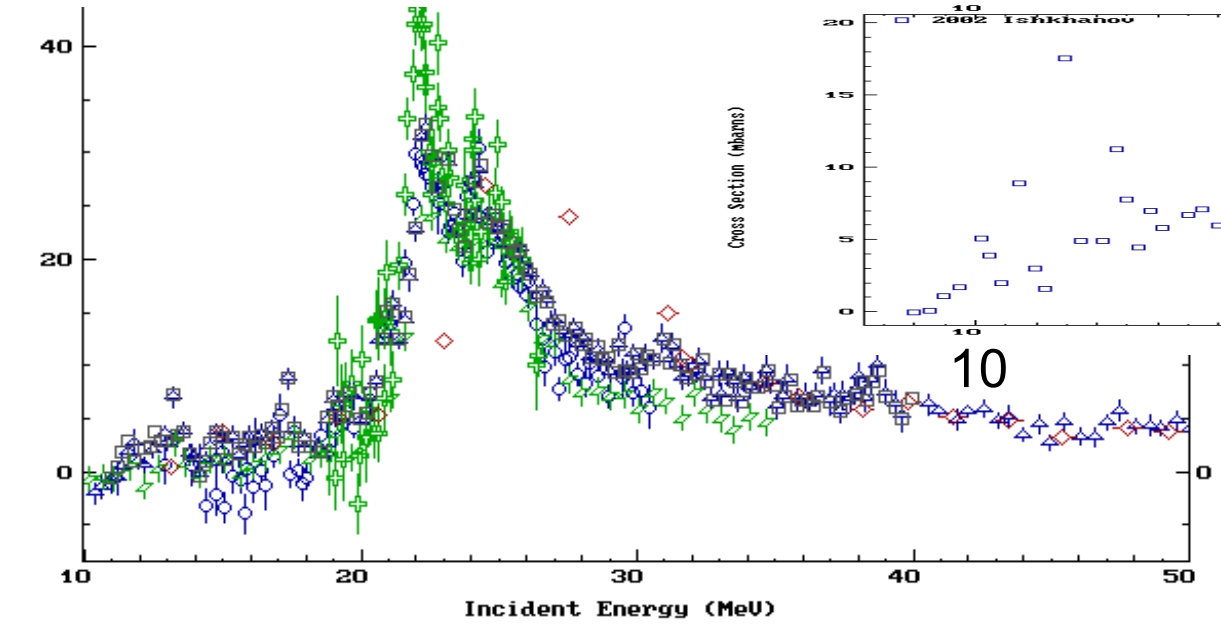


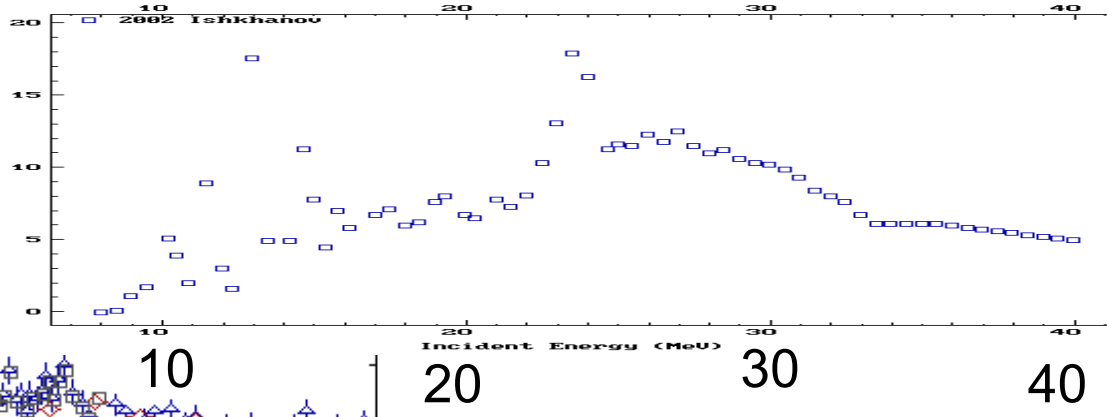
$$\delta\rho_p(t) = \rho_p(t) - (\rho_0)_p$$

Protons









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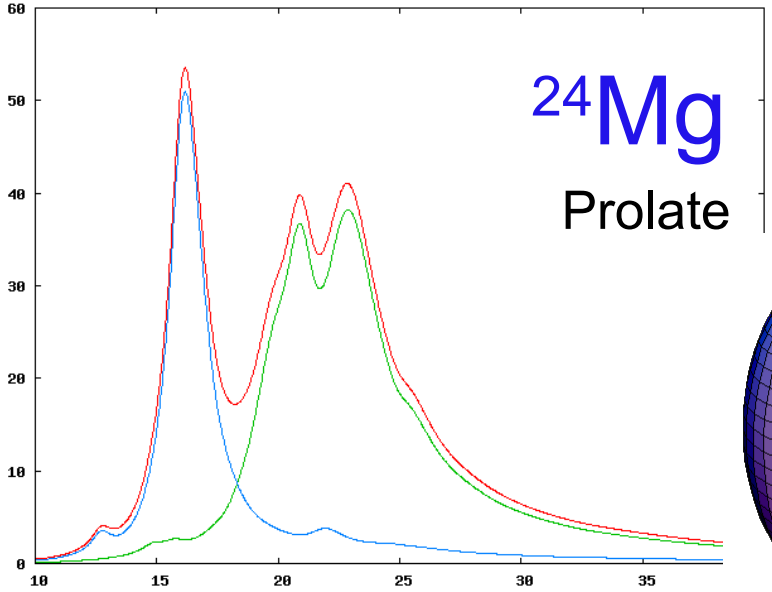
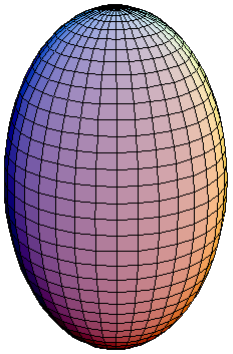
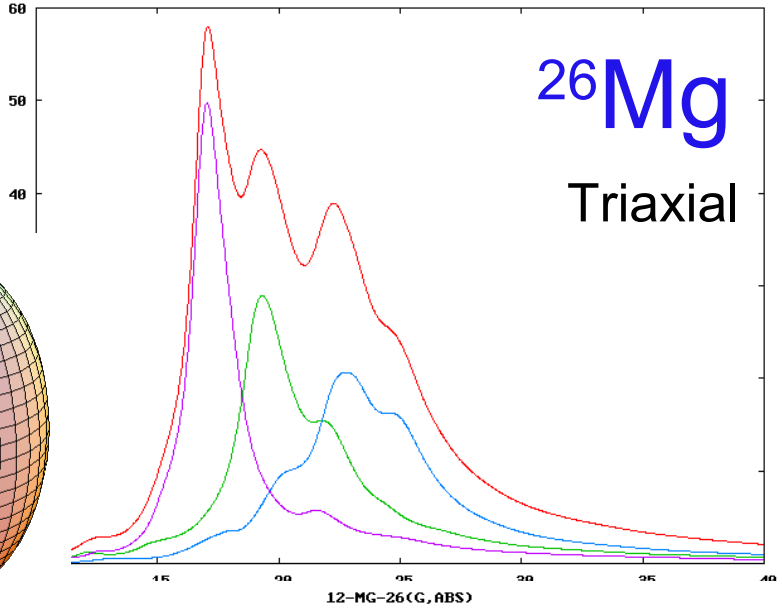
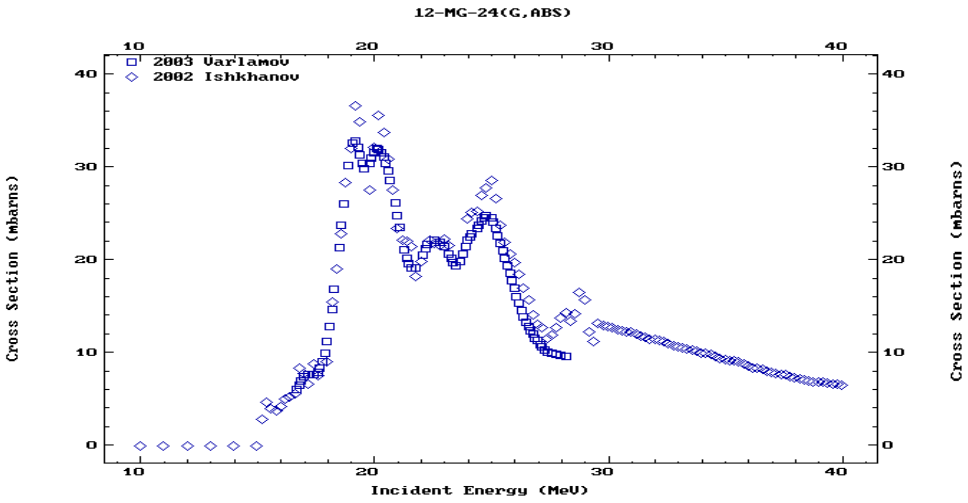
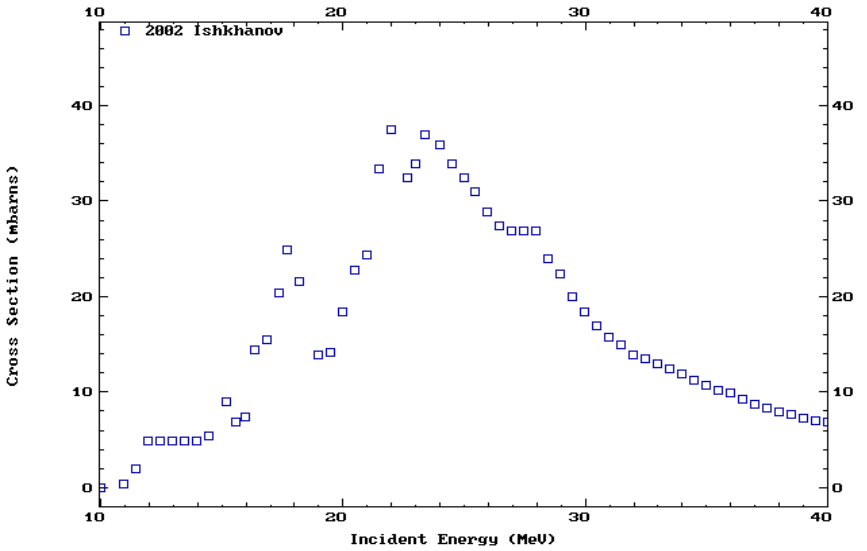
E_x [MeV]











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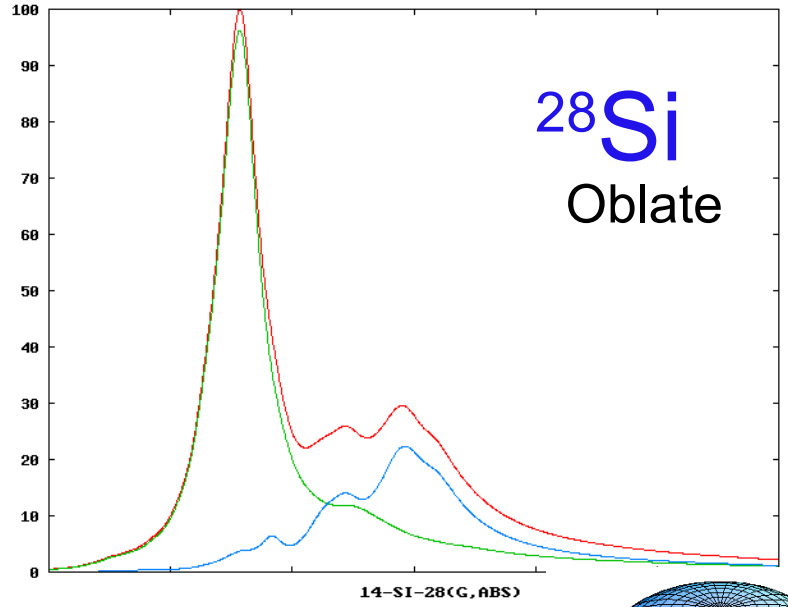
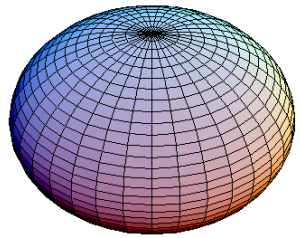
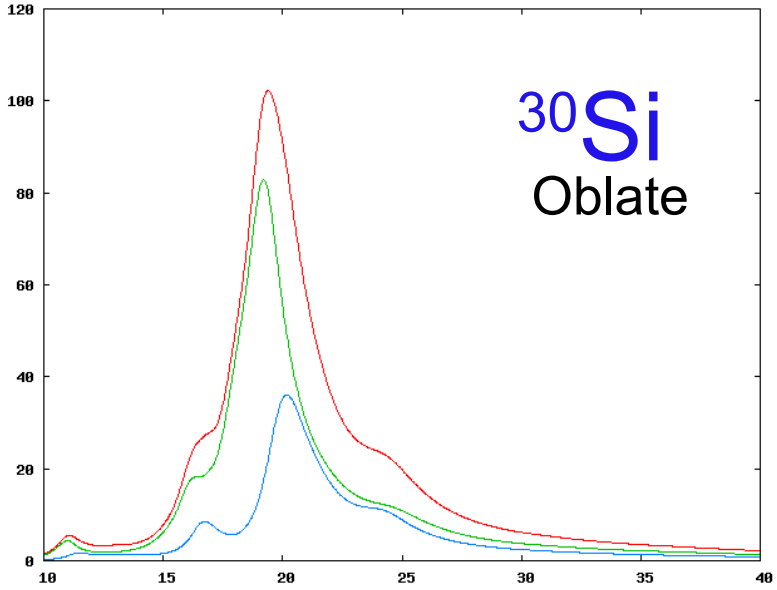
E_x [MeV]

10 20 30 40

E_x [MeV]







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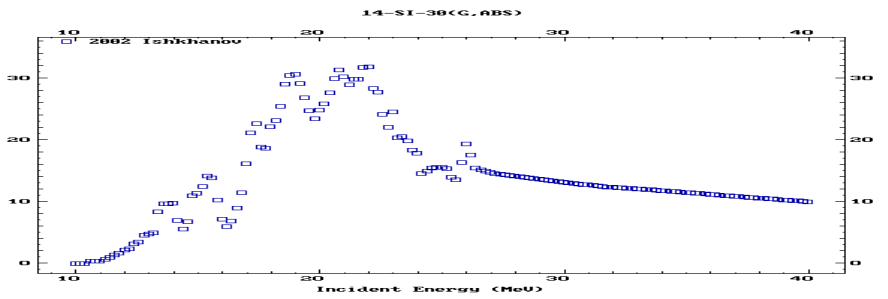
E_x [MeV]



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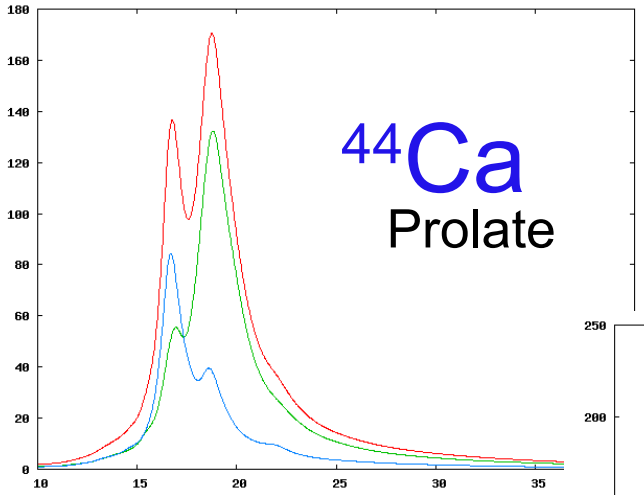
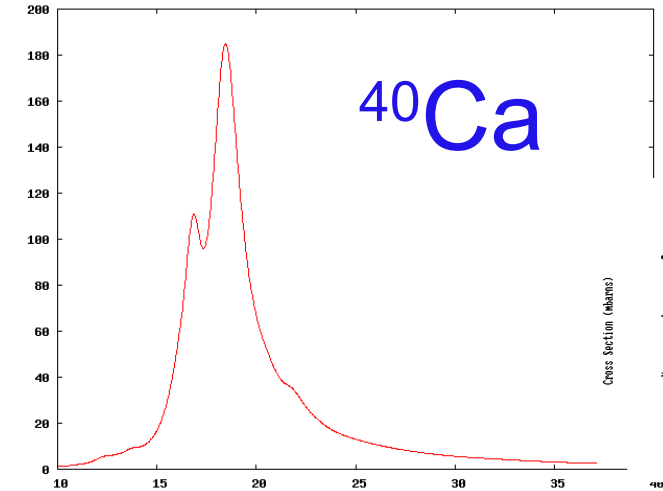
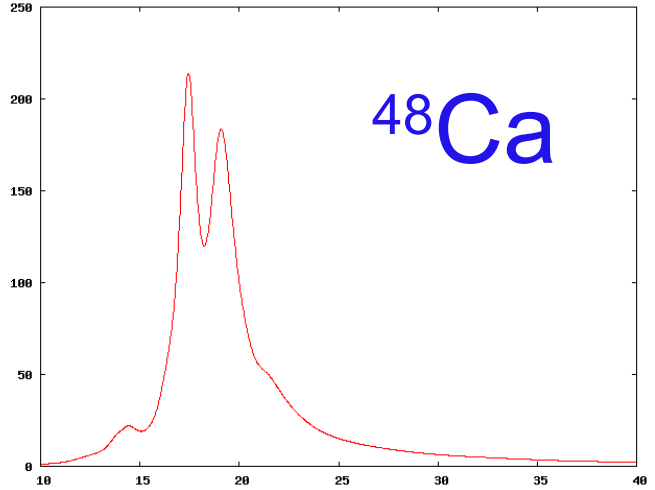
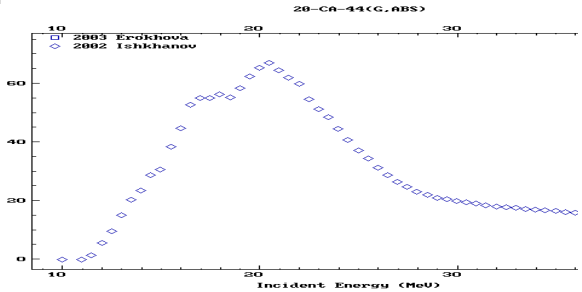
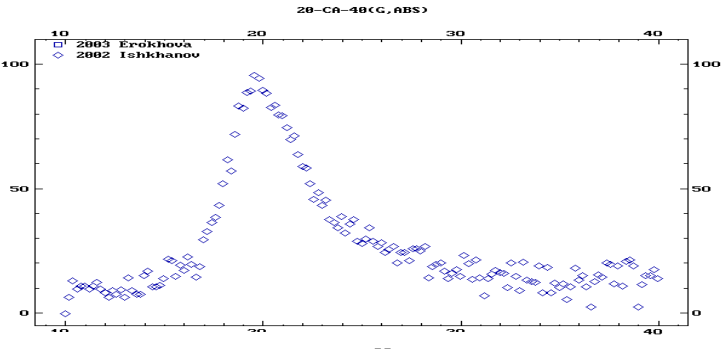
E_x [MeV]

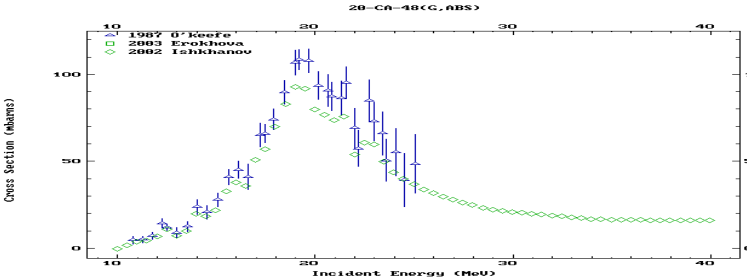












10 20 30

E_x [MeV]

10 20 30 40

E_x [MeV]

10 20 30 40

E_x [MeV]

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

A method to avoid the explicit calculation of the residual fields (interactions)

$$\omega \left| X_i(\omega) \right\rangle = \left(h_0 - \varepsilon_i \right) \left| X_i(\omega) \right\rangle + \hat{Q}\left\{ \delta h(\omega) + V_{\mathrm{ext}}(\omega) \right\} \left| \phi_i \right\rangle$$
$$\omega \left\langle Y_i(\omega) \right| = -\left\langle Y_i(\omega) \right| \left(h_0 - \varepsilon_i \right) - \left\langle \phi_i \right| \left\{ \delta h(\omega) + V_{\mathrm{ext}}(\omega) \right\} \hat{Q} \qquad (1)$$

Residual fields can be estimated by the finite difference method:

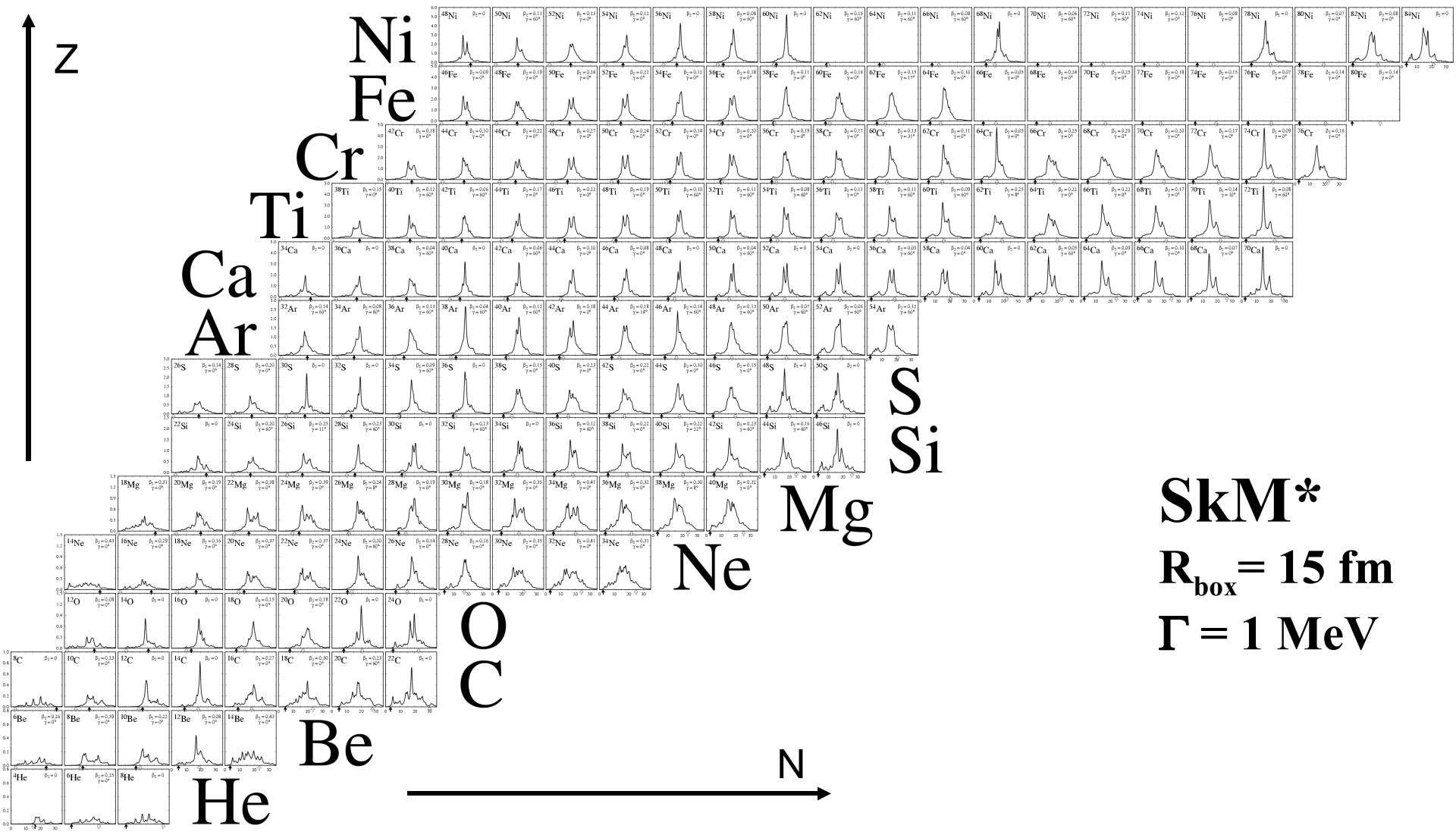
$$\delta h(\omega) = \frac{1}{\eta} \left(h\left[\left\langle \psi' \right|, \left| \psi \right\rangle \right] - h_0 \right)$$
$$\left| \psi_i \right\rangle = \left| \phi_i \right\rangle + \eta \left| X_i(\omega) \right\rangle, \quad \left\langle \psi_i' \right| = \left\langle \phi_i \right| + \eta \left\langle Y_i(\omega) \right|$$

Starting from initial amplitudes $X^{(0)}$ and $Y^{(0)}$, one can use an iterative method to solve eq. (1).

Programming of the RPA code becomes very much trivial, because we only need calculation of the single-particle potential, with different bras and kets.

Fully self-consistent calculation of E1 strength distribution

Inakura, T.N., Yabana, in preparation



SkM*

R_{box} = 15 fm

Γ = 1 MeV

Large Amplitude Collective Motion

Beyond the small-amplitude approximation

- In the small-amplitude limit, the normal modes are obtained by diagonalizing the RPA matrix.

  → “Quantization” is on hand.

- Large amplitude collective motion
  - Real-time approach to non-linear response
  - Adiabatic TDHF
  - Self-consistent collective coordinate method

Real-time approach to non-linear response

- In principle, non-linear response can be studied with the real-time method.
  - Accuracy
  - Applicability

TDHF(TDDFT) calculation in 3D real space

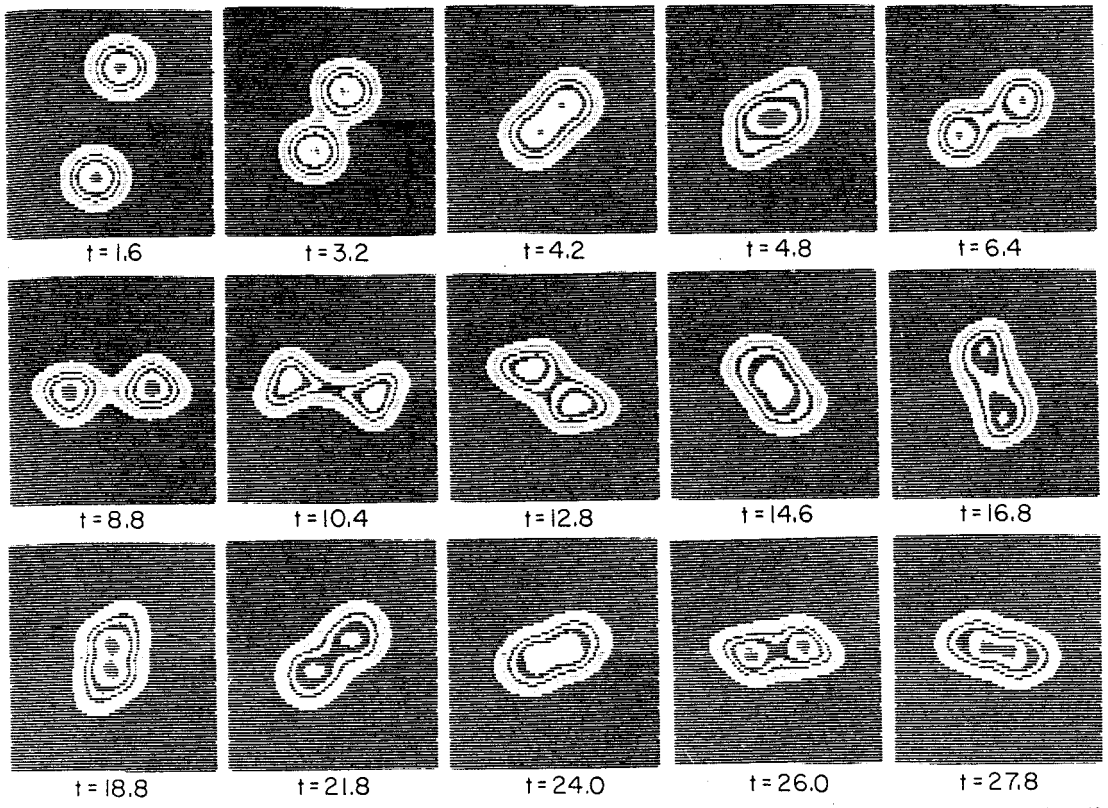


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{lab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

H. Flocard, S.E. Koonin, M.S. Weiss, Phys. Rev. 17(1978)1682.

Ionization by Laser

Electrons in a strong electric field

Laser field, E ~ Electric field of ions binding electrons

Laser frequency ω ~ HOMO-LUMO gap

Re-scattering process: A new probe for electronic structure

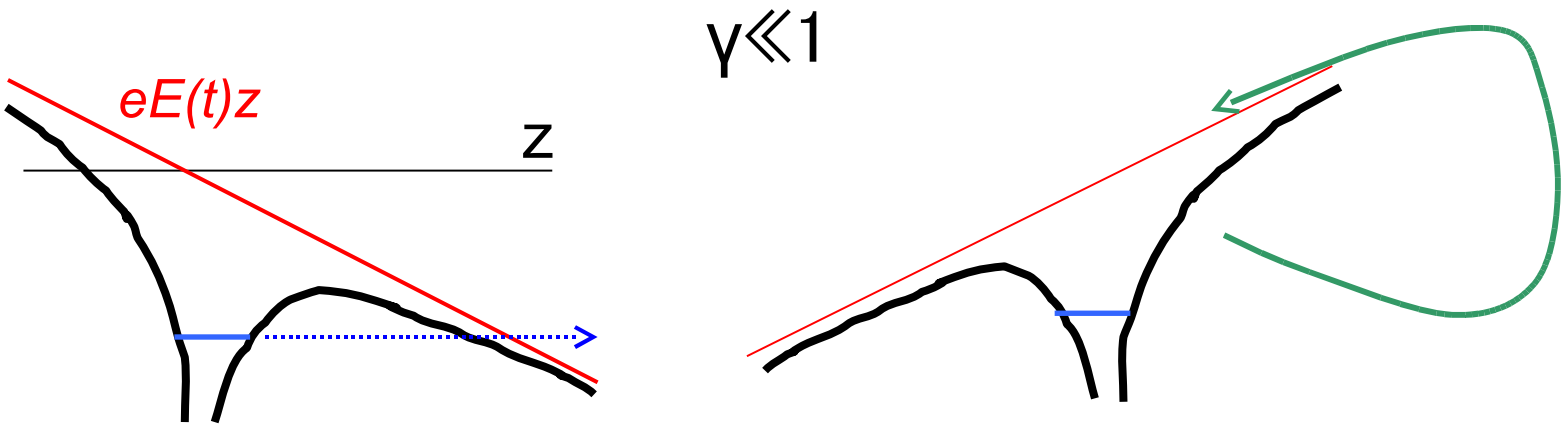
Wave packet split by the laser field

Re-accelerated toward the origin

Scattered by the remaining part of itself

Keldysh parameter

$$\gamma = \tau_{tunnel}\omega_{laser}$$

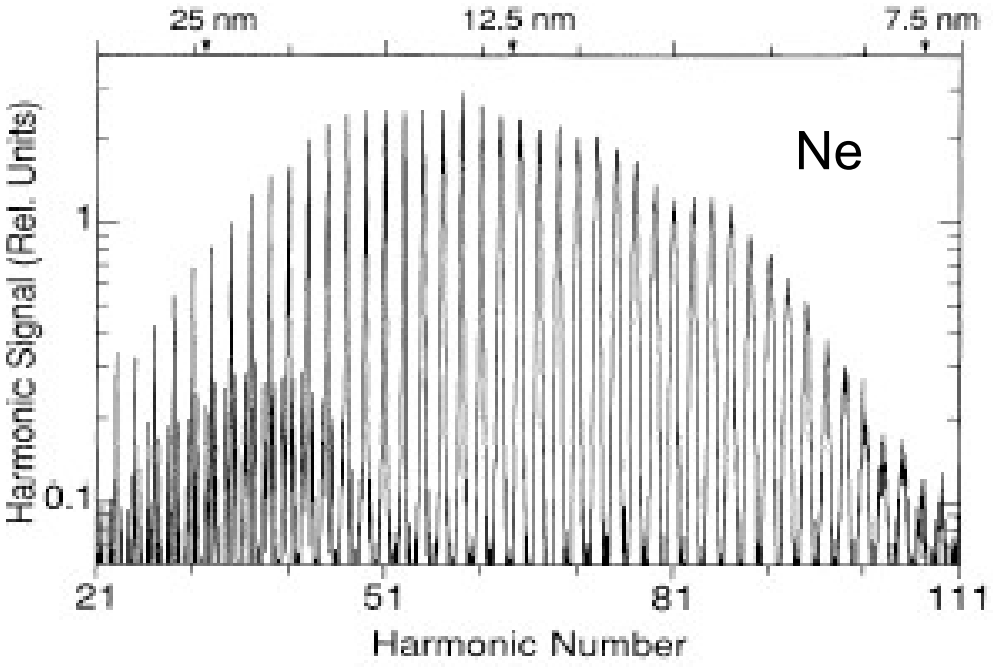


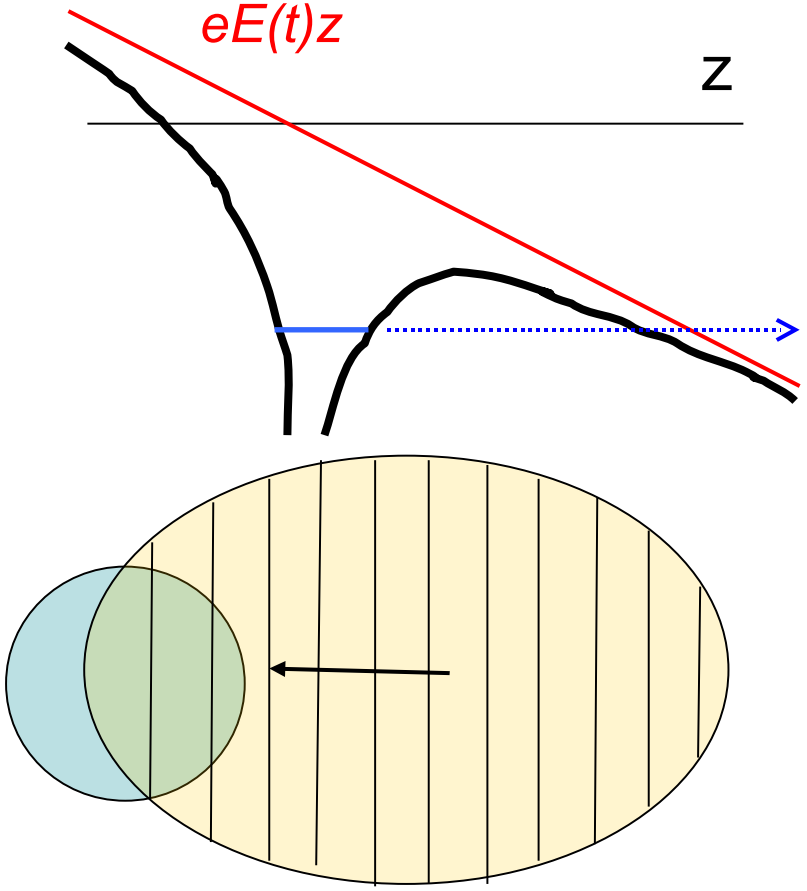
Higher-order harmonic generation

$$\psi(t) = \alpha\,\phi + \beta\, e^{i\vec{k}\cdot\vec{r} - iE_k t/\hbar}$$

$$d(t) = \langle \psi(t) | z | \psi(t) \rangle \approx \alpha^{*}\beta \left\langle \phi \left| z \right| e^{i\vec{k}\cdot\vec{r} - iE_k t/\hbar} \right\rangle + cc$$

$$I(\omega) \propto \left| \int dt e^{i\omega t} d_A(t) \right|^2$$

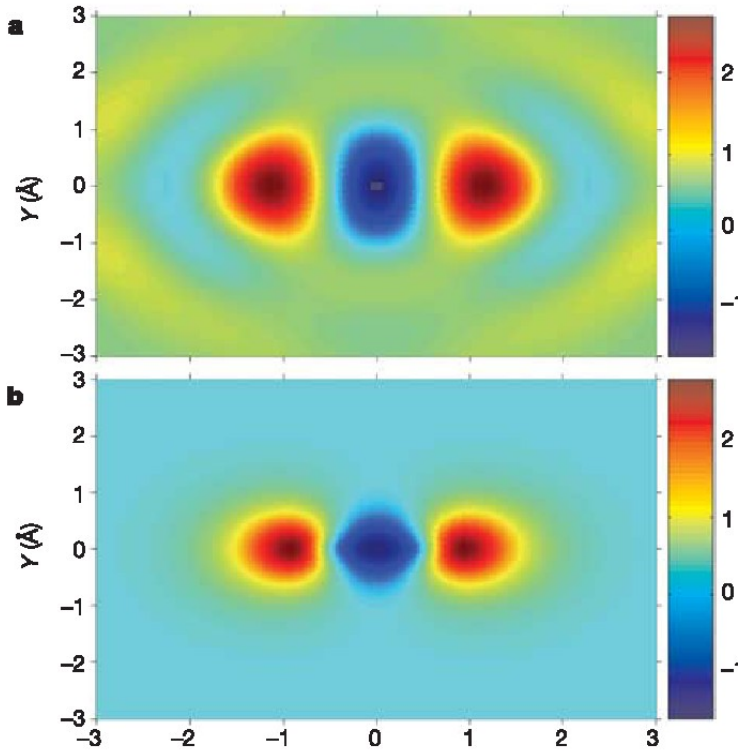




Tomographic imaging of molecular orbitals

J. Itatani[1,2], J. Levesque[1,3], D. Zeidler[1], Hiromichi Niikura[1,4], H. Pépin[3], J. C. Kieffer[3], P. B. Corkum[1] & D. M. Villeneuve[1]

[1]*National Research Council of Canada, 100 Sussex Drive, Ottawa, Ontario K1A 0R6, Canada*
[2]*University of Ottawa, 150 Louis Pasteur, Ottawa, Ontario K1N 6N5, Canada*
[3]*INRS- Energie et Materiaux, 1650 boulevard Lionel-Boulet, CP 1020, Varennes, Québec J3X 1S2, Canada*
[4]*PRESTO, Japan Science and Technology Agency, 4-1-8 Honcho Kawaguchi Saitama, 332-0012, Japan*



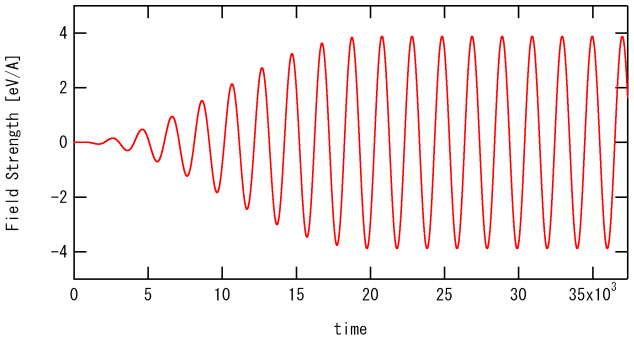
HOMO orbital in N_2

(Molecular tomography)

Ab inito calculation

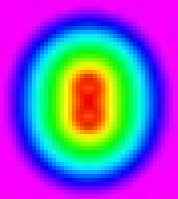
N_2 molecule

$2x10^{14}W/cm^2$, 800nm laser



Calculated by Yabana

50fs



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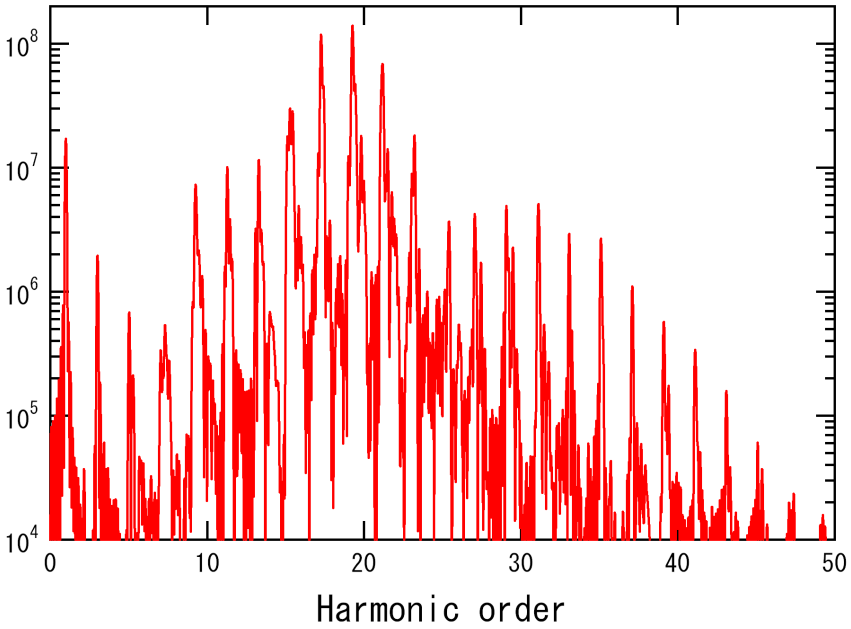
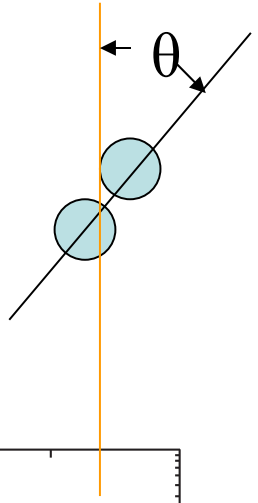
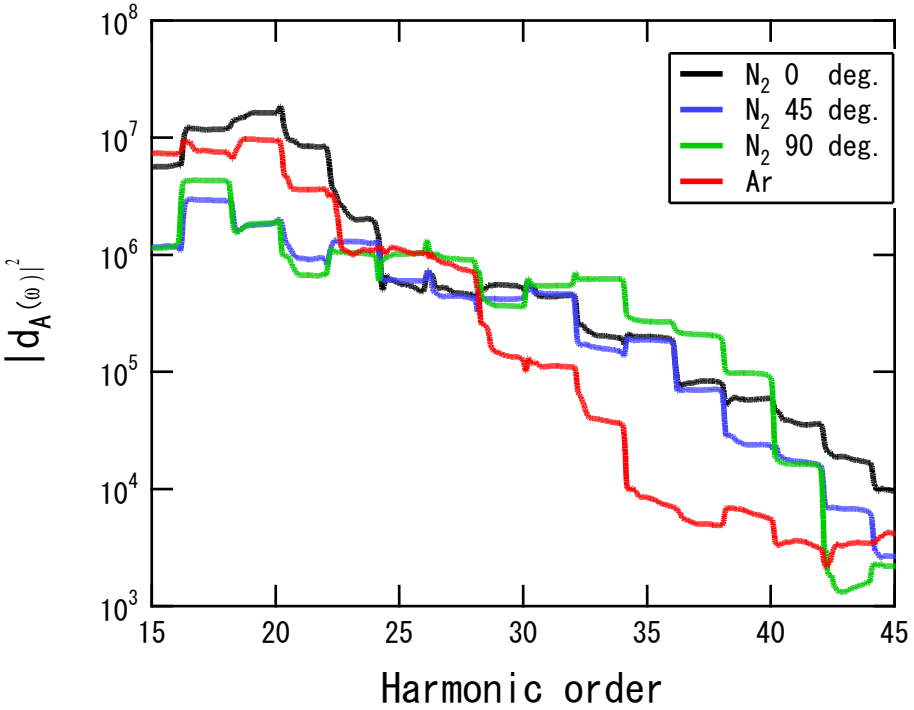


$iE_k t/\hbar\rangle + cc$

Comparison with experiments



Calculation



Experiment

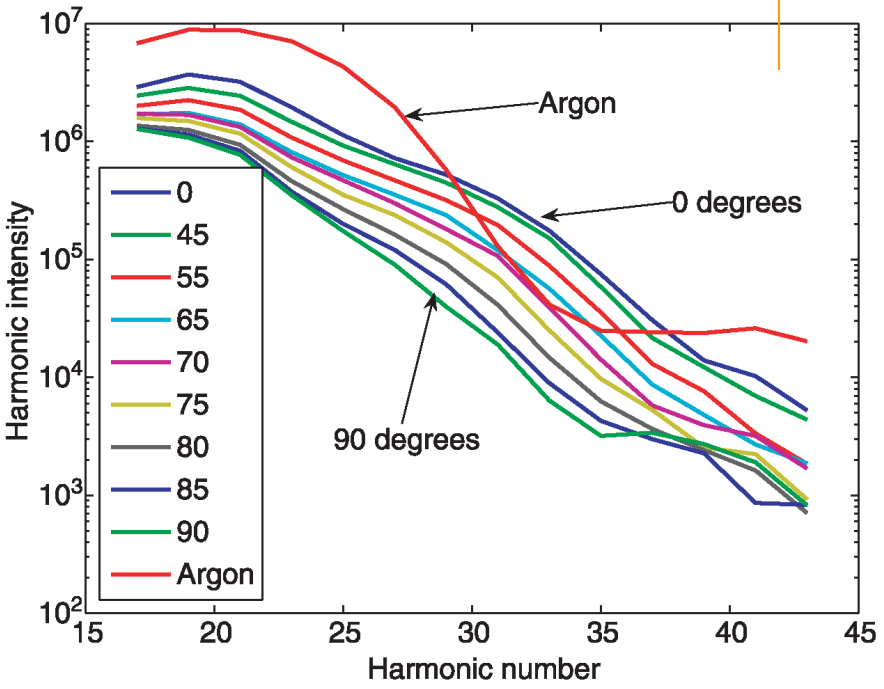
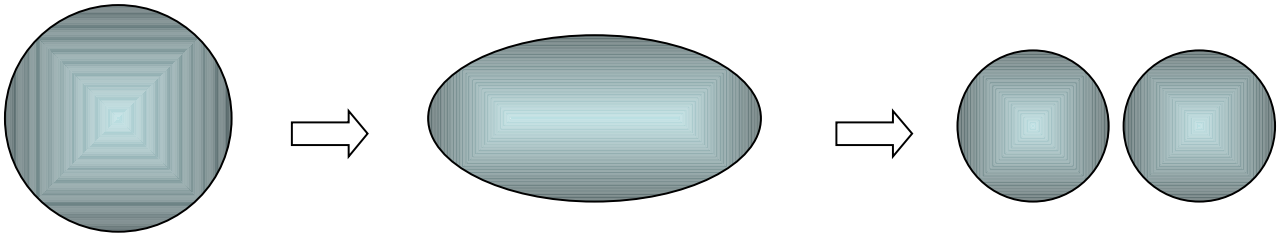


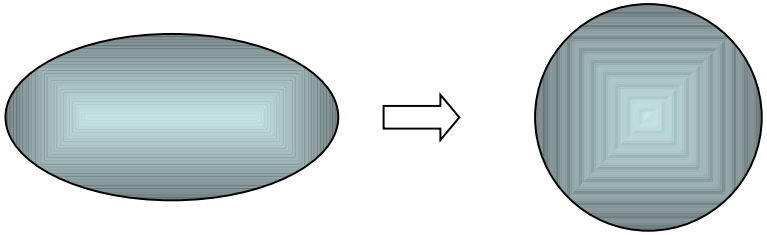
Figure 3 High harmonic spectra were recorded for N_2 molecules aligned at 19 different angles between 0 and 90° relative to the polarization axis of the laser. For clarity, only some of the angles have been plotted above. The high harmonic spectrum from argon is also shown; argon is used as the reference atom. Clearly the spectra depend on both the alignment angle and shape of the molecular orbital.

Large amplitude collective motion (LACM) in nuclei

- Fission



- Decay of superdeformed band



- Shape-coexistence phenomena

$$|\Phi\rangle = c_1 \left| \quad \right\rangle + c_2 \left| \quad \right\rangle$$

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

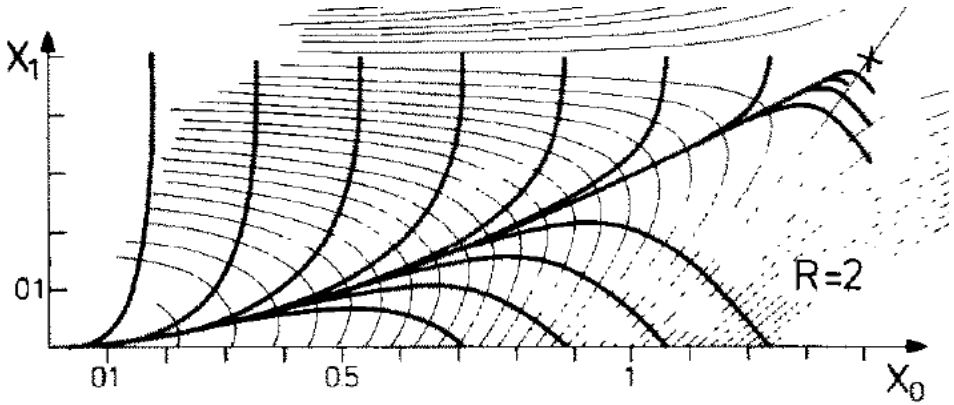
  - Eq. for the collective subspace (zero-th and first-order w.r.t. momenta)

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

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

Goeke, Reinhard, Rowe, NPA359 (1981) 408

  - Non-uniqueness problem "Validity condition" (Goeke-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.

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

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

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

- 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).

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

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

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

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

$$|z\rangle = \exp\left(\frac{1}{2} z_{\mu\nu} a_\mu^+ a_\nu^+\right)|\Phi_0\rangle$$

The TDHF(B) equation becomes in a form

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

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

$$\mathcal{H}(z,z^+) = \frac{\langle z|H|z\rangle}{\langle z|z\rangle}$$

The Holstein-Primakoff-type mapping $\beta_{\mu\nu} = \left[z(1+z^+z)^{1/2}\right]_{\mu\nu}$

leads to

$$i\dot{\beta} = 2\frac{\partial \mathcal{H}}{\partial \beta^+}$$

$$i\dot{\beta}^+ = -2\frac{\partial \mathcal{H}}{\partial \beta}$$

$$\beta_{\mu\nu} = (\xi + i\pi)_{\mu\nu}/\sqrt{2} \longrightarrow$$

$$\dot{\xi}_{\mu\nu} = \frac{\partial \mathcal{H}}{\partial \pi_{\mu\nu}}$$

$$i\dot{\pi}_{\mu\nu} = -\frac{\partial \mathcal{H}}{\partial \xi_{\mu\nu}}$$

TDHF(B) →Small amplitude limit

Small fluctuation around the HF(B) state

$$2\text{qp index}\ \alpha = (\mu\nu)$$

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

$$A_{\alpha\beta} = \langle \Phi_0 | [(aa)_\alpha, [H, (a^+a^+)_\beta]] | \Phi_0 \rangle, \quad B_{\alpha\beta} = \langle \Phi_0 | [(aa)_\alpha, [H, (aa)_\beta]] | \Phi_0 \rangle$$

Rewriting the last term in terms of variables (ξ^α, π_α)

$$\langle \xi,\pi \,|H|\, \xi,\pi \rangle = E_{\mathrm{RPA}} + \frac{1}{2}(\bar{\kappa}^*, \bar{\kappa}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \bar{\kappa} \\ \bar{\kappa}^* \end{pmatrix}, \quad \bar{\kappa} \equiv \beta\,(1 - \beta^+\beta) \approx \beta$$

$$= E_{\mathrm{RPA}} + \frac{1}{2}(A+B)_{\alpha\beta}\xi^\alpha\xi^\beta + \frac{1}{2}(A-B)_{\alpha\beta}\pi_\alpha\pi_\beta$$

Linear point transformation $(\xi^\alpha, \pi_\alpha) \rightarrow (q^\mu, p_\mu)$ leads to

$$= E_{\mathrm{RPA}} + \frac{1}{2}\sum_n \left[p_\mu^2 + \omega_n^2 (q^\mu)^2 \right]$$

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

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

Decoupled classical motion within the point transformation

Klein, Walet, DoDang, Ann. Phys. 208 (1991) 90

Expanding the classical Hamiltonian w.r.t. momentum up to 2nd order

$$H(\xi,\pi) = \frac{1}{2} B^{\alpha\beta}\pi_\alpha \pi_\beta + V(\xi), \quad B^{\alpha\beta} \equiv \left.\frac{\partial^2 H}{\partial \pi_\alpha \partial \pi_\beta}\right|_{\pi=0}$$

Point transformation $(\xi,\pi) \to (q,p)$

$$q^\mu = f^\mu(\xi), \quad \xi^\alpha = g^\alpha(q)$$

$$p_\mu = g^\alpha_{,\mu}\pi_\alpha, \quad \pi_\alpha = f^\mu_{,\alpha} p_\mu$$

$$g^\alpha_{,\mu} \equiv \frac{\partial g^\alpha}{\partial q^\mu} = \frac{\partial \xi^\alpha}{\partial q^\mu}, \quad f^\mu_{,\alpha} \equiv \frac{\partial f^\mu}{\partial \xi^\alpha} = \frac{\partial q^\mu}{\partial \xi^\alpha}$$

Point transformation conserves the quadratic form in momenta.

$$\overline{H}(q,p) = \frac{1}{2}\overline{B}^{\mu\nu} p_\mu p_\nu + \overline{V}(q), \quad \overline{B}^{\mu\nu} \equiv f^\mu_{,\alpha} B^{\alpha\beta} f^\nu_{,\beta}$$

Metric tensor: $B_{\alpha\beta}$: defined by $B_{\alpha\gamma}B^{\gamma\beta} = \delta_\alpha^{\ \beta}$

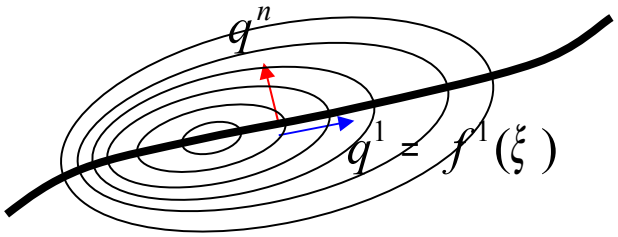
Shift-up and down of indexes: $V^{,\alpha} \equiv B^{\alpha\beta} V_{,\beta}$

Chain rules: $g^\alpha_{,\mu} f^\mu_{,\beta} = \delta_\alpha^{\ \beta}, \quad f^\mu_{,\alpha} g^\alpha_{,\nu} = \delta_\nu^{\ \mu}$ (=canonical variable cond.)

Assuming that there is a decoupled path (1-dim. collective submanifold)

$$q^1 : \text{Collective coordinate}, \quad q^n : \text{Non-collective coord.}$$

Decoupling condition: $q^n = p_n = 0 \Rightarrow \dot{q}^n = \dot{p}_n = 0$



$$\Updownarrow$$

(1) $\overline{V}_{,n} = 0$	(1) $V_{,\alpha} = \overline{V}_{,1} f^1_{,\alpha}$
(2) $\overline{B}^{n1} = 0$ $\Leftrightarrow$	(2) $B^{\alpha\beta} f^1_{,\beta} = \overline{B}^{11} g^{\alpha}_{,1}$
(3) $\overline{B}^{11}_{,n} = 0$	(3) $\overline{B}^{11}_{,\alpha} = \overline{B}^{11}_{,1} f^1_{,\alpha}$

Decoupling condition (1) $\leftrightarrow$ HF(B) with the constraint $q^1 = \left\langle \Phi(q^1) \middle| \hat{Q}(q^1) \middle| \Phi(q^1) \right\rangle$

$$\delta\left(V(\xi) - \frac{\partial \overline{V}}{\partial q^1} q^1 \right) = \delta\left\{ H(\xi, \pi = 0) - \lambda q^1(\xi) \right\} = \delta \left\langle \Phi(q^1) \middle| H - \lambda \hat{Q}(q^1) \middle| \Phi(q^1) \right\rangle = 0$$

Using the decoupling conditions (2) and (3), we may construct the constraint operator $Q(q)$. More precisely speaking, we can determine the 2qp parts of $Q(q)$.

Differentiating the chain relation $V_{,\alpha} = \overline{V}_{,\mu} f^{\mu}_{,\alpha}$

$$V_{,\alpha\beta} = \overline{V}_{,\mu\nu} f^{\mu}_{,\alpha} f^{\nu}_{,\beta} + \overline{V}_{,\mu} f^{\mu}_{,\alpha\beta}$$

The last term indicates that the second derivative of the potential is not covariant. This can be rewritten in a covariant derivative

$$V_{;\alpha\beta} = \overline{V}_{;\mu\nu} f^{\mu}_{,\alpha} f^{\nu}_{,\beta} \qquad V_{;\alpha\beta} \equiv V_{,\alpha\beta} - \Gamma^{\gamma}_{\alpha\beta} V_{,\gamma}\ , \quad \overline{V}_{;\mu\nu} \equiv \overline{V}_{,\mu\nu} - \overline{\Gamma}^{\rho}_{\mu\nu} \overline{V}_{,\rho}$$

Here, two different definitions of the metric tensor are possible:

(i) Riemannian type

Mass tensor as the metric tensor

$$\Gamma^{\gamma}_{\alpha\beta} \equiv \frac{1}{2} B^{\gamma\delta} \left(B_{\delta\alpha,\beta} + B_{\delta\beta,\alpha} - B_{\alpha\beta,\delta} \right)$$ Affine connection

(ii) Symplectic type

Metric tensor $K_{\alpha\beta} = \sum_{\mu} f^{\mu}_{,\alpha} f^{\mu}_{,\beta}\ , \quad K^{\alpha\beta} = \sum_{\mu} g^{\alpha}_{,\mu} g^{\beta}_{,\mu}$ $\qquad K_{\alpha\beta} = B_{\alpha\beta}$

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

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

A certain combination of the decoupling conditions (1-3) leads to the following Local Harmonic Equation (LHE) (with metric tensor K_{ij}):

$$V^{,\beta}_{;\alpha} f^1_{,\beta} = \omega^2 f^1_{,\alpha} \qquad V^{,\beta}_{;\alpha} \equiv B^{\beta\gamma} V_{;\alpha\gamma}, \quad V_{;\alpha\beta} \equiv V_{,\alpha\beta} - \Gamma^{\gamma}_{\alpha\beta} V_{,\gamma}$$

(i) Riemannian LHE

The condition (3) is equivalent to that the decoupled collective path is geodesic with metric tensor of $B_{\alpha\beta}$

$$\delta \int \sqrt{\overline{B}_{11}(q^1)}\, dq^1 = 0 \quad \Rightarrow \quad f^1_{,\alpha\beta} - \Gamma^{\gamma}_{\alpha\beta} f^1_{,\gamma} + \overline{\Gamma}^1_{11} f^1_{,\alpha} f^1_{,\beta} = 0$$

Then, using the condition (2), we can derive the LHE above.

$$\omega^2 = \overline{V}^1_{;1} = \overline{B}^{11}\left(\overline{V}_{,11} - \Gamma^1_{11}\overline{V}_{,1}\right)$$

(ii) Symplectic LHE

Without the condition (3), we can derive the LHE.

$$\omega^2 = \overline{V}^1_{;1} = \overline{B}^{11}\overline{V}_{,11}$$

Either neglect, or determine by a certain condition, the curvature $f^1_{,\alpha\beta}$

Riemannian LHE vs Symplectic LHE

Symplectic LHE is (almost) identical to the "adiabatic" approximation of the Self-consistent Collective Coordinate (SCC) Method

Original formulation: Matsuo, TN, Matsuyanagi, Prog. Theor. Phys. 103 (2000) 959
Gauge-invariant formulation: Hinohara et al, PTP 117 (2007) 451

We believe that the Symplectic LHE (ASCC) is superior to the Riemannian LHE in the following reasons:

- Extension to lift the restriction to the point transformation can be consistently achieved.
- Both formalisms coincide with the RPA at equilibrium. However, in case of superconducting nuclei, the "extended" symplectic LHE naturally becomes identical to the QRPA.
- Nambu-Goldstone modes are automatically separated from the decoupled collective variables, as zero-energy solutions.

Separation of Nambu-Goldstone modes

Extended “point” transformation

$$q^\mu = f^\mu(\xi) + \frac{1}{2} f^{(1)\mu\alpha\beta}\pi_\alpha\pi_\beta + O(\pi^4) \qquad \xi^\alpha = g^\alpha(q) + \frac{1}{2} g^{(1)\alpha\mu\nu} p_\mu p_\nu + O(p^4)$$

$$p_\mu = g^\alpha_{,\mu}\pi_\alpha + O(\pi^3) \qquad \pi_\alpha = f^\mu_{,\alpha} p_\mu + O(p^3)$$

This extension leads to the modification of mass parameter, but the other formulation is kept invariant. $\widetilde{B}^{\alpha\beta} \equiv B^{\alpha\beta} - \overline{V}_{,\mu} f^{(1)\mu\alpha\beta}$

(1) Symmetry operator *S* = momentum

TN, Walet, DoDang, PRC61 (1999) 014302

$$p_s = g^\alpha_{,s}\pi_\alpha + O(\pi^3) \xrightarrow[\{p_s, H\}_{\mathrm{PB}} = 0]{} g^\alpha_{,s} V_{,\alpha} = 0 \quad \Rightarrow \quad V_{;\alpha\beta} g^\alpha_{,s} = 0$$

(2) Symmetry operator *S* = coordinate

$$q^s = f^s(\xi) + \frac{1}{2} f^{(1)s\alpha\beta}\pi_\alpha\pi_\beta + O(\pi^4)$$

$$\Longrightarrow \quad \widetilde{B}^{\alpha\beta} f^s_{,\beta} = B^{\alpha\beta} f^s_{,\beta} - \overline{V}_{,\mu} f^{(1)\mu\alpha\beta} f^s_{,\beta}$$

$$= B^{\alpha\beta} f^s_{,\beta} - \overline{V}_{,\mu} f^{(1)s\alpha\beta} f^\mu_{,\beta} \qquad (\because \{q^\mu, q^\nu\}_{\mathrm{PB}} = 0)$$

$$= B^{\alpha\beta} f^s_{,\beta} - V_{,\beta} f^{(1)s\alpha\beta} = 0 \qquad (\because \{q^s, H\}_{\mathrm{PB}} = 0)$$

Collective path and re-quantization

Solve the constrained MF eq. and LHE to obtain self-consistent solutions

Symplectic LHE

(CMF) $V_{,\alpha} = \overline{V}_{,1} f^{1}_{,\alpha}$

(LHE) $V^{,\beta}_{;\alpha} f^{1}_{,\beta} = \omega^{2} f^{1}_{,\alpha}$

$V^{,\beta}_{;\alpha} \equiv B^{\beta\gamma}\left(V_{,\alpha\lambda} - \overline{V}_{,1} f^{1}_{,\alpha\gamma}\right)$

Adiabatic SCC

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

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

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

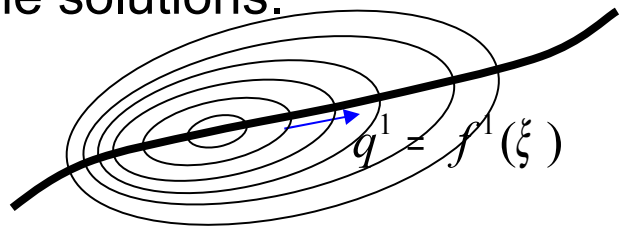
$\left. - \frac{1}{2B(q)}\left[\left[\hat{H}, (\partial V/\partial q)\hat{Q}(q)\right], \hat{Q}(q)\right]\middle|\phi(q)\right\rangle = 0$

We obtain a series of “Slater determinants”, as the solutions.

$|\phi(q_1)\rangle, |\phi(q_2)\rangle, |\phi(q_3)\rangle, \cdots \longrightarrow$ GCM

$\overline{B}(q_1), \overline{B}(q_2), \overline{B}(q_3), \cdots$

$\overline{V}(q_1), \overline{V}(q_2), \overline{V}(q_3), \cdots \longrightarrow$ “Collective Hamiltonian”



$$\overline{H}(q,p) = \frac{1}{2}\overline{B}(q)p^2 + \overline{V}(q) \Rightarrow \frac{1}{2}\sqrt{\overline{B}(q)}\left(\frac{\partial}{i\partial q}\right)\sqrt{\overline{B}(q)}\left(\frac{\partial}{i\partial q}\right) + \overline{V}(q)$$

Applications to simple models

Applications to O(4) models

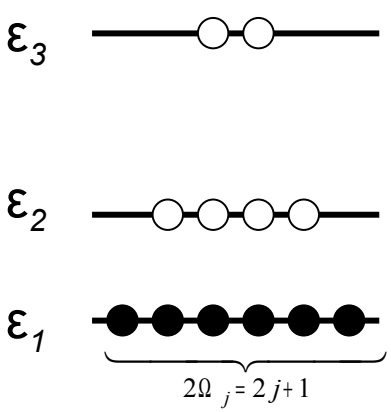
Model Hamiltonian

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

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

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

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

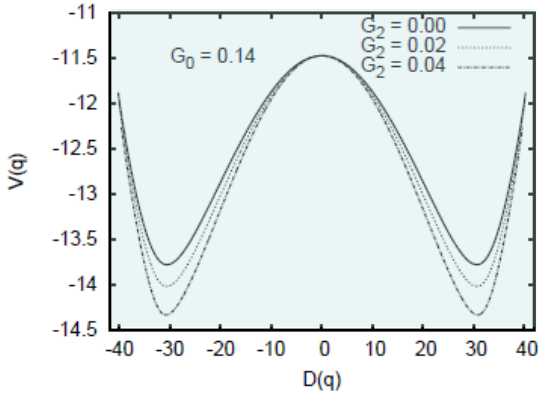
Hinohara, TN, Matsuo, Matsuyanagi, PTP115 (2006) 567

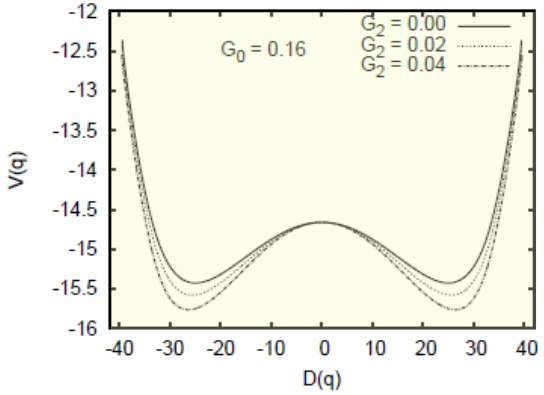
Potential

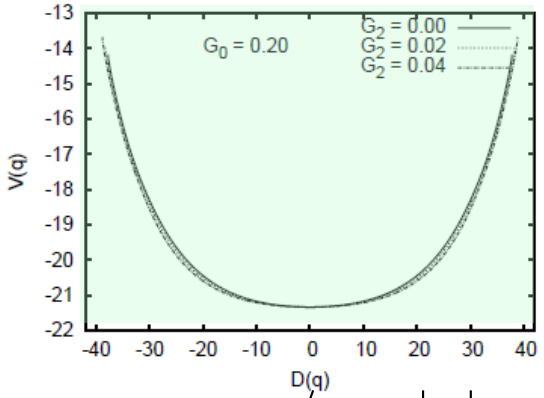
Mass: M=1/B

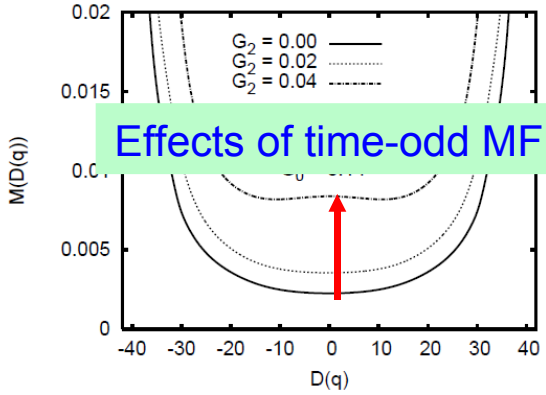
Cranking Mass

Larger G_0

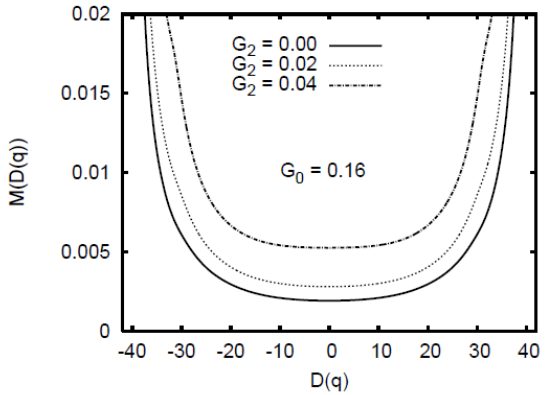


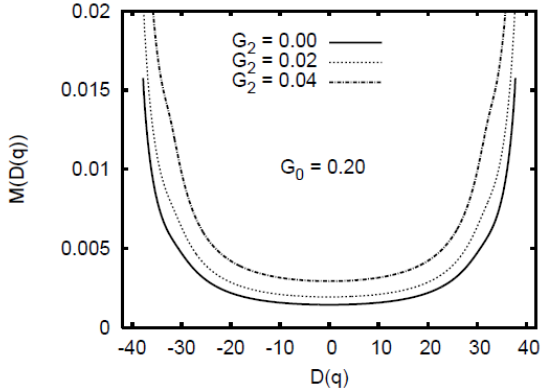


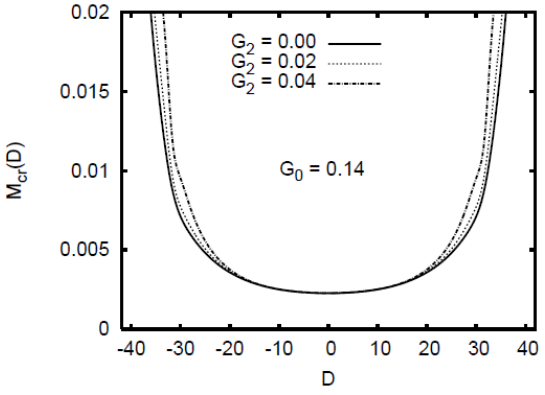


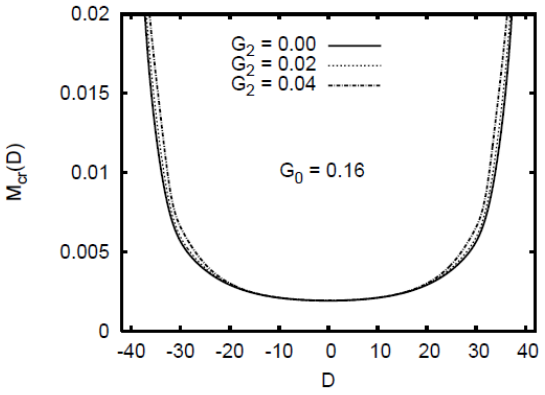


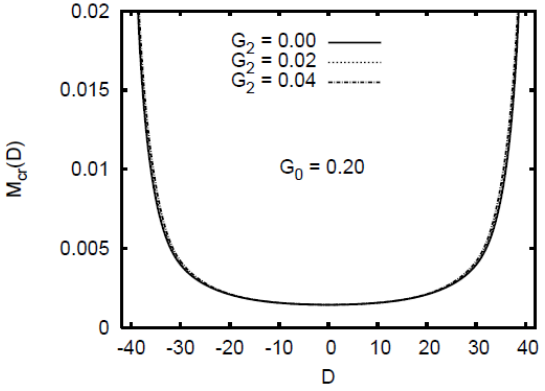
Effects of time-odd MF









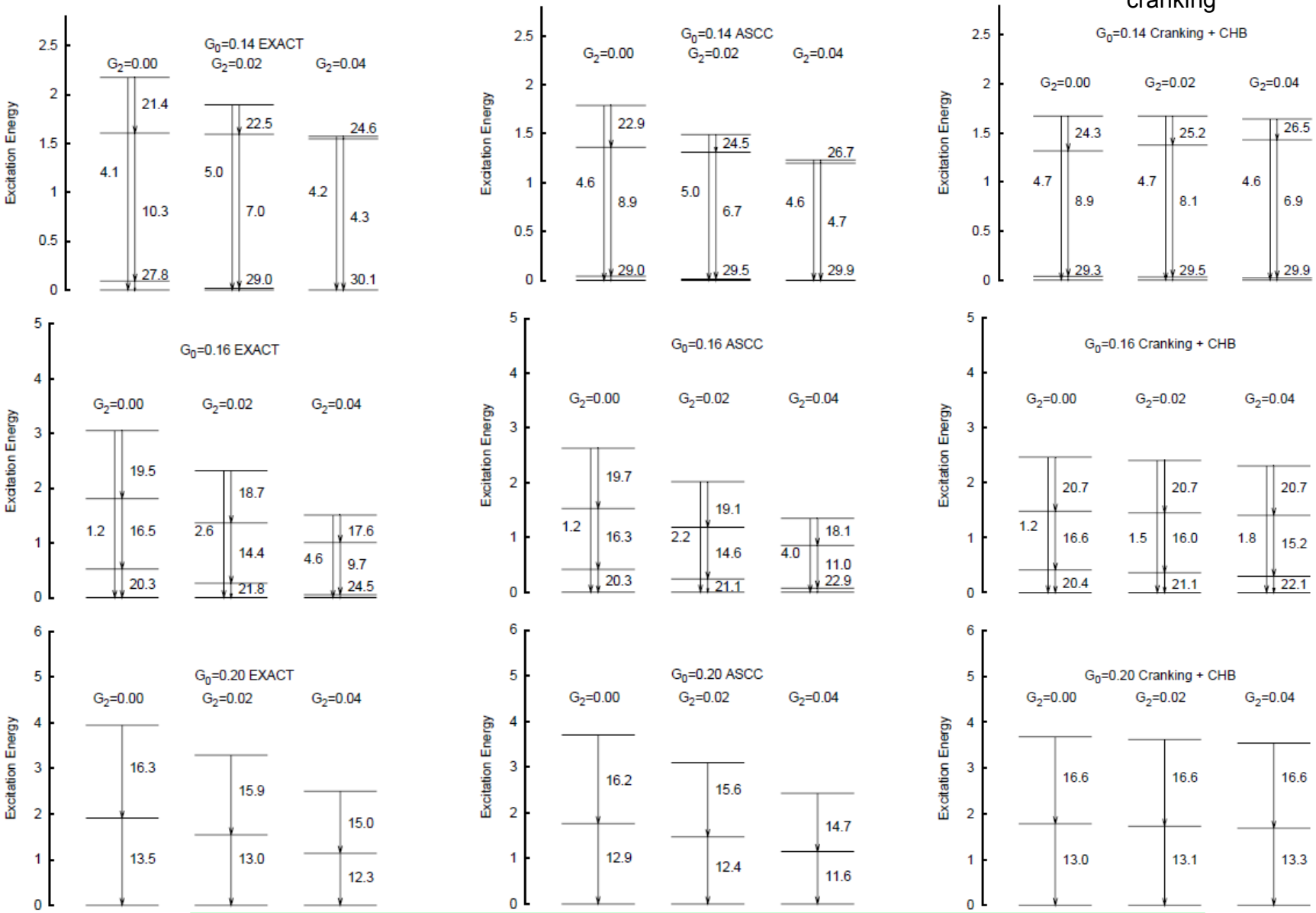


$$D(q) \equiv \left\langle \phi\,(q) \middle| Q \middle| \phi\,(q) \right\rangle$$

Exact

Adiabatic SCC

CHB with $M_{cranking}$



Time-odd effects are neglected in the cranking mass !

Curvature effects

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

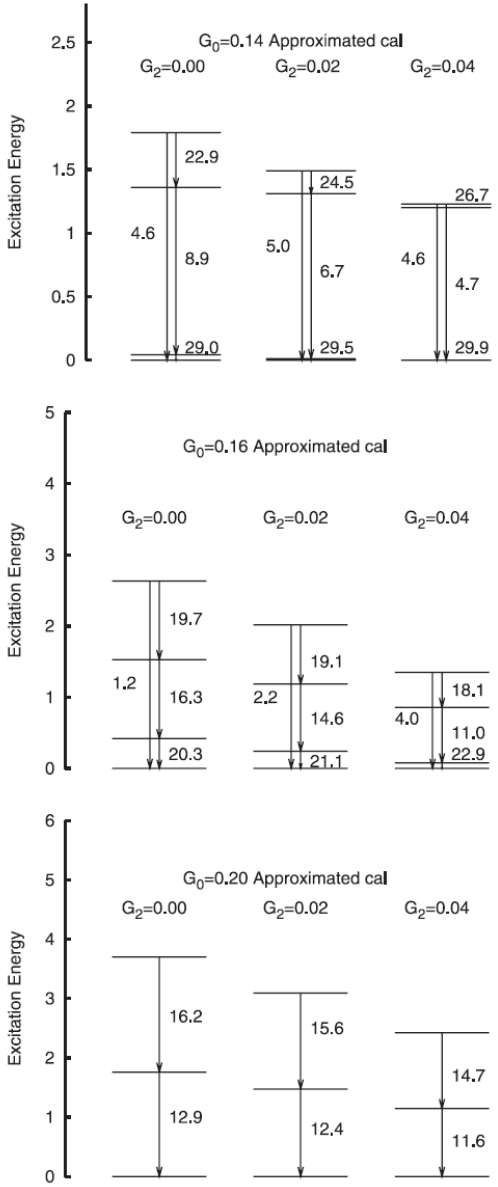
$$\updownarrow$$

$$f^{1}_{,\alpha\beta}$$

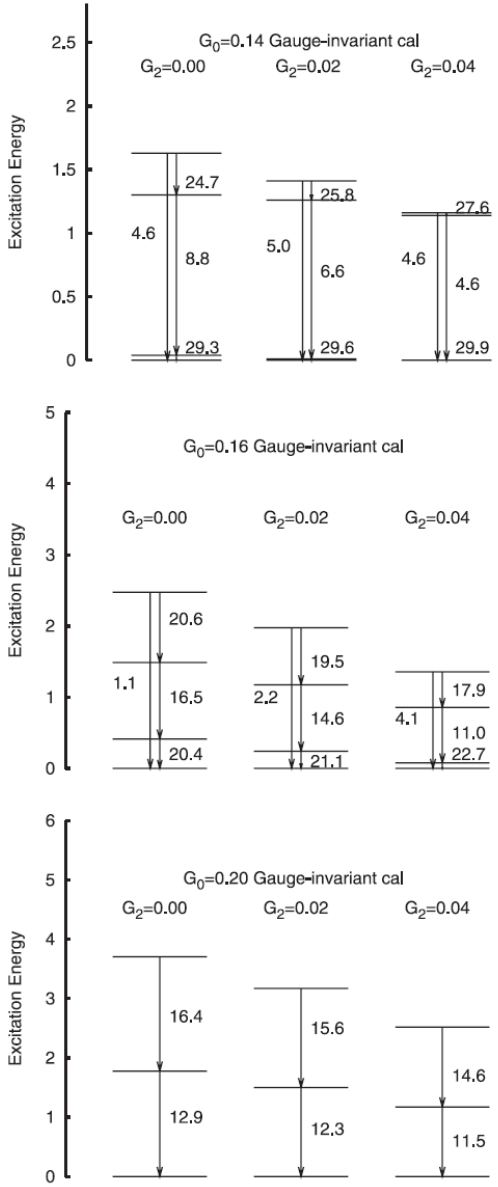
In this model, requiring the gauge invariance, we can determine them.

The curvature effects are weak.

Neglected calc



Full calc



Model of protons and neutrons

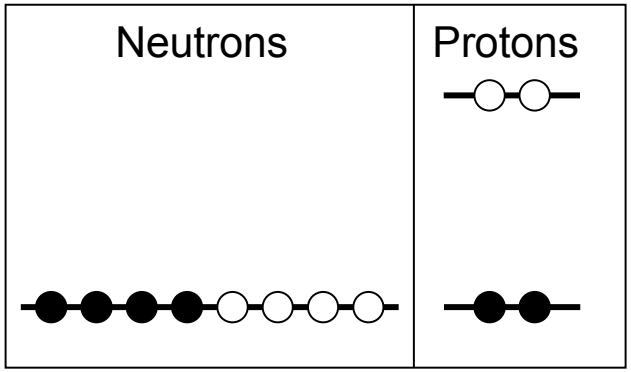
T.N. & Walet, PRC58 (1998) 3397

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

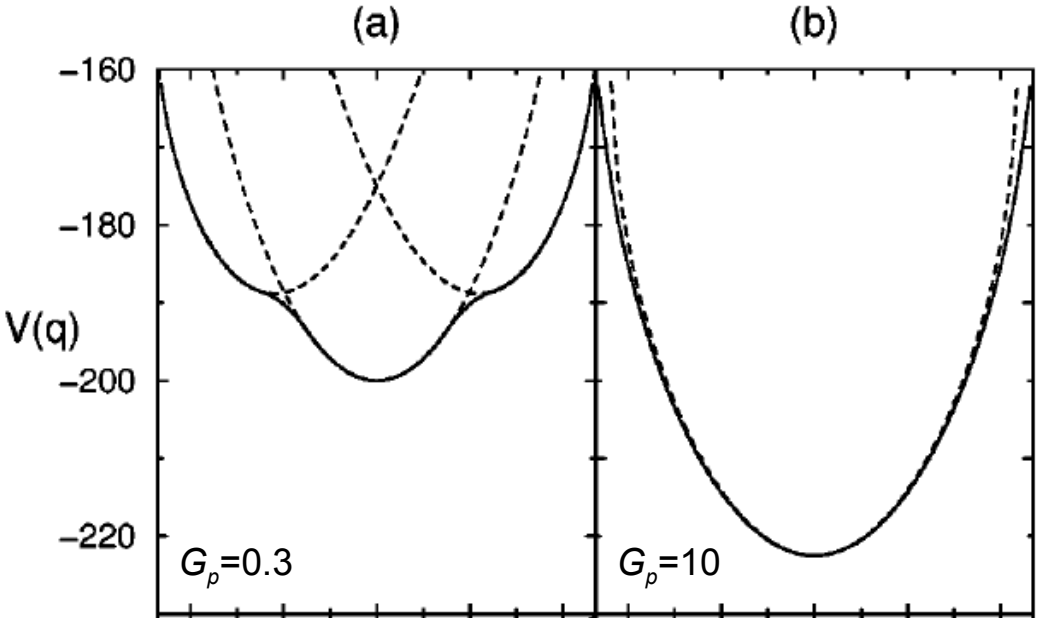
$$H_n = \sum_{i \in n, m_i} \epsilon_i c^\dagger_{j_i m_i} c_{j_i m_i} - G_n P^\dagger_n P_n - \tfrac{1}{2}\kappa Q^2_n\,,$$

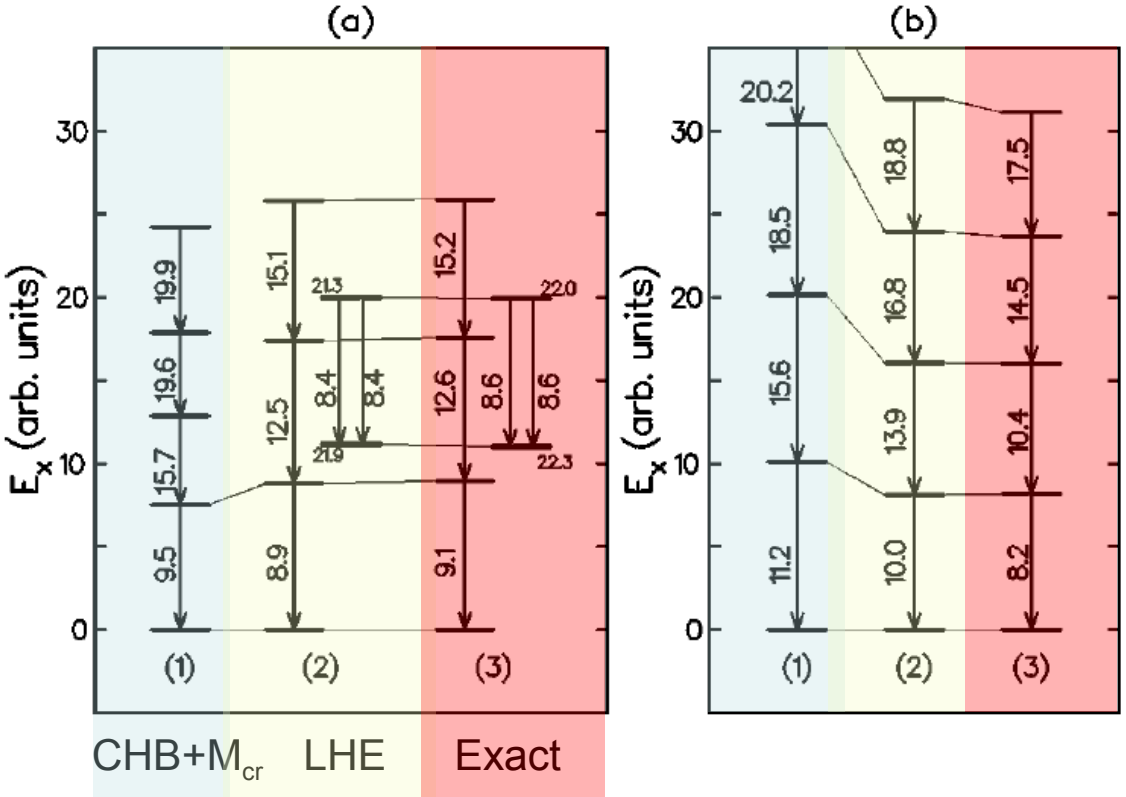
$$H_p = \sum_{i \in p, m_i} \epsilon_i c^\dagger_{j_i m_i} c_{j_i m_i} - G_p P^\dagger_p P_p - \tfrac{1}{2}\kappa Q^2_p\,,$$

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



Upper orbital has a larger quadrupole moment



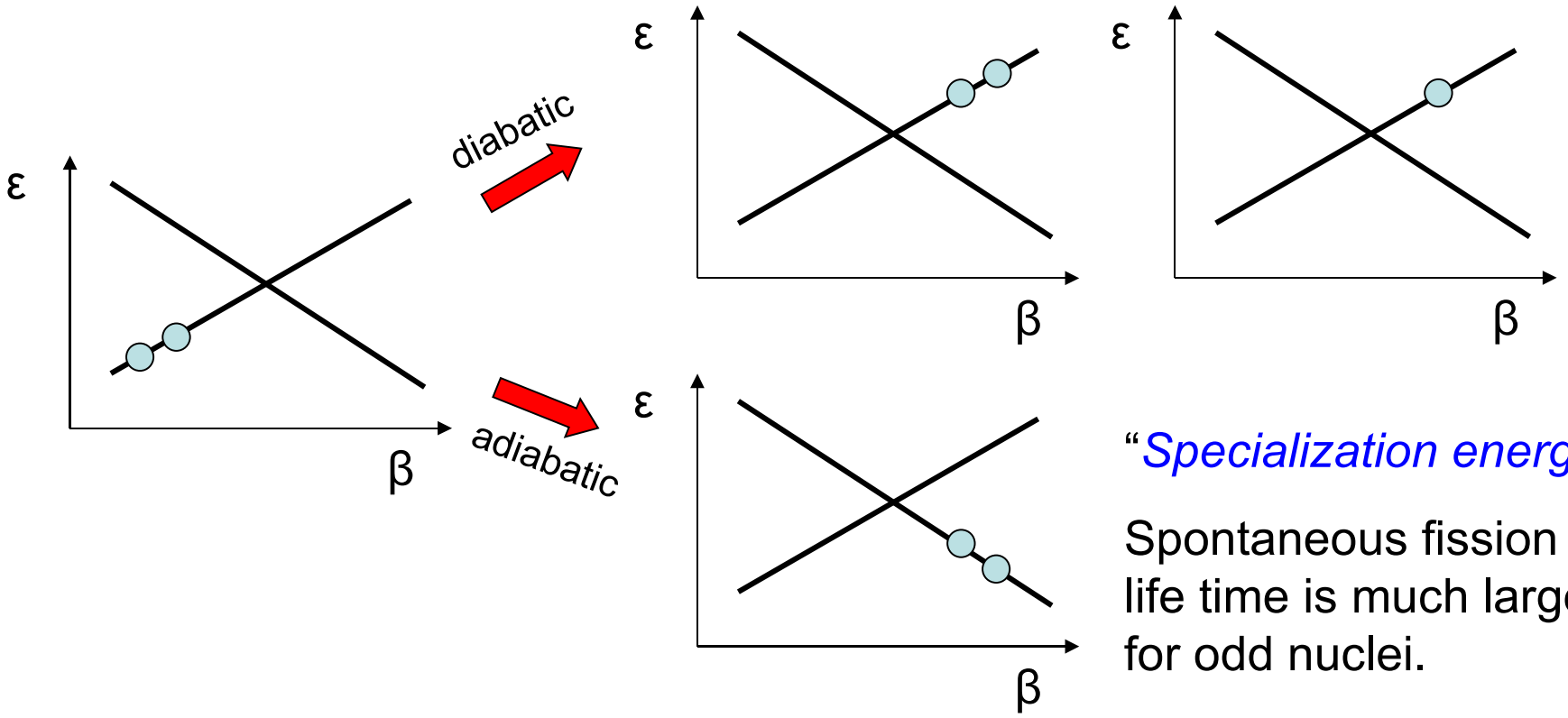


Adiabatic vs Diabatic Dynamics

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.



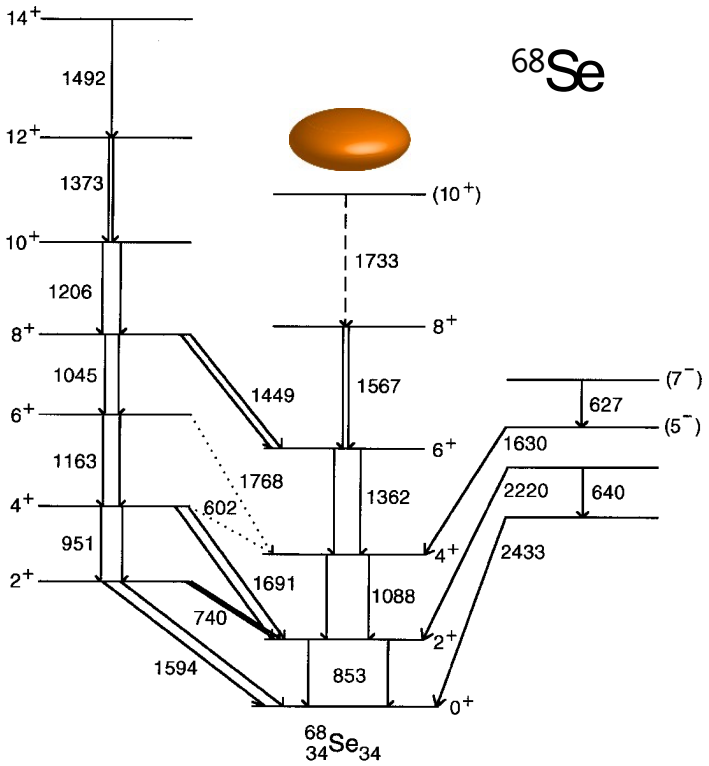
"*Specialization energy*"

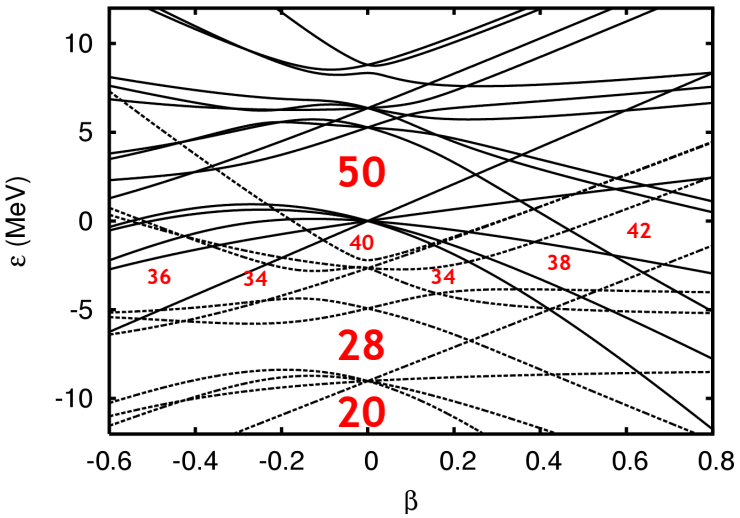
Spontaneous fission life time is much larger for odd nuclei.

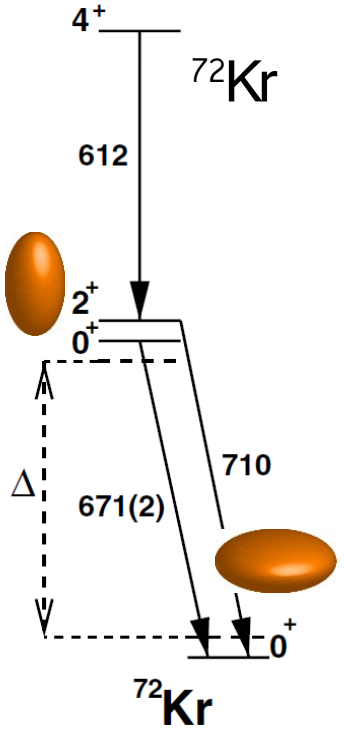
Applications to more realistic models: Separable-force model

Calculations carried out by Dr Nobuo Hinohara (YITP, Japan)

Shape coexistence in N~Z~40 region





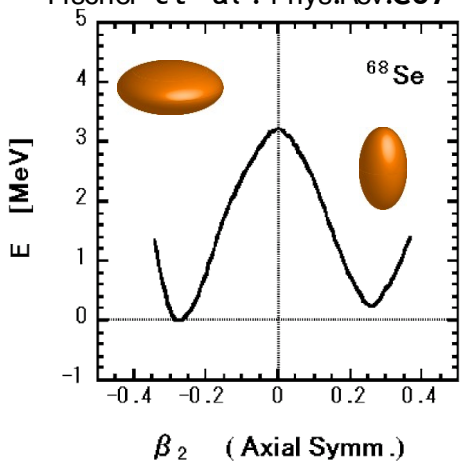


Z,N = 34,36 (oblate magic numbers)

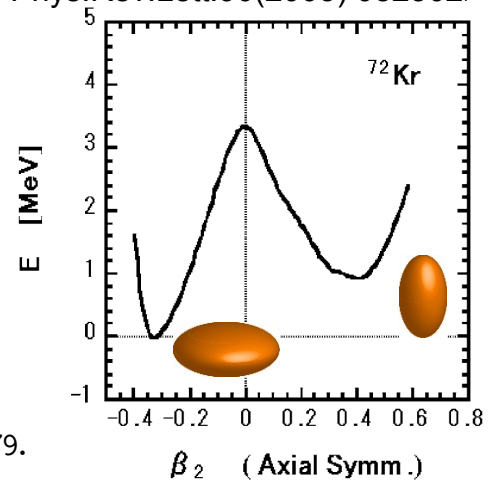
Z,N = 38 (prolate magic number)

Fischer *et al.* Phys.Rev.**C67** (2003) 064318.

Bouchez *et al.* Phys.Rev.Lett.**90**(2003) 082502.



- oblate–prolate shape coexistence
- oblate ground state
- shape coexistence/mixing



Skyrme–HFB: Yamagami *et al.* Nucl.Phys.**A693** (2001) 579.

Microscopic theory to describe shape coexistence

Large-Scale Shell Model Calculation

- Dimension becomes too large for medium-heavy nuclei
  (10^{13} dim for ^{80}Zr, ^{40}Ca core) → Too hard to perform !
- ^{68}Se: Kaneko *et al*. Phys.Rev.**C70** (2004)051301.
  Model Space: ^{56}Ni core, *fpg*-shell 1.6 x 10^{8} dim

GCM

- ^{72}Kr: Bender *et al*. Phys. Rev. **C74** (2006) 024312.
- Skyrme interaction
- Generator Coordinate: axial symmetric deformation

→ The triaxial deformation is ignored.

Adiabatic TDHF

- Adiabatic Self-consistent Collective Coordinate Method
  - ^{68}Se, ^{72}Kr: Kobayasi *et al*. (Prog.Theor.Phys.**112**(2004), **113**(2005))
- Almehed *et al*. (Phys. Lett. **B604** (2004)163.)

→ Importance of triaxial deformation is discussed

Pairing + Quadrupole Model (^{68}Se, ^{72}Kr)

Microscopic Hamiltonian

SP energy + Pairing (Monopole, Quadrupole) + Quadrupole interaction

Model Space

two major shells (N_{sh}=3,4) (^{40}Ca core)

Parameters

sp energy: Modified Oscillator
interaction strength

monopole pairing and quadrupole int. strength:
adjusted to the pairing gaps and deformations of Skyrme-HFB
(Yamagami *et al*. NPA693(2001))

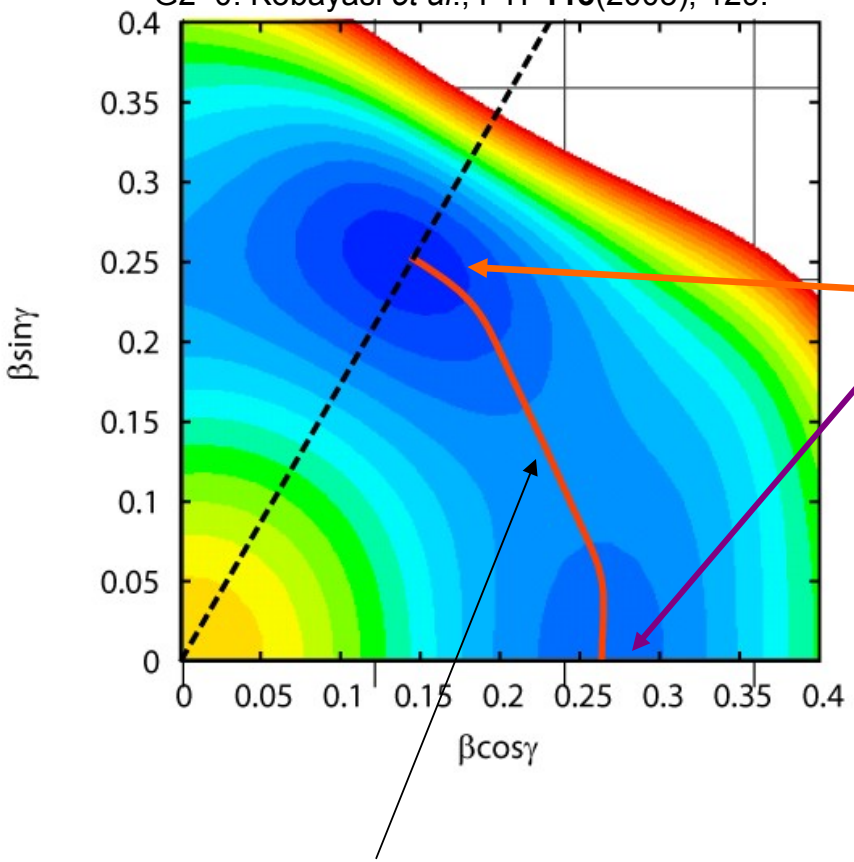
quadrupole pairing strength G_2:

- $G_2 = 0$
- $G_2 = (G_2)_{self}$ (self-consistent value) Sakamoto and Kishimoto PLB245 (1990) 321.

$(G_2)_{self}$ restores the Galilean invariance in RPA order,
which was broken by the monopole pairing.

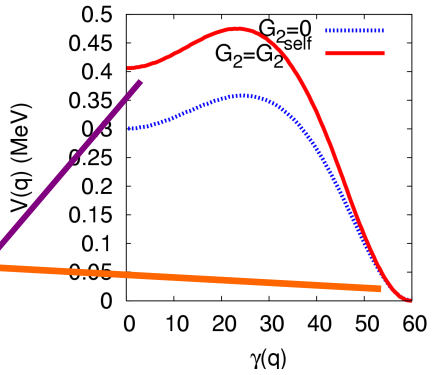
Collective path in ^{68}Se

G2=0: Kobayasi *et al.*, PTP**113**(2005), 129.

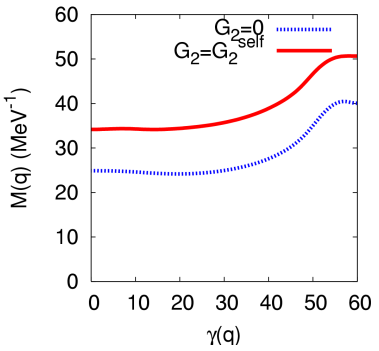


collective path

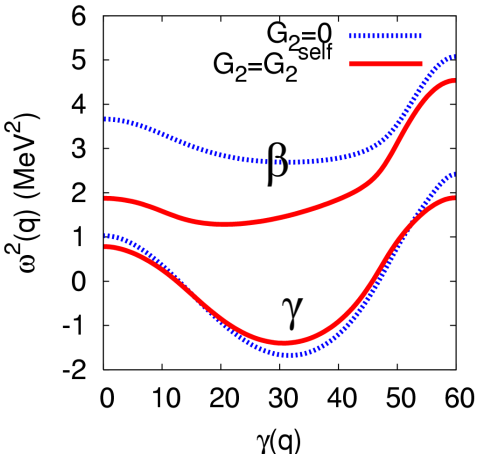
Collective potential



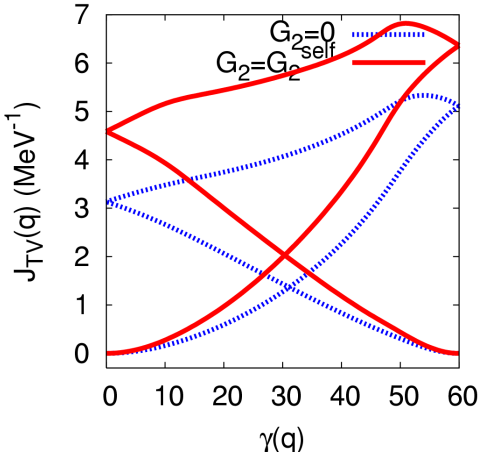
Collective mass



Moving-frame QRPA frequency



Moment of Inertia



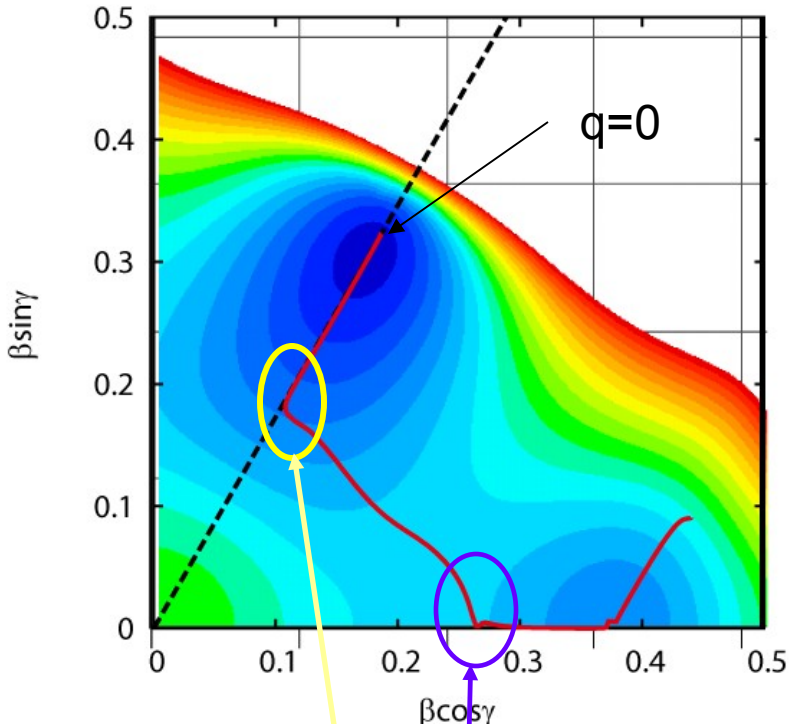
- Triaxial deformation connects two local minima
- Enhancement of the collective mass and MoI by the quadrupole pairing

→ Due to the contribution from the time-odd component

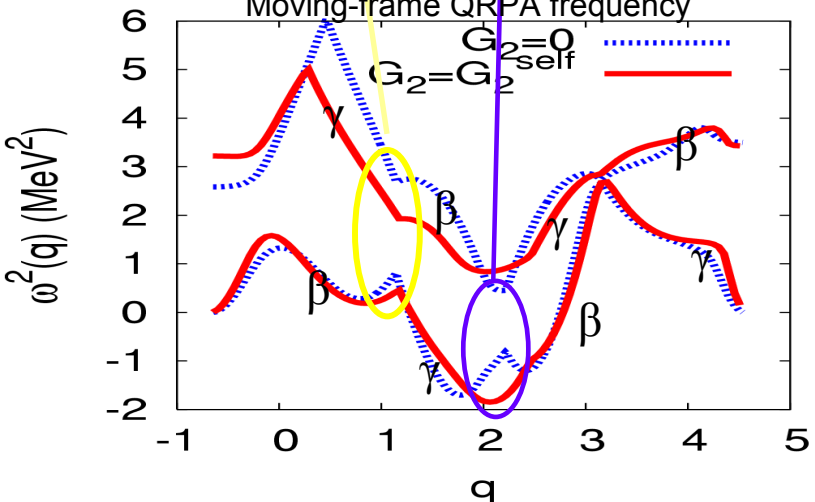
Prog.Theor.Phys.115(2006)567.

Collective path in ^{72}Kr

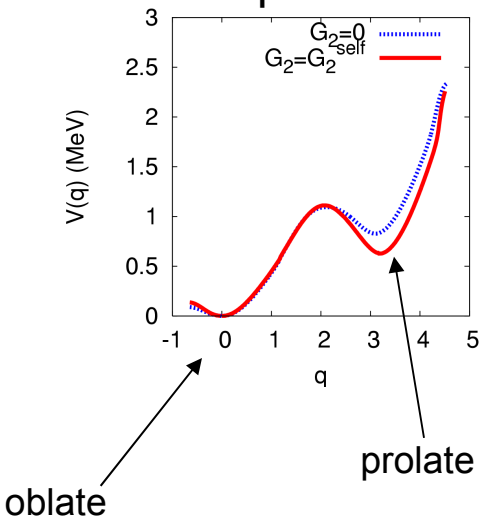
G2=0: Kobayasi *et al.*, PTP**113**(2005), 129.



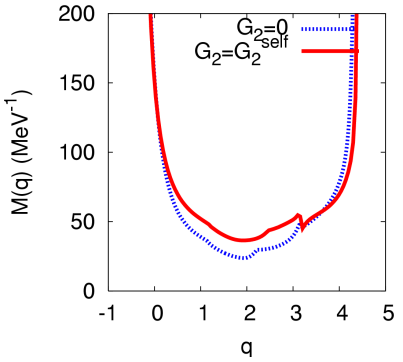
Moving-frame QRPA frequency



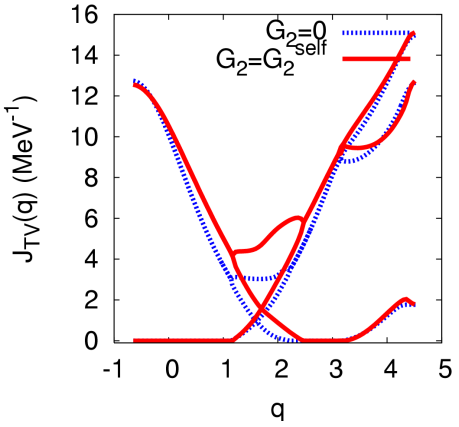
Collective potential



Collective mass



Moment of Inertia



- Bifurcation of the path
- Triaxial degrees of freedom: important
- Enhancement of the collective mass and MoI by the quadrupole pairing

Basic Scheme of ASCC Method (2)

3rd Step: Requantize the collective Hamiltonian.

Collective wave function

vibrational wavefunctions

$$\Psi_{IMk}(q,\Omega) = \sum_{K=0}^{I} \Phi_{IKk}(q)\,\langle \Omega | IMK \rangle$$

Collective Hamiltonian

K: 3-axis component of angular momentum

3-axis: quantization axis, symmetry axis(γ=0°)

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial q^2} + \sum_{i=1}^{3} \frac{1}{2}\mathcal{J}_i^{-1}(q)\hat{I}_i^2 + V(q) \right) \Psi_{IM,k}(q,\Omega) = E_{I,k}\Psi_{IM,k}(q,\Omega)$$

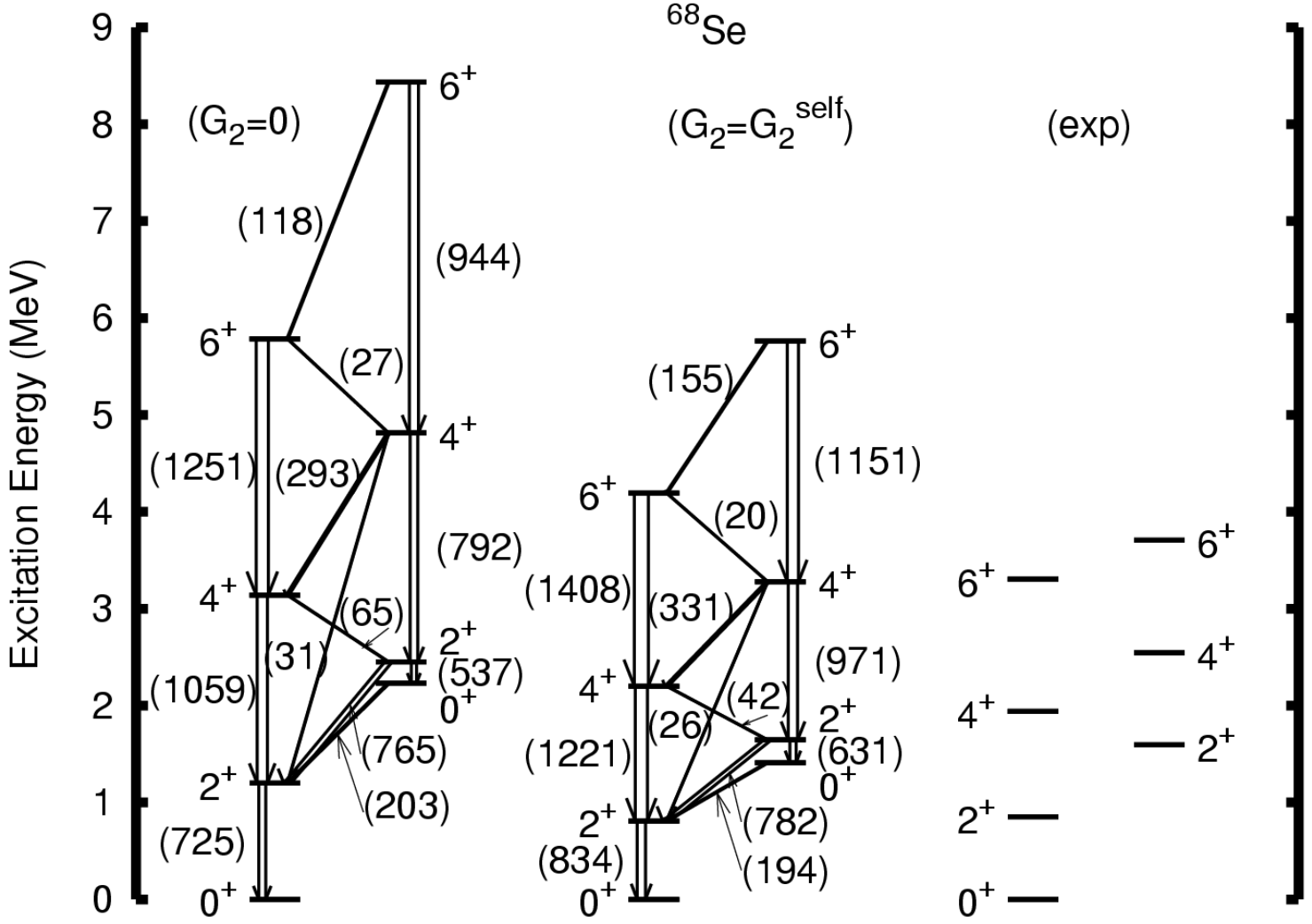
boundary conditions for collective wave functions

- periodic boundary condition at γ=0°and 60°for ^{68}Se
  Kumar and Baranger Nucl. Phys. **A92** (1967) 608.
- box boundary condition for ^{72}Kr

4th Step: Calculate EM transitions

E2 transitions, spectroscopic quadrupole moments …

Energy spectra of ^{68}Se



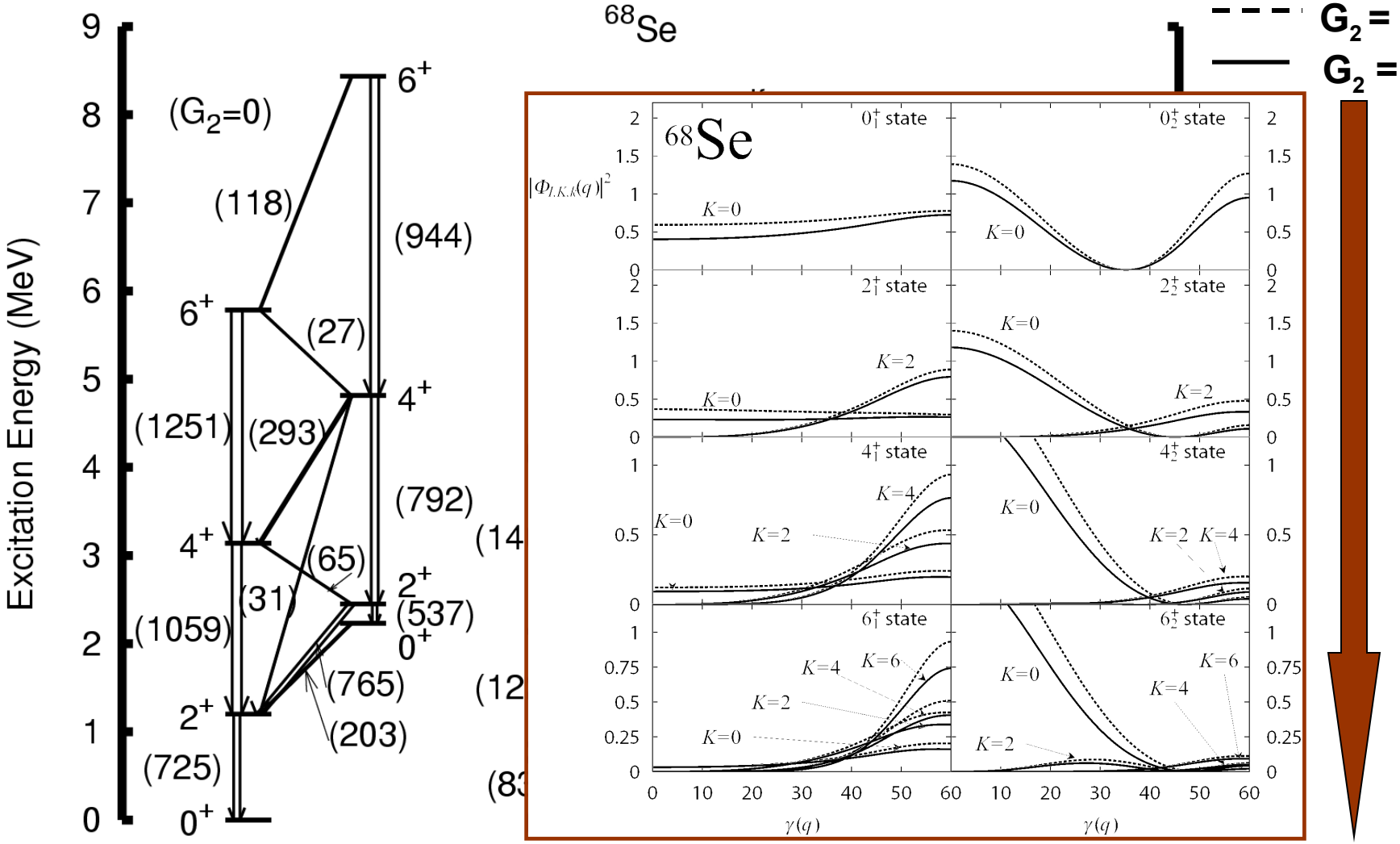
- **two rotational bands**
- **0_2^+ state**
- **quadrupole pairing reduces ex.energy**

( ) …B(E2) e^2 fm^4

effective charge: e_{pol} = 0.904

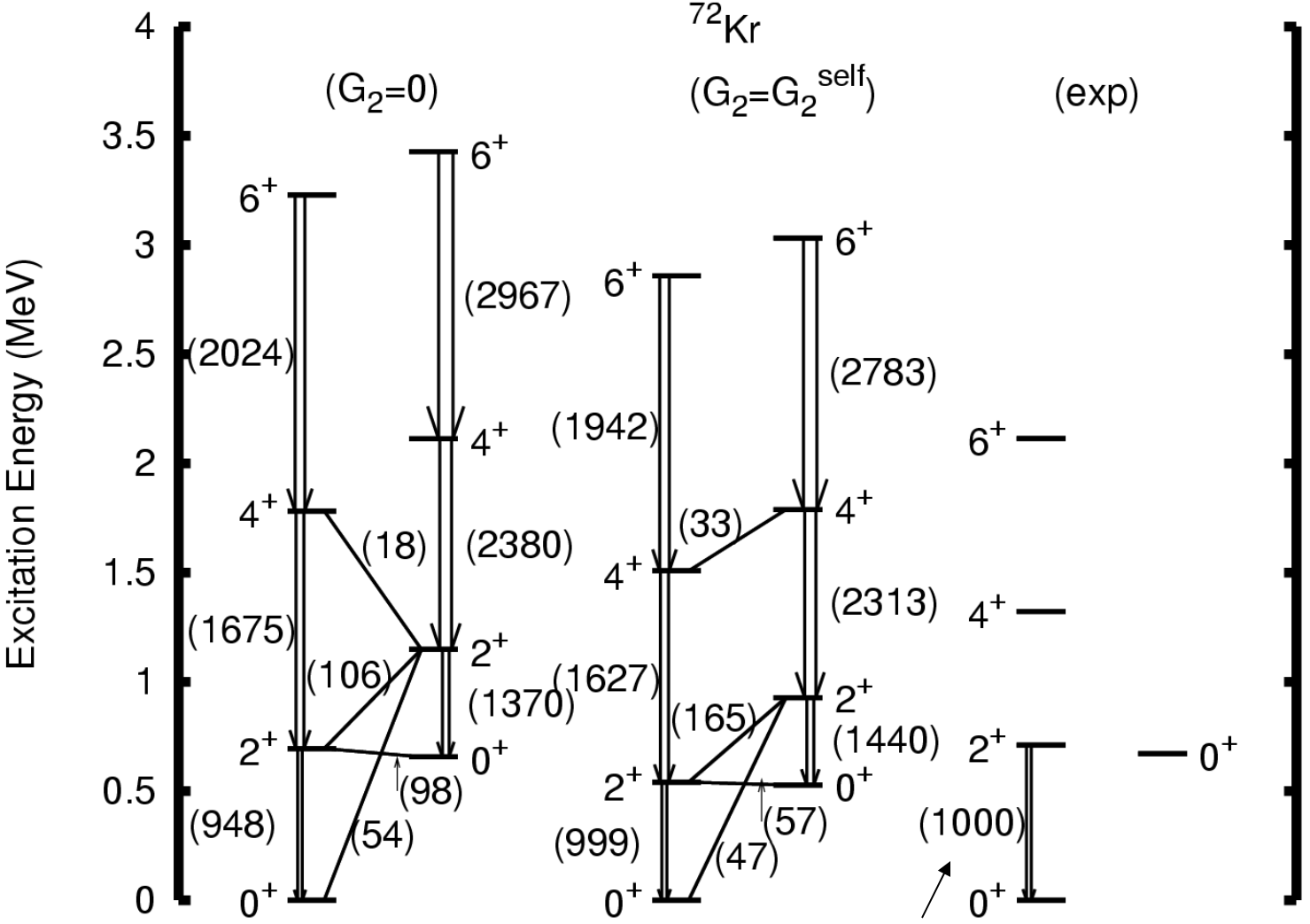
EXP : Fischer et al., Phys.Rev.**C67** (2003) 064318.

Collective Wavefunctions of ^{68}Se



- I = 0: oblate and prolate shapes are strongly mixed via a triaxial degree of freedom
- ground band: mixing of different K states、excited band: K=0 dominant
- oblate-prolate mixing: strong in 0^+ states, reduced as angular momentum increases

Energy Spectra of ^{72}Kr



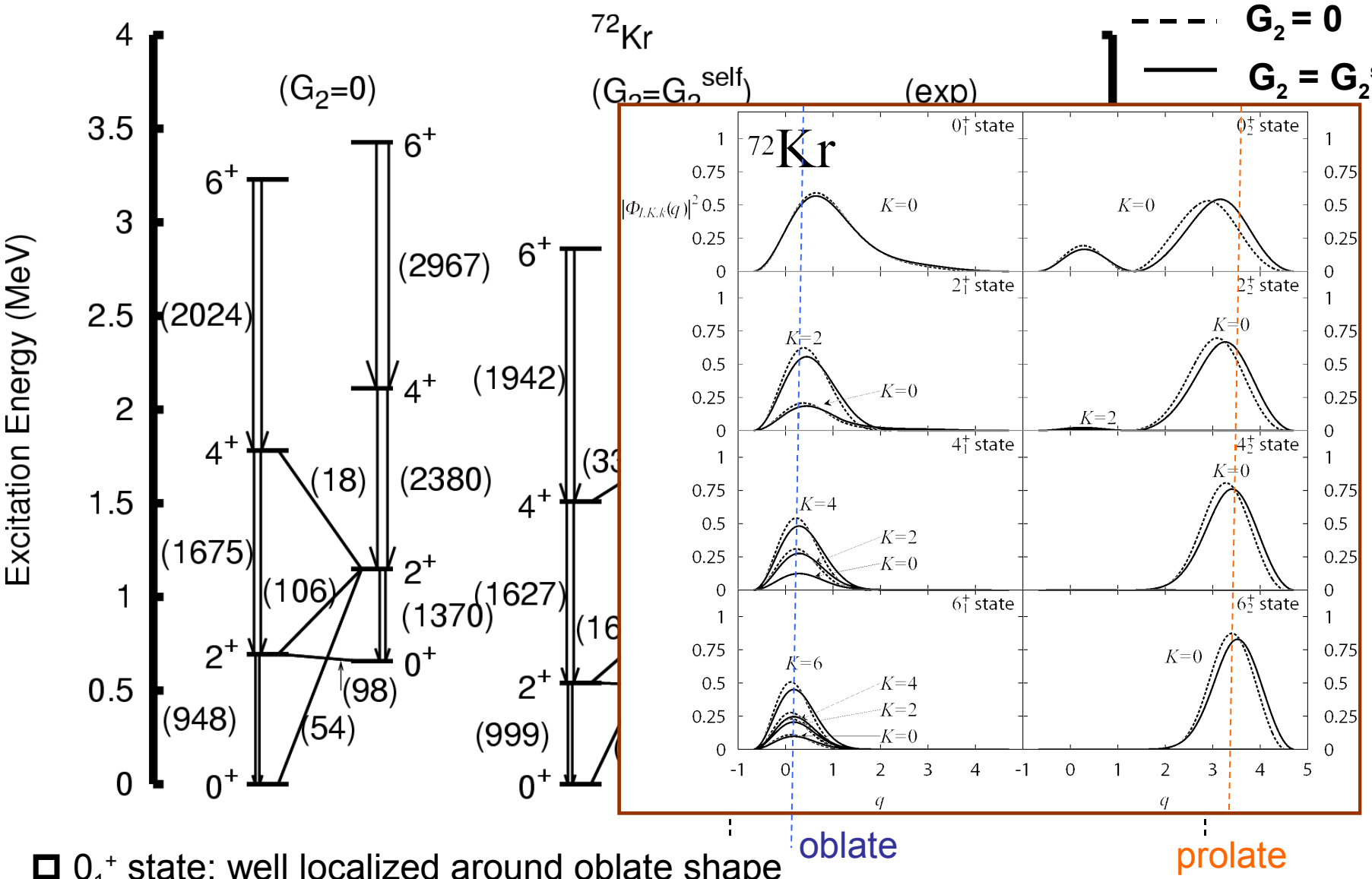
effective charge is adjusted to this value

( ) …B(E2) e² fm⁴

- two rotational bands
- small inter-band B(E2): shape mixing rather weak

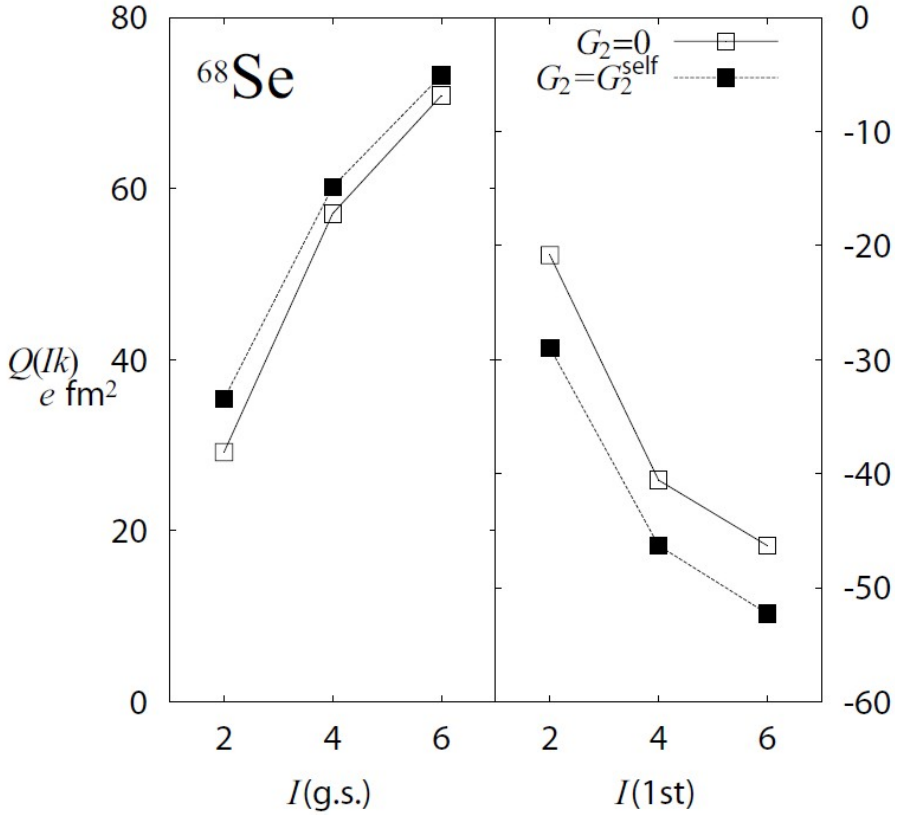
EXP : Fischer et al., Phys.Rev.**C67** (2003) 064318, Bouchez, et al., Phys.Rev.Lett.90 (2003) 082502.
Gade, et al., Phys.Rev.Lett.**95** (2005) 022502, **96** (2006) 189901

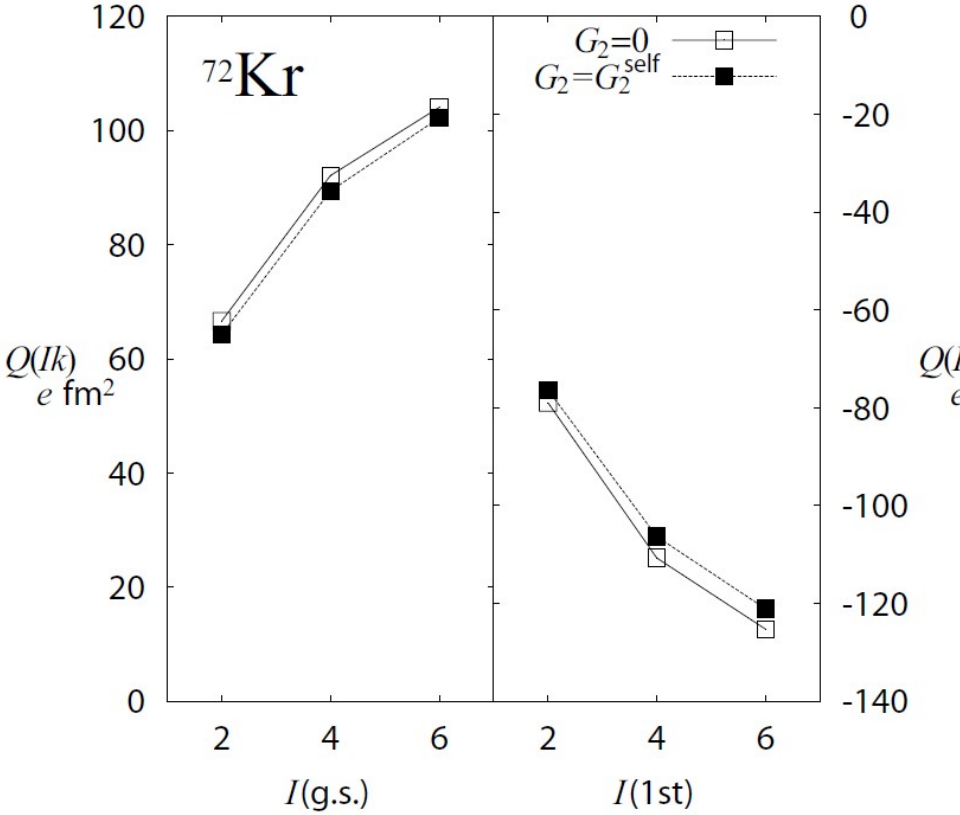
Collective wavefunctions of ^{72}Kr



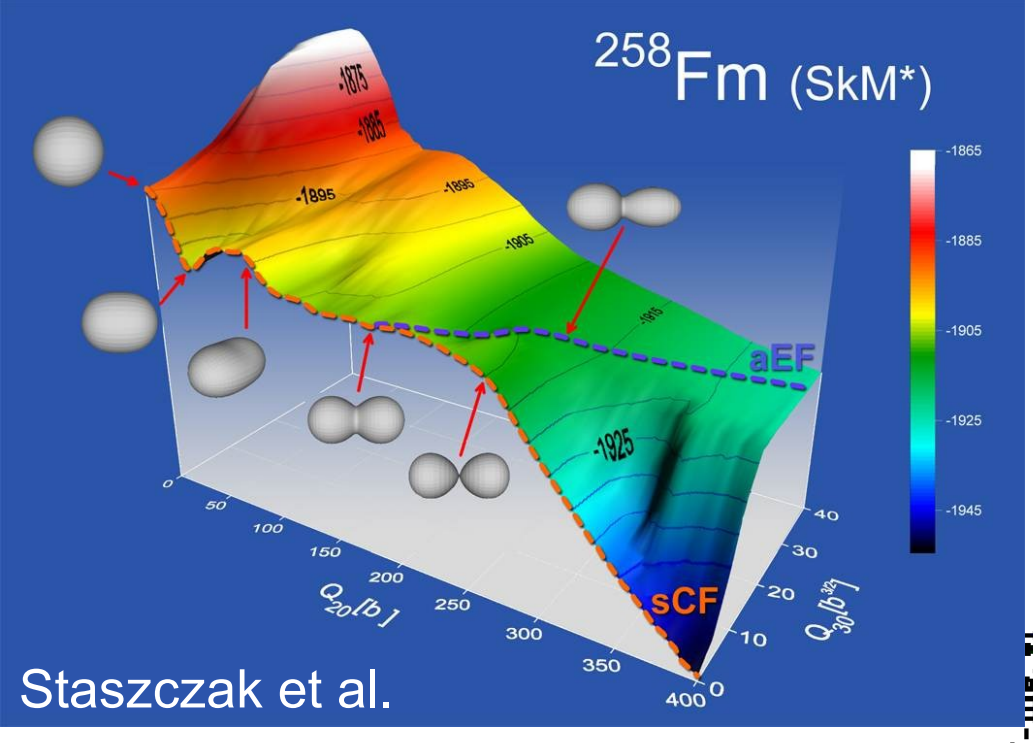
- 0_1^+ state: well localized around oblate shape
- 0_2^+ state: weak oblate-prolate shape mixing
- other states: well defined shape character

Spectroscopic quadrupole moment



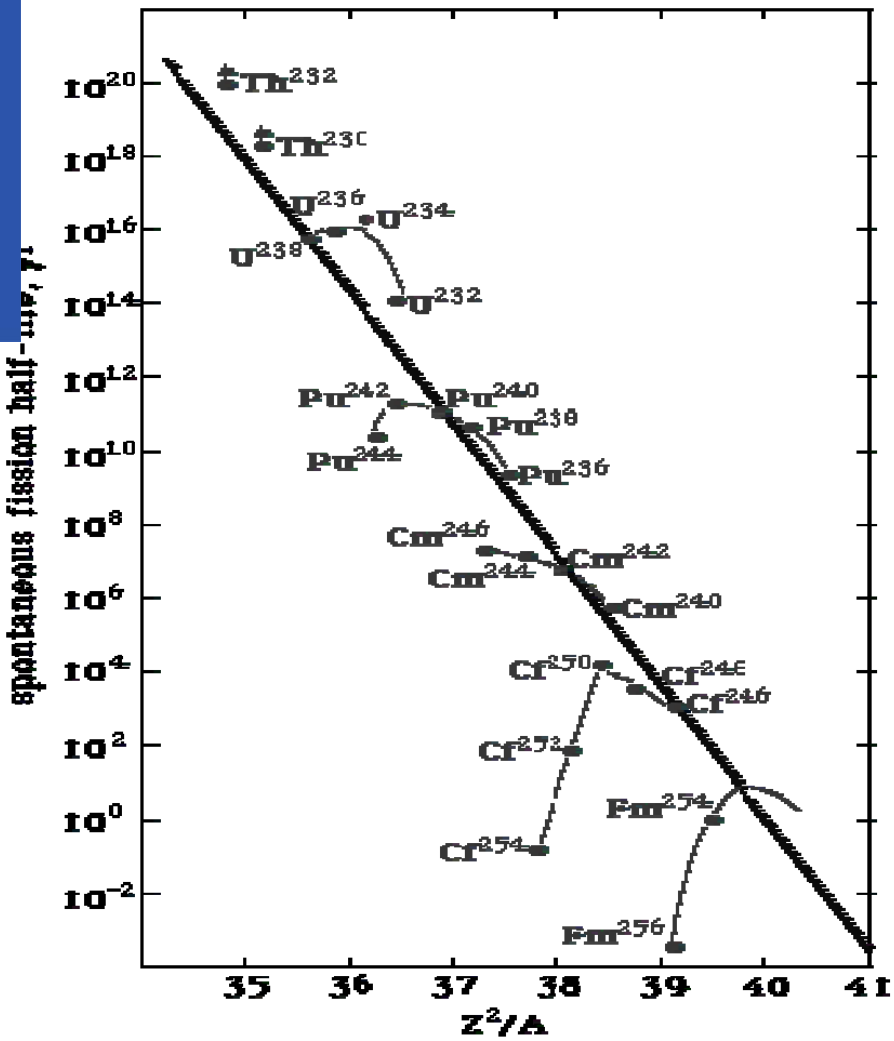


Fission



- Optimal path to fission
- Diabatic vs Adiabatic dynamics
- Collective mass parameters

Self-consistent, self-determined, microscopic description of nuclear fission



Summary

- Liquid-drop, shell, unified models, cranking model
- Nuclear structure at high spin and large deformation
- Sum-rule approaches to giant resonances
- Basic theorem for the Time-dependent density-functional theory (TDDFT)
- Linearized TDDFT (RPA) and elementary modes of nuclear excitation
- Theories of large-amplitude collective motion
- Anharmonic vibrations, shape coexistence phenomena