Giant Resonances and Sum rule

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\(^+\)) | \[
\int f_j(r)Y_{j\mu} \]
| Quadrupole (2\(^+\)) |
| Octupole (3\(^-\)) |
| Isovector (T=1) | Monopole (0\(^+\)) | \[
\int \tau_i f_\lambda(r) Y_{\lambda\mu} \]
| Dipole (1\(^-\)) |
| Quadrupole (2\(^+\)) |
| Gamow-Teller (1\(^+\)) | \[
\int \tau_i \sigma_{j\lambda} f_\lambda(r) \]
| Spin-monopole (1\(^+\)) |
| Spin-dipole (0\(^-\), 1\(^-\), 2\(^-\)) | \[
\int \tau_i f_\lambda(r)(\hat{\sigma} \times Y_{1\lambda})_{\mu} \]
Sum rule

\[ m_i = \sum_n E_n \langle n|F|0\rangle^2 \quad \Rightarrow \quad \text{(Energy - weighted) Sum Rule} \]

\[ m_p = \sum_n E_n' \langle n|F|0\rangle^2 \]

Odd-\( p \) moments can be expressed by the ground-state expectation value.

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

\[ m_3 = \sum_n E_n' \langle n|F|0\rangle^2 = \frac{1}{2} \langle 0|[F,[H,[H,F]]]|0\rangle \]

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

\[ m_1 = \frac{1}{2m} \langle 0|\sum_i (\nabla f)^2 \rangle |0\rangle \]

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

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

Physical meaning of sum rule

Nucleus under an impulse external field

\[ V(t) = F\delta(t) = \delta(t) \sum_i f(\vec{r}_i) \]

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:

\[ \vec{v}(\vec{r}) = -\nabla f(\vec{r}) \]

Energy transferred to nucleon \( i \)

\[ \Delta \varepsilon_i = \frac{\left|\nabla f(\vec{r}_i)\right|^2}{2m} \]

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

\[ \sum_n E_n \langle n|F|0\rangle^2 = \frac{1}{2m} \langle 0|\sum_i (\nabla f)^2 \rangle |0\rangle \]

The energy absorbed by nucleus:

(Exc. energy) \times (probability)
Meaning of $m_3$

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

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

If $f(\vec{r}) = r^4 Y_{4\mu}(\vec{r})$ and the Hamiltonian does not have momentum dependence,

$$G = -\frac{m}{2} \{ H, F \} = \frac{1}{2} \sum \left( \nabla r^4 Y_{4\mu}(\vec{r}) \right) \cdot \nabla_i$$

The state $e^{iG}|0\rangle$ introduces the displacement field $\tilde{d}(\vec{r}) = \nabla r^4 Y_{4\mu}(\vec{r})$

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

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Isoscalar giant resonance

$$\hat{F} = \sum_i f(\vec{r}_i) \quad f(\vec{r}) = r^4 Y_{4\mu}(\vec{r})$$

The previous formulae lead to

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

$$E(\eta) = \langle 0 | e^{-iG} H e^{iG} | 0 \rangle, \quad G = \frac{1}{2} \sum \left( \nabla r^4 Y_{4\mu} \right) \cdot \nabla_i$$

For instance, for the quadrupole operator, with zero-range interactions,

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

$\langle T \rangle$: Kinetic energy expectation value

Giant quadrupole resonance energy

$$\omega_0^2 = \frac{m_3}{m_i} = \frac{4\langle T \rangle}{mA\langle r^2 \rangle} \approx 2\omega^2, \quad \langle \langle T \rangle \rangle \approx mA\langle r^2 \rangle / 2$$
Fermi Liquid Properties

\[ m_\gamma \propto \frac{1}{2} \frac{\partial^2}{\partial \eta^2} E(\eta) \bigg|_{\eta=0} \propto \langle T \rangle \]

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

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

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

and a property of the density operator \( \int \rho(\vec{r}) f(\vec{r}) d\vec{r} = \sum_{\bar{r}} f(\bar{r}) \)

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 \( f(\vec{r}) = r^\pm Y_{\lambda\mu}(\vec{r}) \)

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

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

Transition density of the Tassie model for the giant resonance
Time-Dependent Density Functional Theory (TDDFT)

Walter Kohn

- Nobel Prize in Chemistry 1998
- Harvard (Van Vleck, Schwinger)
  - "While I did not yet know in what subfield of physics I wanted to do my thesis, I was sure it would not be in solid state physics."
  - Green's function variational method for low-energy neutron-deuteron scattering (Failed?)
  - QED, Field theory of nucleons and mesons (Feel completely useless)
- Polaroid Laboratory
  - charged particles falling on a photographic plate lead to a photographic image (Solid-state physics, Van Vleck)
  - "Since you are familiar with solid state physics, ..."
- Copenhagen
  - No one, including Niels Bohr, had even heard the expression "Solid State Physics."
  - Very exciting work was going on in Copenhagen, which eventually led to the great "Collective Model of the Nucleus" of A. Bohr and B. Mottelson, both of whom had become close friends.
- École Normale Supérieure (Nozières)
  - I knew that there was a 1-to-1 correspondence between a weak perturbing potential $v(r)$ and the corresponding small change $\Delta n(r)$ of the density distribution.
  - It seemed such a remarkable result that I did not trust myself.
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;
    \[ \Psi(\vec{r}_1, \ldots, \vec{r}_N) \]
- 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

**Density** \( \rho(\vec{r}) \) determines \( \nu(\vec{r}) \),

except for arbitrary choice of zero point.

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

\[ H = H + \sum_i \nu(\vec{r}_i) \]

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

**Existence of one-to-one mapping:** \( \nu(\vec{r}) \leftrightarrow \Psi^v \leftrightarrow \rho(\vec{r}) \)

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

\( v \)-representative
\[ \psi(\vec{r}) \leftrightarrow \Psi_{gs}^{v} \]

Here, we assume the non-degenerate g.s.

*Reductio ad absurdum:* Assuming different \( \psi(\vec{r}) \) and \( \psi'(\vec{r}) \) produces the same ground state \( \Psi_{gs}^{v} \)

\[
(H + V)\Psi_{gs}^{v} = E_{gs}^{v} \Psi_{gs}^{v} \quad V = \sum_{i} \psi(\vec{r}_i)
\]

\[
- (H + V')\Psi_{gs}^{v} = E_{gs}^{v'} \Psi_{gs}^{v'} \quad V' = \sum_{i} \psi'(\vec{r}_i)
\]

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

\( V \) and \( V' \) are identical except for constant. \( \Box \) Contradiction

\[ \Psi_{gs}^{v} \leftrightarrow \rho_{v} \]

Again, *reductio ad absurdum*

assuming different states \( \Psi_{gs}^{v}, \Psi_{gs}^{v'} \) with \( \psi(\vec{r}), \psi'(\vec{r}) \) produces the same density \( \rho_{v} \)

\[
E_{gs}^{v} = \langle \Psi_{gs}^{v} | H + V | \Psi_{gs}^{v} \rangle
\]

\[
E_{gs}^{v} < E_{gs}^{v'} + \int d\vec{r} [\psi(\vec{r}) - \psi'(\vec{r})] \rho_{v}(\vec{r})
\]

Replacing \( V \) \( \ni \) \( V' \)

\[
E_{gs}^{v'} < E_{gs}^{v'} + \int d\vec{r} [\psi'(\vec{r}) - \psi(\vec{r})] \rho_{v}(\vec{r})
\]

\[ E_{gs}^{v} + E_{gs}^{v'} < E_{gs}^{v'} + E_{gs}^{v} \]

Contradiction!

Here, we assume that the density \( \rho_{v} \) is \( v \)-representative.

For degenerate case, we can prove one-to-one \( \psi(\vec{r}) \leftrightarrow \rho_{v}(\vec{r}) \)
Hohenberg-Kohn Theorem (2)

The second theorem

There is an 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) \( \nu(\vec{r}) \leftrightarrow \Psi_{\nu} \leftrightarrow \rho_{\nu} \)

Many-body wave function \( \Psi[\rho(\vec{r})] \) is a functional of density \( \rho(\vec{r}) \).

Energy functional for external potential \( \nu(\vec{r}) \)

\[ E_{\nu}[\rho] = \langle \Psi[\rho]|H + V|\Psi[\rho]\rangle \]

\[ E_{\nu}[\rho] = E^{\nu<}_{\nu} < E_{\nu}[\rho] \]

Variational principle holds for \( \nu \)-representative density.

\[ E_{\nu}[\rho] = F_{H \nu}[\rho] + \int \rho(\vec{r})\nu(\vec{r})d\vec{r} \]

\( F_{H \nu}[\rho] \) : \( \nu \)-independent universal functional

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

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

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 \( A[\rho(\vec{r})] = \langle \Psi[\rho]|\hat{A}|\Psi[\rho]\rangle \)
v-representative \( \square \) N-representative

Levy (1979, 1982)

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

Ritz’ Variational Principle

\[
\begin{align*}
\text{Min} \langle \Psi(r_1, \ldots, r_N) | H | \Psi(r_1, \ldots, r_N) \rangle &\Rightarrow \Psi_{gs}(r_1, \ldots, r_N) \\
H \Psi_{gs}(r_1, \ldots, r_N) &= E_{gs} \Psi_{gs}(r_1, \ldots, r_N)
\end{align*}
\]

Decomposed into two steps

\[
\begin{align*}
\text{Min} \langle \Psi | H | \Psi \rangle &= \text{Min}_{\rho(r)} \left[ \text{Min}_{\Psi \rightarrow \rho(r)} \langle \Psi | H | \Psi \rangle \right] \\
F[\rho(\bar{r})] &= \text{Min}_{\Psi \rightarrow \rho(r)} \langle \Psi | H | \Psi \rangle
\end{align*}
\]

One-to-one Correspondence

External potential

Minimum-energy state

Density

\[V(\bar{r})\]

\[|\Psi\rangle_{V}\]

\[\rho(\bar{r})\]

\[\rho_v(\bar{r})\]
Title: Time-dependent “HK” theorem

Runge & Gross (1984)

One-to-one mapping between time-dependent density \( \rho(t) \) 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 \( t_0 \)

\[
v(r, t) = \sum_{k=0}^{\infty} \frac{1}{k!} v_k(r)(t-t_0)^k
\]

The initial state is arbitrary.
This condition allows an impulse potential, but forbids adiabatic switch-on.

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Schrödinger equation:

\[
i \frac{\partial}{\partial t} \langle \Psi(t) \rangle = \hat{H}(t) \langle \Psi(t) \rangle
\]

Current density follows the equation

\[
i \frac{\partial}{\partial t} j(r, t) = \langle \Psi(t) \rvert \hat{j}(r), H(t) \lvert \Psi(t) \rangle
\]

Different potentials, \( v(r, t) \), \( v'(r, t) \), make time evolution from the same initial state into \( \hat{\Psi}(t), \hat{\Psi}'(t) \)

\[
v_k(r) - v_k'(r) \neq c \quad \text{for } k
\]

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

\[
w_k(r) = \left( \frac{\partial}{\partial t} \right)^k \{ v(r, t) - v'(r, t) \}_{t=t_0} = v_k(r) - v_k'(r) \neq c
\]

\[\therefore \quad j(r, t) \neq j'(r, t) \quad \text{Continuity eq} \quad \rho(r, t) \neq \rho'(r, t)\]

at \( t > t_0 \)
**Problem 1:** Two external potentials are different, when their expansion
\[ v(r,t) = \sum_{k=0}^{\infty} \frac{1}{k!} v_k(r)(t-t_0)^k \]
has different coefficients at the zero-th order
\[ v_0(r) - v_0'(r) \neq c \]
Using eq. (1), show
\[ \frac{\partial}{\partial t} \left\{ j(r,t) - j'(r,t) \right\} \bigg|_{t=t_0} = -\rho(r,t_0) \nabla w_0(r) \]
\[ w_0(r) = \left\{ v(r,t) - v'(r,t) \right\} \bigg|_{t=t_0} = v_0(r) - v_0'(r) \neq c \]
Next, if \( v_0(r) - v_0'(r) = c \), but \( v_1(r) - v_1'(r) \neq c \),
then, show
\[ \left( \frac{\partial}{\partial t} \right)^2 \left\{ j(r,t) - j'(r,t) \right\} \bigg|_{t=t_0} = -\rho(r,t_0) \nabla w_1(r) \]

**Problem 2:** Using the continuity equation and the following equation
\[ \left( \frac{\partial}{\partial t} \right)^{k+1} \left\{ j(r,t) - j'(r,t) \right\} \bigg|_{t=t_0} = -\rho(r,t_0) \nabla w_k(r) \]
\[ w_k(r) = \left( \frac{\partial}{\partial t} \right)^k \left\{ v(r,t) - v'(r,t) \right\} \bigg|_{t=t_0} = v_k(r) - v_k'(r) \neq c \]
prove that
\[ \left( \frac{\partial}{\partial t} \right)^{k+2} \left\{ \rho(r,t) - \rho'(r,t) \right\} \bigg|_{t=t_0} = \nabla \cdot \left\{ \rho(r,t_0) \nabla w_k(r) \right\} \]
Then, show that the right-hand side cannot vanish identically, with
\[ \nabla w_k(r) \neq 0 \]
One-to-one Correspondence

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

From the first theorem, we have \( \mathcal{L}(r,t) \). Thus, the variation of the following function determines \( \mathcal{L}(r,t) \).

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

\[
S[\rho] = \tilde{S}[\rho] - \int_{t_0}^{t_1} dt \int dr \rho(r,t) v(r,t)
\]

The universal functional \( \tilde{S}[\rho] \) 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

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

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

$$\bar{S}[\rho] = S[\rho] - \int_0^t \langle \Phi_0[\rho](t') | i \frac{\partial}{\partial t} - T | \Phi_0[\rho](t') \rangle$$

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

The functional depends on $\Phi(\vec{r}, t)$ and the initial state $\Phi_0$. 
Time-dependent quantities

Information on excited states

\[ |\Psi(0)\rangle = \sum_n c_n |\Phi_n\rangle \Rightarrow |\Psi(t)\rangle = \sum_n c_n e^{-iE_n t} |\Phi_n\rangle \]

Energy projection

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} |\Psi(t)\rangle e^{-iE t} dt = \sum_n c_n |\Phi_n\rangle \delta(E-E_n) \]

Finite time period \( T \sim 1/\Gamma \)  □ Finite energy resolution

\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} |\Psi(t)\rangle e^{-iE t} d\Gamma t = \sum_n c_n \frac{\Gamma/2}{\pi (E-E_n)^2 + (\Gamma/2)^2} |\Phi_n\rangle \]

TDHF(TDDFT) calculation in 3D real space

Small-amplitude limit
(Random-phase approximation)

One-body operator under a TD external potential
\[ i \frac{\partial}{\partial t} \rho(t) = [\hat{h}_{\text{ext}}(\rho(t)) + V_{\text{ext}}(t), \rho(t)] \]

Assuming that the external potential is weak,
\[ \rho(t) = \rho_0 + \delta \rho(t) \quad h(t) = h_0 + \delta h(t) = h_0 + \frac{\delta h}{\delta \rho} \cdot \delta \rho(t) \]

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

Let us take the external field with a fixed frequency \( \omega \),
\[ V_{\text{ext}}(t) = V_{\text{ext}}(\omega) e^{-i \omega t} + V_{\text{ext}}^*(\omega) e^{i \omega t} \]

The density and residual field also oscillate with \( \omega \),
\[ \delta \rho(t) = \delta \rho(\omega) e^{-i \omega t} + \delta \rho^*(\omega) e^{i \omega t} \]
\[ \delta h(t) = \delta h(\omega) e^{-i \omega t} + \delta h^*(\omega) e^{i \omega t} \]

The linear response (RPA) equation
\[ \omega \delta \rho(\omega) = [h_0, \delta \rho(\omega)] + [\delta h(\omega) + V_{\text{ext}}(\omega), \rho_0] \]

Note that all the quantities, except for \( \omega \) and \( h_0 \), are non-hermitian.
\[ \delta \rho(t) = \sum_{i=1}^{N} [|\delta \psi_i(t) \rangle \langle \phi_i| + |\phi_i \rangle \langle \delta \psi_i(t)|] \]
\[ \delta \rho(\omega) = \sum_{i=1}^{N} [X_i(\omega) \langle \phi_i | + | \phi_i \rangle \langle Y_i(\omega)|] \]

This leads to the following equations for \( X \) and \( Y \):
\[ \omega \langle X_i(\omega)| = (h_0 - \varepsilon_i) \langle X_i(\omega)| + \hat{Q} \langle \delta h(\omega) + V_{\text{ext}}(\omega)| \phi_i \rangle \]
\[ \omega \langle Y_i(\omega)| = -\langle Y_i(\omega)| h_0 - \varepsilon_i \rangle - \langle \phi_i | \delta h(\omega) + V_{\text{ext}}(\omega) \rangle \hat{Q} \]
\[ \hat{Q} = \sum_{i=1}^{N} (i - | \phi_i \rangle \langle \phi_i |) \]

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

\[ \omega X(\omega) = \frac{1}{\hbar} \left( \hbar \psi_0^2 \right) + Q \left[ \frac{\hbar}{\nu^2} \right] \]

\[ \omega Y(\omega) = -\frac{1}{\hbar} \left( \hbar \psi_0^2 \right) - \left[ \frac{\hbar}{\nu^2} \right] Q \]

If we expand the X and Y in particle orbitals:

\[ |X(\omega)\rangle = \sum_{m} \phi_m |X_m(\omega)\rangle \quad |Y(\omega)\rangle = \sum_{m} \phi_m |Y_m(\omega)\rangle \]

Taking overlaps of Eq.(1) with particle orbitals

\[ \begin{pmatrix} A & B \\ B' & A' \end{pmatrix} \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = \begin{pmatrix} |X_m(\omega)\rangle \\ |Y_m(\omega)\rangle \end{pmatrix} \]

\[ \lambda_{m} = (\epsilon_{m} - \epsilon_{n}) \delta_{mn} + \langle \phi_{m} | \frac{\partial}{\partial \nu} | \phi_{n} \rangle \]

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

- Diagonalization of the matrix
Green’s function method

\[ \omega \delta \rho(\omega) = \left[ h_0, \delta \rho(\omega) \right] + \left[ \delta H(\omega) + V_{\text{ext}}(\omega), \rho_\omega \right] \]  

(2)

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

\[ \delta \rho(\omega)|\phi_i\rangle\langle \phi_i| = (\omega + \epsilon_i - h_0)^{-1}[V_{\text{ext}}, \rho_\omega]|\phi_i\rangle\langle \phi_i| \]  

(3-1)

\[ |\phi_i\rangle\langle \phi_i| \delta \rho(\omega) = |\phi_i\rangle\langle \phi_i| \left[ \delta \rho(\omega), \rho_\omega \right] (\omega - \epsilon_i + h_0)^{-1} \]  

(3-2)

Sum up with respect to occupied orbitals \(i\), then, add (3-1) and (3-2), using the orthonormalization condition for KS orbitals (\( \int \delta \rho(\omega) = [\rho_\omega, \delta \rho(\omega)] \)):

\[ \delta \rho(\omega) = \sum_i \left( G_i(\epsilon_i + \omega)V_{\text{ext}}|\phi_i\rangle\langle \phi_i| + |\phi_i\rangle\langle \phi_i| \left[ V_{\text{ext}}G_i(\epsilon_i - \omega) \right] \right) \]

\[ G_i(\epsilon_i) = (E - \epsilon_i)^{-1} \]

If the \( V_{\text{ext}} \) is local, we can rewrite this as follows:

\[ \delta \rho(\omega) = \sum_i \int d\mathbf{r} \left\{ G_i(\epsilon_i + \omega)V_{\text{ext}}(\mathbf{r}^\prime)|\phi_i(\mathbf{r}^\prime)\rangle\langle \phi_i(\mathbf{r}^\prime)| + |\phi_i(\mathbf{r}^\prime)\rangle\langle \phi_i(\mathbf{r}^\prime)| V_{\text{ext}}(\mathbf{r}^\prime)G_i(\epsilon_i - \omega) \right\} \]

\[ = \sum_i \int d\mathbf{r} \Pi_i(\mathbf{r}, \omega)V_{\text{ext}}(\mathbf{r}; \omega) \]

where the independent-particle response function is defined by

\[ \Pi_i(\mathbf{r}, \omega; \omega + i\eta) = \sum_i \int d\mathbf{r} \left\{ \phi_i(\mathbf{r})G_i^{\text{scf}}(\mathbf{r}^\prime; \epsilon_i - \omega)|\phi_i(\mathbf{r}^\prime)\rangle + |\phi_i(\mathbf{r}^\prime)\rangle\langle \phi_i(\mathbf{r}^\prime)| \right\} \]

\[ G_i^{\text{scf}}(E) = (E \pm i\eta - h_0)^{-1} \]

Green’s function method (cont.)

An advantage of the Green’s function method is that we can treat the continuum exactly.\hspace{1cm}Shlomo and Bertsch, NPA243 (1975) 507.

\[ \Pi_i(\mathbf{r}, \omega; \omega + i\eta) = \sum_i \int d\mathbf{r} \left\{ \phi_i(\mathbf{r})G_i^{\text{scf}}(\mathbf{r}^\prime; \epsilon_i - \omega)|\phi_i(\mathbf{r}^\prime)\rangle + |\phi_i(\mathbf{r}^\prime)\rangle\langle \phi_i(\mathbf{r}^\prime)| \right\} \]

\[ G_i^{\text{scf}}(E) = (E \pm i\eta - h_0)^{-1} \]

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

\[ G_i^{\text{scf}}(E) = 2m \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \frac{\mu_l(\mathbf{r})V_l^{\text{scf}}(\mathbf{r})}{W[\mu_l, V_l^{\text{scf}}]} Y_{lm}(\mathbf{r}) Y_{lm}^{*}(\mathbf{r}) \]

In case \( h_0 \) is deformed, we can construct the Green’s function by using the following identity:

\[ T.N. \text{ and Yabana, JCP114 (2001) 2550; PRC71 (2005) 024301.} \]

\[ G_i^{\text{ad}}(E) = G_i^{\text{scf}}(E) + G_i^{\text{scf}}(E)[h_0 - h_0^{\text{ad}}]^{-1}G_i^{\text{ad}}(E) \]
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:

\[ \partial \tilde{h}(\omega) = \frac{\partial \tilde{h}}{\partial \tilde{\rho}} \cdot \tilde{\rho}(\omega) \]

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

\[ \hat{h}[\rho(t)] = \hat{h}_0 + \partial \hat{h}(t), \quad \partial \hat{h}(t) = \frac{\partial \hat{h}}{\partial \rho} \cdot \tilde{\rho}(t) \]

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

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

Skyrme TDDFT in real space

Time-dependent Hartree-Fock equation

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

3D space is discretized in lattice

Single-particle orbital:

\[ \varphi_i(r, t) = \{ \varphi_i(k, t_n) \}_{k=1, \ldots, Mr}, \quad i = 1, \ldots, N \]

\[ N: \text{Number of particles} \]

\[ Mr: \text{Number of mesh points} \]

\[ Mt: \text{Number of time slices} \]

Spatial mesh size is about 1 fm.

Time step is about 0.2 fm/c

Calculation of time evolution

Time evolution is calculated by the finite-order Taylor expansion

\[ \psi_i(t + \Delta t) = \exp \left( -i \int_{t}^{t+\Delta t} h(t') dt' \right) \psi_i(t) \]

\[ \approx \sum_{n} \left( -i \Delta t \frac{h(t + \Delta t/2)^n}{n!} \right) \psi_i(t) \]

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

\[ \Delta t \varepsilon_{\text{max}} \ll 1 \]

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

Real-time calculation of response functions

1. Weak instantaneous external perturbation

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

2. Calculate time evolution of

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

3. Fourier transform to energy domain

\[ \frac{dB(\omega; \hat{F})}{d\omega} = -\frac{1}{\pi \eta} \text{Im} \int \langle \Psi(t) | \hat{F} | \Psi(t) \rangle e^{i\omega t} dt \]
Real-time dynamics of electrons in photoabsorption of molecules

1. External perturbation $t=0$

$V_{ex}(\mathbf{r}, t) = -\varepsilon_i \delta(t)$, \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

\[ \frac{\hbar}{i} \frac{\partial}{\partial t} \psi_i(\mathbf{r}, t) = \hbar [\hat{\eta}_i(\mathbf{r})] \psi_i(\mathbf{r}, t) \]

[Exp]  
TDDFT

PZ+LB94

Photoabsorption cross section in C$_3$H$_6$ isomer molecules


- 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.

\[ \delta \rho_n(t) = \rho_n(t) - (\rho_0)_n \]

Time-dep. transition density

\[ \delta \rho_p(t) = \rho_p(t) - (\rho_0)_p \]

Protons

Neutrons

16^O

\[ \delta \rho_n(t) = \rho_n(t) - (\rho_0)_n \]
Finite Amplitude Method

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

\[ \omega X_i(\omega) = (\hbar_0 - \varepsilon_i) X_i(\omega) + Q [\hat{\mathbf{p}}] X_i(\omega) \phi \]

\[ \omega Y_i(\omega) = -\langle Y_i(\omega) | h_0 - \varepsilon_i \rangle - \langle \phi | [\hat{\mathbf{p}}] X_i(\omega) \phi \rangle \]

(1)

Residual fields can be estimated by the finite difference method:

\[ \hat{\mathbf{p}} = \frac{1}{\hbar} \left( \frac{\psi^*}{\psi} \right) \]

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*  
\( R_{\text{box}} = 15 \text{ fm} \)  
\( \Gamma = 1 \text{ MeV} \)
基底状態に関する計算

- 系統的計算が汎用的に行うに可能に
  - Ab-inito計算の助けを借りて、Energy functionalを最適化（目標：質量誤差500 keV以下）
- 偶核の計算
  - (100テラ級のPCクラスターがあれば、1,2時間で偶偶核全種の結果を出せる汎用コード)
- 奇核の計算
  - Odd-even mass differenceは実験をよく再現 (Pairing channelのfunctionalには依存)
  - Filling approx.の正当性
  - スピン・パリティを正確に予言することは未だ困難な課題

Jaguar Cray XT4 at ORNL
No. 2 on Top500
- 11,706 processor nodes
- Each compute/service node contains 2.6 GHz dual-core AMD Opteron processor and 4 GB/8 GB of memory
- Peak performance of over 119 Teraflops
- 250 Teraflops after Dec.'07 upgrade
- 600 TB of scratch disk space
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
Large amplitude collective motion (LACM) in nuclei

- Fission
- Decay of superdeformed band
- Shape-coexistence phenomena

\[
|\Phi\rangle = c_1 |\text{state}_1\rangle + c_2 |\text{state}_2\rangle
\]

Adiabatic theories of LACM

- Baranger-Veneroni, 1972-1978
  \[
  \rho(t) = e^{i\Pi(t)} \rho(0) e^{-i\Pi(t)}
  \]
  • Expansion with respect to \[ \]
- Villars, 1975-1977
  • Eq. for the collective subspace (zero-th and first-order w.r.t. momenta)
    \[
    \delta \langle \Phi(q)| H - \frac{\partial V}{\partial q} Q(q)|\Phi(q) \rangle = 0
    \]
    \[
    \delta \langle \Phi(q)| H, Q(q) | + iM(q)^{-1} \frac{\partial}{\partial q} |\Phi(q) \rangle = 0
    \]
  • 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, $Q,P \cong$
    Infinitesimal generator, is not
    guaranteed.

  \[
  \delta \langle \Phi(q) \rvert H - \frac{\partial V}{\partial q} Q(q) \rvert \Phi(q) \rangle = 0 \\
  \delta \langle \Phi(q) \rvert [H, Q(q)] + i M(q) \rvert P(q) \rvert \Phi(q) \rangle = 0 \\
  \delta \langle \Phi(q) \rvert H, P(q) \rvert - i C(q) Q(q) \rvert \Phi(q) \rangle = 0
  \]

- 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
    $(q, p)$.

  \[
  \delta \langle \Phi(q, p) \rvert H - \frac{\partial H}{\partial q} Q - \frac{\partial H}{\partial p} P \rvert \Phi(q) \rangle = 0 \\
  H = \langle \Phi(q, p) \rvert H \rvert \Phi(q, p) \rangle
  \]

  “Adiabatic” approx. \LACM
  (Matsuo, TN, Matsuyanagi, 2000)
The TDHF(B) equation can be described by the classical form.

For instance, using the Thouless form

\[ z = \exp \left( \frac{1}{2} z_{\mu} a_{\mu}^* \right) \Phi_0 \]

The TDHF(B) equation becomes in a form

\[ H(z, z^*) = \frac{z [H] z^*}{(z | z)} \]

The Holstein-Primakoff-type mapping leads to

\[ \beta_{\mu\nu} = \left[ z (1 + z^*) \right]^{\mu\nu} \]

The last term in terms of variables \((\xi, \pi)\)

\[ \langle \xi, \pi | H | \xi, \pi \rangle = E_{RPA} + \frac{1}{2} \left( \alpha + \frac{1}{2} \left[ \sum_{\mu \nu} \alpha^2 a^\dagger a^\dagger a a \right] \right) \]

Rewriting the last term in terms of variables \((\xi, \pi)\)

Linear point transformation \((\xi, \pi) \rightarrow (q, p)\) leads to

\[ q^\nu = \sqrt{\frac{1}{\alpha_{\mu}} \sum_{\mu} \left( X^\mu + Y^\mu \right)} \xi^\mu, \quad p^\nu = \sqrt{\frac{1}{2} \sum_{\mu} (X^\mu - Y^\mu)} \pi^\mu, \]

The TDHF(B) equation can be described by the classical form.
Decoupled classical motion within the point transformation

Expanding the classical Hamiltonian w.r.t. momentum up to 2nd order
\[ H(\xi, \pi) = \frac{1}{2} B^{\alpha\beta}(\xi) \pi_\alpha \pi_\beta + V(\xi), \quad B^{\alpha\beta} = \frac{\partial^2 H}{\partial \pi_\beta \partial \pi_\alpha} \]

Point transformation \((\xi, \pi) \rightarrow (q, p)\)
\[ q^\alpha = f^\alpha(\xi), \quad \xi^\alpha = g^\alpha(q) \]
\[ p_\mu = g^\alpha_\mu \pi_\alpha, \quad \pi_\alpha = f^\mu_\alpha p_\mu \quad g^\alpha_\mu = \frac{\partial g^\gamma_\alpha}{\partial q^\mu} \frac{\partial g^\mu_\beta}{\partial q^\gamma}, \quad f^\mu_\alpha = \frac{\partial f^\nu_\beta}{\partial q^\mu} \frac{\partial f^\nu_\beta}{\partial q^\gamma} \]

Point transformation conserves the quadratic form in momenta.
\[ \bar{H}(q, p) = \frac{1}{2} \bar{B}^{\alpha\beta} p_\alpha p_\beta + \bar{V}(q), \quad \bar{B}^{\alpha\beta} = f^\mu_\alpha B^{\beta\mu} f^\nu_\beta \]

Metric tensor: \( B_{\alpha\beta} \) : defined by \( B_{\alpha\beta} B^{\beta\alpha} = \delta^\alpha_\beta \)
Shift-up and down of indexes: \( V^\alpha = B^{\alpha\beta} V_\beta \)
Chain rules: \( g^\alpha_\mu f^\beta_\mu = \delta^\beta_\alpha \), \( f^\alpha_\mu g^\mu_\beta = \delta^\alpha_\beta \) (=canonical variable cond.)

Assuming that there is a decoupled path (1-dim. collective submanifold)
\( q^I \) : Collective coordinate, \( q^\alpha \) : Non-collective coord.

Decoupling condition: \( q^\alpha = p_\alpha = 0 \Rightarrow \dot{q}^\alpha = \dot{p}_\alpha = 0 \)

Decoupling condition (1) \( \square \H(q) \) with the constraint \( q^I = \langle \Phi(q^I) | \hat{Q}(q^I) | \Phi(q^I) \rangle \)
\[ \delta \left( V(\xi) - \frac{\partial \bar{V}}{\partial q^I} q^I \right) = \delta \left( H(\xi, \pi = 0) - \lambda q^I(\xi) \right) = \delta \langle \Phi(q^I) | H - \lambda \hat{Q}(q^I) | \Phi(q^I) \rangle = 0 \]
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 \( Q(q) \).
Here, two different definitions of the metric tensor are possible:

(i) Riemannian type

Metric tensor

\[ G_{\alpha \beta} = \partial_{[\alpha} f^{\mu}_{\beta]} + \partial_{\beta} f^{\mu}_{\alpha} \]

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

\[ V_{\alpha \beta} = \bar{V}_{\alpha \beta} f^{\mu}_{\beta} \quad V_{\alpha \beta} = V_{\alpha \beta} - \Gamma^\mu_{\alpha \beta} V_{\mu} \quad \bar{V}_{\alpha \beta} = \bar{V}_{\alpha \beta} - \Gamma^\mu_{\alpha \beta} \bar{V}_{\mu} \]

(ii) Symplectic type

Metric tensor

\[ K_{\alpha \beta} = \sum_{\mu} f^{\mu}_{\alpha} f^{\mu}_{\beta}, \quad K^{\alpha \beta} = \sum_{\mu} g^{\alpha \mu} g^{\beta \mu} \]

\[ \Gamma^\alpha_{\beta \gamma} = \frac{1}{2} K^{\alpha \gamma} (K_{\alpha \beta} + K_{\beta \alpha} - K_{\alpha \gamma}) = g^{\alpha \mu} f^{\mu}_{\beta} \]

With this metric, the decoupled space is assumed to be “flat”. \( \mathcal{K}_{\mu \nu} = \delta_{\mu \nu} \)

A certain combination of the decoupling conditions (1-3) leads to the following Local Harmonic Equation (LHE) :

\[ V_{\alpha \beta} f^{\gamma}_{\beta} = \omega^2 f^{\gamma}_{\beta} \quad V_{\alpha \beta} = B^{\beta}_{\alpha \gamma}, \quad V_{\alpha \beta} = V_{\alpha \beta} - \Gamma^\gamma_{\alpha \beta} V_{\gamma} \]

(i) Riemannian LHE

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

\[ \delta \int \sqrt{B_{ij}(q)} dq = 0 \quad \Rightarrow \quad f^{\gamma}_{\beta} = -\Gamma^\gamma_{\alpha \beta} f^{\gamma}_{\beta} + \Gamma^\gamma_{\alpha \beta} f^{\gamma}_{\beta} = 0 \]

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

\[ \omega^2 = B^{\gamma \beta}_{\alpha \gamma} (\bar{V}_{\gamma \beta} - \Gamma^\gamma_{\gamma \beta} \bar{V}_{\beta}) \]

(ii) Symplectic LHE

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

\[ \omega^2 = B^{\gamma \beta}_{\alpha \gamma} \bar{V}_{\beta \gamma} \quad V_{\alpha \beta} = V_{\alpha \beta} - \Gamma^\mu_{\alpha \beta} V_{\mu} = V_{\alpha \beta} - f^{\mu}_{\alpha \beta} \bar{V}_{\mu} \]

We need to determine the curvature \( f^{\mu}_{\alpha \beta} \)
Riemannian LHE vs Symplectic LHE

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.

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


---

Extended Point Transformation

Extended “point” transformation

\[
q^\mu = f^\mu (\xi) + \frac{1}{2} f^{(1)\mu\nu} \pi_\mu \pi_\nu + O(\pi^4)
\]

\[
\xi^\mu = g^\mu (q) + \frac{1}{2} g^{(1)\mu\nu} p_\mu p_\nu + O(p^4)
\]

\[
p_\mu = g^\mu_\nu \pi_\nu + O(\pi^4)
\]

\[
\pi_\mu = f^\mu_\nu p_\nu + O(p^4)
\]

This extension leads to the modification of mass parameter, but the other formulation is kept invariant.

\[
\tilde{B}^{\mu\nu} = B^{\mu\nu} - \tilde{\nabla}_\mu f^{(1)\mu\nu}
\]

Extended Local Harmonic Equations

\[
\tilde{V}_{\alpha\beta} f_{,\beta} = \omega^\gamma f_{,\alpha}^\gamma
\]

\[
\tilde{V}_{\alpha\beta}^\gamma = \tilde{B}^{\alpha\beta} V_{\gamma\nu} \quad V_{\alpha\beta} = V_{\alpha\beta} - \Gamma^\nu_{\alpha\beta} V_{\gamma}
\]

\[
\tilde{B}_{\alpha\beta} = B_{\alpha\beta} - \tilde{\nabla}_\nu f^{(1)\mu\nu} = B_{\alpha\beta} - \tilde{\nabla}_\nu f^{(1)\mu\nu}
\]

\[
V_{\alpha\beta} \equiv V_{\alpha\beta} - \Gamma^\gamma_{\alpha\beta} V_{\gamma}
\]

\[
= V_{\alpha\beta} - \frac{1}{2} B^{\alpha\beta} (B_{\gamma\nu,\beta} + B_{\nu\alpha,\beta} - B_{\alpha\beta,\Delta}) V_{\gamma} \quad \text{(Riemannian case)}
\]

\[
= V_{\alpha\beta} - f^\mu_{\alpha\beta} \tilde{\nabla}_\mu \quad V_{\alpha\beta} = f^\mu_{\alpha\beta} \tilde{\nabla}_\mu \quad \text{(Symplectic case)}
\]
Separation of Nambu-Goldstone modes

\[ S(\xi, \pi) = (\Psi(t)|\hat{S}|\Psi(t)) = S^{(0)}(\xi) + S^{(1)}(\xi) \pi_+ + \frac{1}{2} S^{(2)}(\xi) \pi_+ \pi_- + O(\pi^3) \]

\[ [\hat{S}, \hat{H}] = 0 \implies [S, H]_{\text{fin}} = 0 \implies \begin{cases} S^{(1)} V_\pi = 0 \\ S^{(0)} B^{0+} - S^{(2)} B^{0-} V_\pi = 0 \end{cases} \]

(1) Symmetry operator \( S = \text{momentum} \)

\[ p_\pi = g^{\alpha} \pi_\alpha + O(\pi^3) \]

\[ g^{\alpha}_\pi V_\alpha = 0 \quad V_{\alpha\beta} g^{\alpha}_\pi = 0 \]

(2) Symmetry operator \( S = \text{coordinate} \)

\[ q' = f^+ f^{(1)+} \pi_+ + O(\pi^4) \quad \hat{B}^{0f} f_{\beta}^{(1)+} = B^{0f} f_{\beta}^{(1)+} - V_\pi f^{(1)+} f_{\beta}^{(1)+} \]

\[ f^+ = S^{(0)} \quad f^{(1)+} = S^{(1)+} \quad \Rightarrow \]

\[ \therefore \quad \hat{V}^{\beta}_\pi f_{\beta}^{(1)+} = 0 \quad \text{and} \quad \hat{g}^{\alpha}_\pi g^{(1)+} = 0 \]

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

Properties of symplectic LHE

We need to determine, \( f^{(1)+} \) and \( f^{(1)+}_\pi \), which are related to \( a'\alpha \)-part of \( \hat{Q} \) and \( \hat{N} \).

These cannot be determined by solution of the LHE. ☐ Stuck! (1999)

Hinohara et al, PTP 117 (2007) 451

- Gauge invariance:

  The symplectic LHE is invariant under the following transformation:

  \[ q^+ \Rightarrow q^+ + cq^N, \quad p^N \Rightarrow p^N + cp^+ \]

  \[ \hat{V}^N \Rightarrow \hat{V}^N - c\hat{V}^+ \]

  Therefore, it requires the gauge fixing condition.

(2) The “strong” canonicity condition:

\[ [\hat{Q}(q), \hat{N}] = 0 \]

(1) and (2) can determine those unknown quantities.
Collective path and re-quantization

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

**Symplectic LHE**

(CMF) \[ V_{\alpha} = V_{\alpha}^f \]

(LHE) \[ V_{\alpha}^p f_{\alpha} = \omega^p f_{\alpha} \]

**Adiabatic SCC**

(CMF) \[ \delta(\phi(q)) \hat{H} - (\partial V / \partial q) \hat{Q}(q) \phi(q) = 0 \]

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

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

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

\[ \{ \phi(q_1), \phi(q_2), \phi(q_3), \ldots \} \]

**GCM**

\[ \{ \hat{B}(q_1), \hat{B}(q_2), \hat{B}(q_3), \ldots \} \]

\[ \{ \hat{V}(q_1), \hat{V}(q_2), \hat{V}(q_3), \ldots \} \]

**“Collective Hamiltonian”**

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

---

Adiabatic SCC (Symplectic LHE) — Applications to simple models —
Applications to O(4) models

Model Hamiltonian

\[ H = -\hbar \omega \left( \frac{1}{2} g_1 \left( \phi_0^\dagger \phi_0 + \phi_0^\dagger \phi_0 \right) - \frac{1}{2} g_2 \left( \phi_2^\dagger \phi_2 + \phi_2^\dagger \phi_2 \right) \right) \]

\[ P_0 = \sum_{m \in \mathbb{N}} c_{j-m} c_{j m} , \quad P_2 = \sum_{m \in \mathbb{N}} \sigma_{j m} c_{j-m} c_{j m} \]

\[ Q = \sum_{m \in \mathbb{N}} \sigma_{j m} c_{j m} \]

\[ \sigma_{j m} = \begin{cases} 1 & \text{if} \quad |m| < \Omega_j / 2 \\ -1 & \text{if} \quad |m| > \Omega_j / 2 \end{cases} \]

Parameters

\( \epsilon_1 = 0, \epsilon_2 = 1.0, \epsilon_3 = 3.5 \)
\( d_1 = 2.0, d_2 = 1.0, d_3 = 1.0 \)
\( \Omega_1 = 14, \Omega_2 = 10, \Omega_3 = 4 \)

Hinohara, TN, Matsuo, Matsuyanagi. PTP115 (2006) 567
Curvature effects

\[ \tilde{\chi}(\rho) = \sum_{\nu} \phi_{\nu}(\rho) \rho_{\nu} + \text{h.c.} \]

In this model, requiring the gauge invariance, we can determine them. The curvature effects are weak.
**Model of protons and neutrons**

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

\[ H = H_n + H_p + H_{np}. \]

\[ H_n = \sum_{i \in n} \, \epsilon \psi_{i_n} \phi_i \bar{\phi}_n - G_n \rho_n \rho_n^* - \frac{1}{2} \kappa \mathcal{Q}_n^2. \]

\[ H_p = \sum_{i \in p} \, \epsilon \psi_{i_p} \phi_i \bar{\phi}_p - G_p \rho_p \rho_p^* - \frac{1}{2} \kappa \mathcal{Q}_p^2. \]

\[ H_{np} = -\kappa \mathcal{Q}_n \mathcal{Q}_p. \]

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.
**Fission**

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

**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
Lecture Materials

Theor. Nucl. Phys. Lab. HP
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References:
(1) DFT theorems with translational/rotational invariance
    (B. Giraud’s idea)
(2) HF, BCS, HFB, TDHF
    Ring-Schuck, “Nuclear Many-Body Theories”
(3) Equivalence between TDHF(B) and classical dynamics