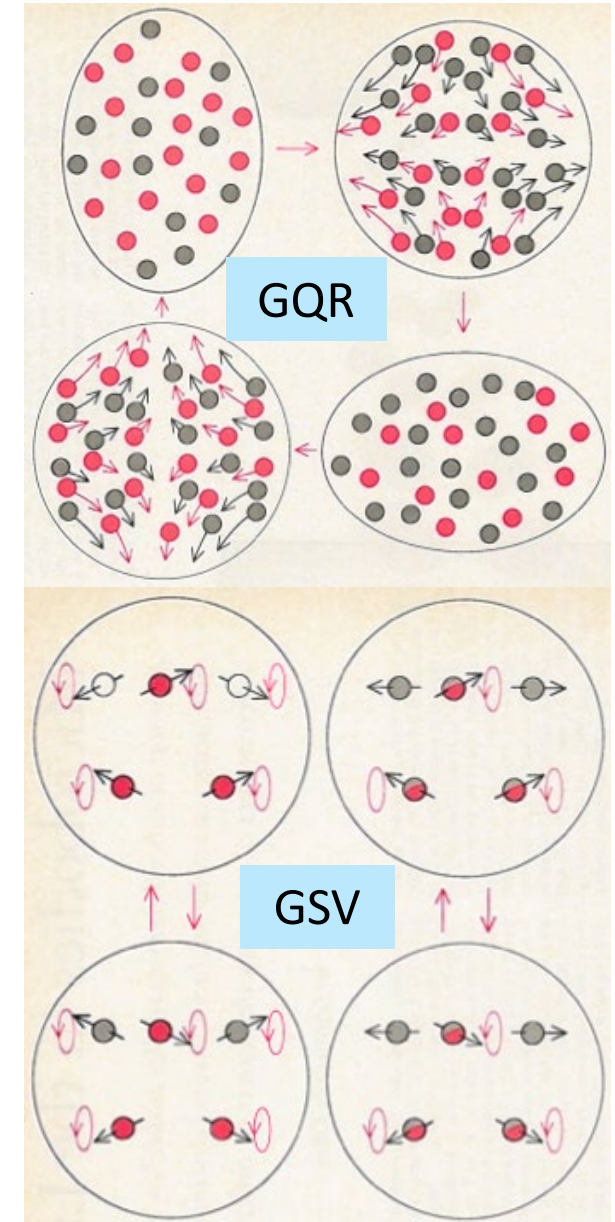
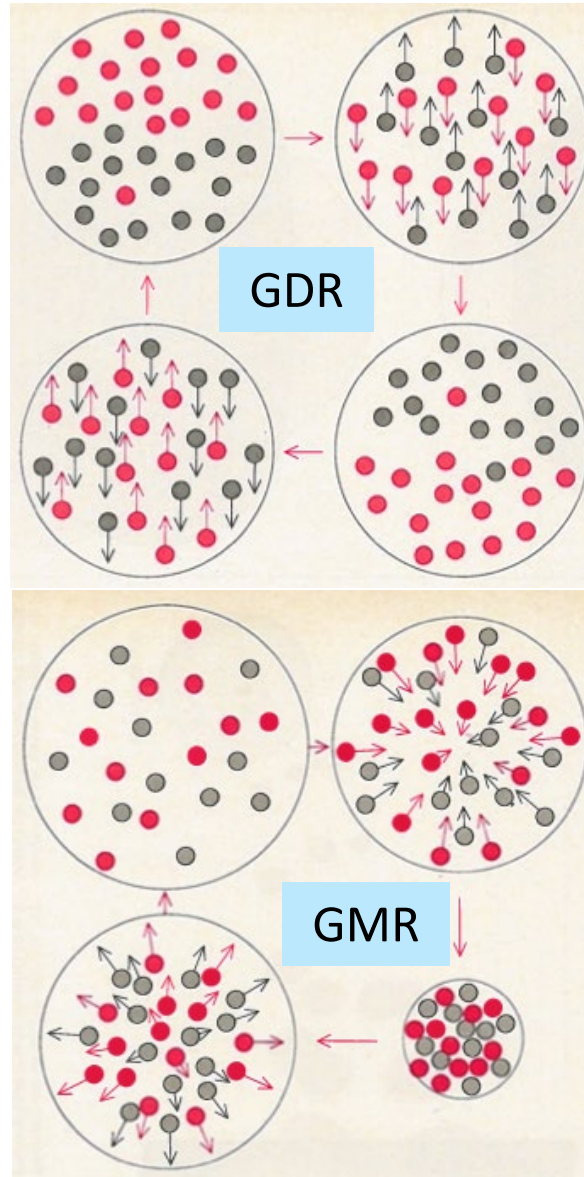


Time-Dependent Density Functional Theory

Time-Dependent Phenomena in Nuclei

Small-amplitude oscillations:

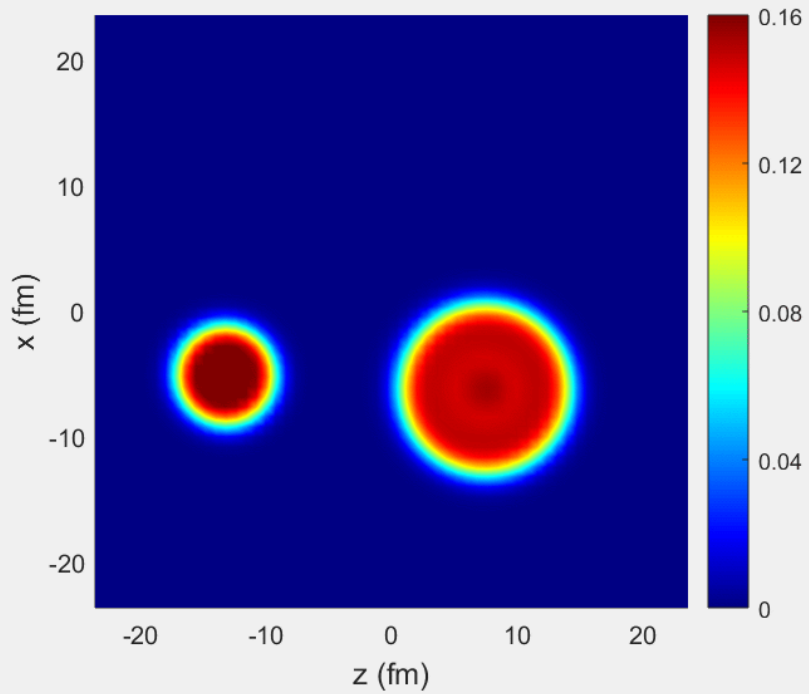
- Giant Dipole Resonance
- Giant Quadrupole Resonance
- Giant Monopole Resonance
- Giant Spin Vibrations



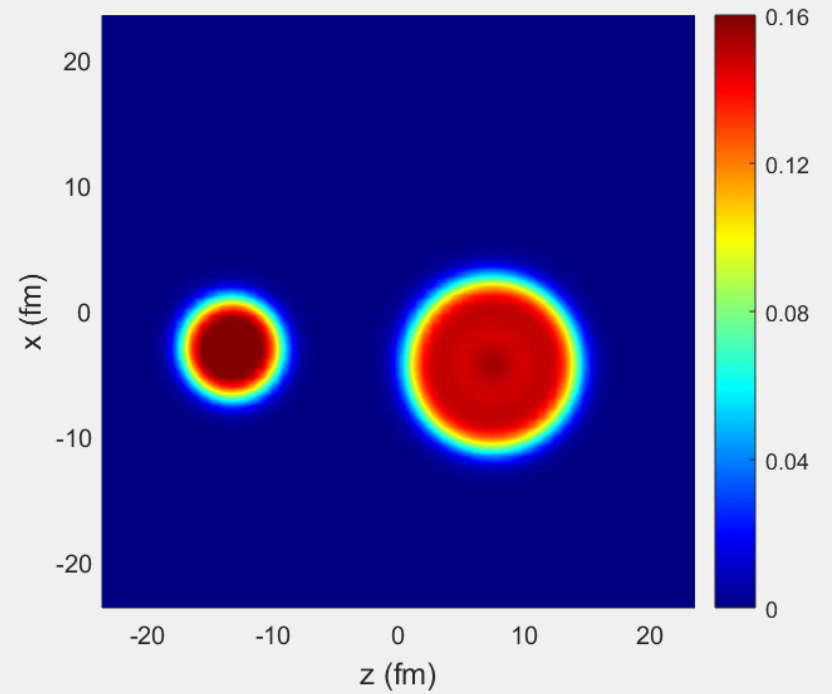


Multi-nucleon transfer reactions

$^{40}\text{Ar} + ^{208}\text{Pb}$, $E_{\text{lab}} = 256 \text{ MeV}$, $b = 5.50 \text{ fm}$, density at time = 40 fm/c



$^{40}\text{Ar} + ^{208}\text{Pb}$, $E_{\text{lab}} = 256 \text{ MeV}$, $b = 6.40 \text{ fm}$, density at time = 40 fm/c



Elements of Time-Dependent Density Functional Theory

A. The Runge-Gross Theorem

Runge-Gross theorem: under certain quite general conditions, there is a one-to-one correspondence between time-dependent one-body densities $n(\mathbf{r},t)$ and time-dependent one-body potentials $v_{\text{ext}}(\mathbf{r},t)$, for a given initial state. That is, a given evolution of the density can be generated by at most one time-dependent potential.

... define a fictitious system of noninteracting electrons moving in a time-dependent effective potential, whose density is precisely that of the real system. This effective potential is known as the **time-dependent Kohn-Sham potential**.

Just as in ground-state density functional theory (DFT), it consists of an external part, the Hartree potential, and the exchange-correlation potential, $v_{\text{xc}}(\mathbf{r}, t)$, which is a functional of:

- the entire history of the density, $n(\mathbf{r}, t)$,
- the initial interacting wavefunction, $\Psi(0)$, and
- the initial Kohn-Sham wavefunction, $\Phi(0)$.

B. One-to-one correspondence

N nonrelativistic electrons, mutually interacting via the Coulomb repulsion, in a **time-dependent external potential**.

The evolution of the wavefunction is governed by the time-dependent Schroedinger equation:

$$\hat{H}(t)\Psi(t) = i\frac{d\Psi(t)}{dt}, \quad \Psi(0) \text{ given}$$

$$\hat{T} = -\frac{1}{2} \sum_{i=1}^N \nabla_i^2$$

$$\hat{V}_{ee} = \frac{1}{2} \sum_{i \neq j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},$$

$$\hat{V}_{\text{ext}} = \sum_{i=1}^N v_{\text{ext}}(\mathbf{r}_i, t),$$

...electron density:
$$n(\mathbf{r}, t) = N \int d^3r_2 \dots \int d^3r_N |\Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N, t)|^2, \quad \int d^3r n(\mathbf{r}, t) = N.$$

R-G Theorem: the densities $n(\mathbf{r}, t)$ and $n'(\mathbf{r}, t)$ that evolve from a common initial state $\Psi(t=0)$ under the influence of two potentials $v_{\text{ext}}(\mathbf{r}, t)$ and $v'_{\text{ext}}(\mathbf{r}, t)$, eventually differ if the potentials differ by more than a purely time-dependent (\mathbf{r} -independent) function:

$$\Delta v_{\text{ext}}(\mathbf{r}, t) = v_{\text{ext}}(\mathbf{r}, t) - v'_{\text{ext}}(\mathbf{r}, t) \neq c(t).$$

→ one-to-one mapping between densities and potentials, which implies **that the potential is a functional of the density**.

C. Time-dependent Kohn-Sham Equations

...system of noninteracting electrons that satisfy time-dependent Kohn-Sham equations:

$$i \frac{\partial \varphi_j(\mathbf{r}, t)}{\partial t} = \left[-\frac{\nabla^2}{2} + v_{\text{KS}}[n](\mathbf{r}, t) \right] \varphi_j(\mathbf{r}, t),$$

The corresponding density: $n(\mathbf{r}, t) = \sum_{j=1}^N |\varphi_j(\mathbf{r}, t)|^2,$

Is by definition identical to that of the real, interacting system.

$$v_{\text{KS}}(\mathbf{r}, t) = v_{\text{ext}}(\mathbf{r}, t) + v_{\text{H}}(\mathbf{r}, t) + v_{\text{xc}}(\mathbf{r}, t),$$

External potential

Exchange-correlation potential

$$v_{\text{H}}(\mathbf{r}, t) = \int d^3 r' \frac{n(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|},$$

The **exchange-correlation potential** → a functional of the entire history of the density, $n(\mathbf{r}, t)$, the initial interacting wavefunction $\Psi(0)$, and the initial Kohn-Sham wavefunction, $\Phi(0)$.

D. Adiabatic approximation to the K-S Equations

The exact exchange-correlation potential depends on the entire history of the density, as well as the initial wavefunctions of both the interacting and the Kohn-Sham systems:

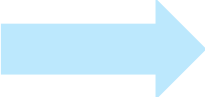
$$v_{\text{xc}}[n, \Psi(0), \Phi(0)](\mathbf{r}, t) = v_{\text{KS}}[n, \Psi(0), \Phi(0)](\mathbf{r}, t) - v_{\text{ext}}(\mathbf{r}, t) - v_{\text{H}}[n](\mathbf{r}, t)$$

Functionals of the initial density.

$V_{\text{exc}}(\mathbf{r}, t)$ has a functional dependence on all $n(\mathbf{r}, t')$ for $0 \leq t' \leq t$. The potential remembers the density's past, it has **memory**.

The **adiabatic approximation** \rightarrow ignore all dependence on the past, and allow only a dependence on the instantaneous density (local in time):

$$v_{\text{xc}}^{\text{adia}}[n](\mathbf{r}, t) = v_{\text{xc}}^{\text{approx}}[n(t)](\mathbf{r})$$


$$v_{\text{xc}}^{\text{adia}}[n](\mathbf{r}, t) = v_{\text{xc}}^{\text{GS}}[n_{\text{GS}}](\mathbf{r})|_{n_{\text{GS}}(\mathbf{r}')=n(\mathbf{r}', t)}$$

uniform electron gas

E. Initial-state dependence and memory

...memory due to initial-state dependence, and memory due to the history-dependence of the density:

$$v_{\text{xc}}[n, \Psi(0), \Phi(0)](\mathbf{r}, t) = v_{\text{KS}}[n, \Psi(0), \Phi(0)](\mathbf{r}, t) - v_{\text{ext}}(\mathbf{r}, t) - v_{\text{H}}[n](\mathbf{r}, t)$$

Memory arises in TDDFT because of the **reduced nature of the density as a basic variable**: If the wavefunction of the system was known, there would be no memory dependence, since the wavefunction at time t contains the complete information about the system at time t .

ALDA $v_{\text{xc}}^{\text{ALDA}}(\mathbf{r}, t) = v_{\text{xc}}^{\text{unif}}[n(\mathbf{r}, t)]$

An adiabatic approximation will work well if the system is slowly-varying so that it remains in a slowly-evolving lowest-energy state.

TDDFT in Nuclear Physics

A. No pairing - Hartree-Fock

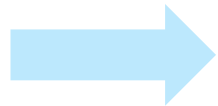
One-body operators

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

Density operator: $\rho(t) = \sum_{k=1}^N |\phi_k(t)\rangle \langle \phi_k(t)|,$

expressed in the time-dependent canonical single-particle basis.

$$[\langle \phi_k(t) | \phi_l(t) \rangle = \delta_{kl}].$$



$$i \frac{\partial}{\partial t} |\phi_k(t)\rangle = h(t) |\phi_k(t)\rangle$$

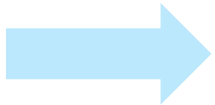
TDHF s.p. equations

Self-consistent and density-dependent (ALDA) potentials

B. Pairing - Hartree-Fock-Bogoliubov

$$i \frac{\partial}{\partial t} R = [\mathcal{H}, R],$$

$$R \equiv \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}, \quad \mathcal{H} \equiv \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}.$$


$$i \frac{\partial}{\partial t} \rho(t) = [h(t), \rho(t)] + \kappa(t)\Delta^*(t) - \Delta(t)\kappa^*(t),$$

$$i \frac{\partial}{\partial t} \kappa(t) = h(t)\kappa(t) + \kappa(t)h^*(t)$$

$$+ \Delta(t)[1 - \rho^*(t)] - \rho(t)\Delta(t).$$

Density operator

Pairing tensor

TD-HFB equations

BCS approximation in the canonical basis

TD-HFB state:
$$|\Psi(t)\rangle = \prod_{k>0} \{u_k(t) + v_k(t)c_k^\dagger(t)c_{\bar{k}}^\dagger(t)\}|0\rangle.$$

Time-reversed orbital

BCS approximation:
$$\Delta_{k\bar{l}} = -\Delta_k \delta_{kl} \quad \rightarrow \text{Diagonal pairing field.}$$

$$i \frac{d}{dt} \rho_k(t) = \kappa_k(t) \Delta_{\bar{k}}^*(t) - \kappa_{\bar{k}}^*(t) \Delta_k(t),$$

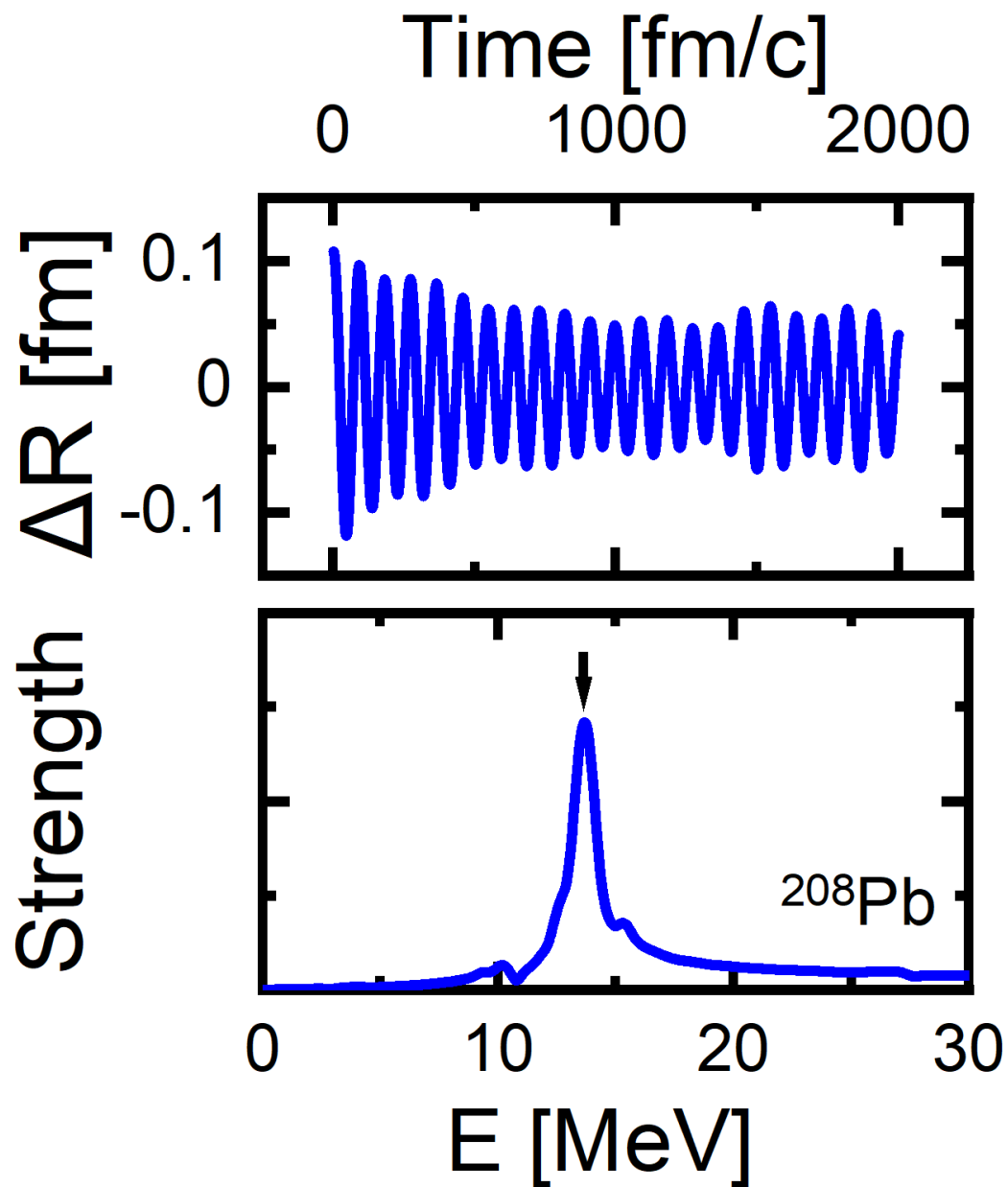
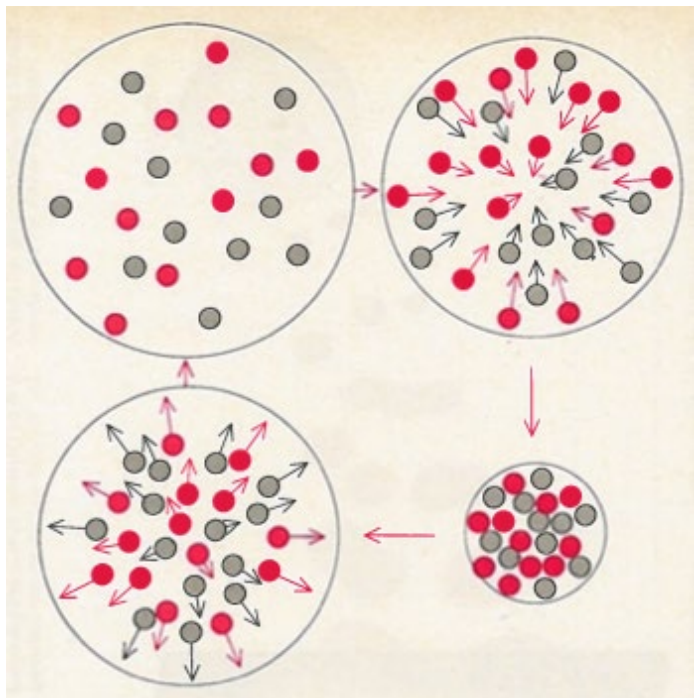
$$i \frac{d}{dt} \kappa_k(t) = [\eta_k(t) + \eta_{\bar{k}}(t)] \kappa_k(t) + \Delta_k(t) [2\rho_k(t) - 1],$$

$$i \frac{\partial}{\partial t} |\phi_k(t)\rangle = [h(t) - \eta_k(t)] |\phi_k(t)\rangle,$$

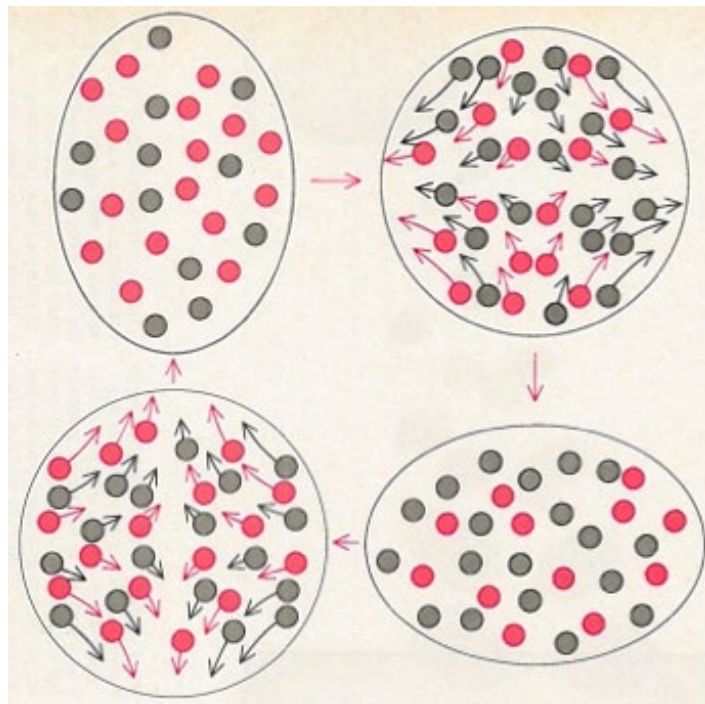
$$i \frac{\partial}{\partial t} |\phi_{\bar{k}}(t)\rangle = [h(t) - \eta_{\bar{k}}(t)] |\phi_{\bar{k}}(t)\rangle.$$

...where
$$\eta_k(t) \equiv \langle \phi_k(t) | h(t) | \phi_k(t) \rangle + i \langle \frac{\partial \phi_k}{\partial t} | \phi_k(t) \rangle.$$

Isoscalar Monopole Vibrations

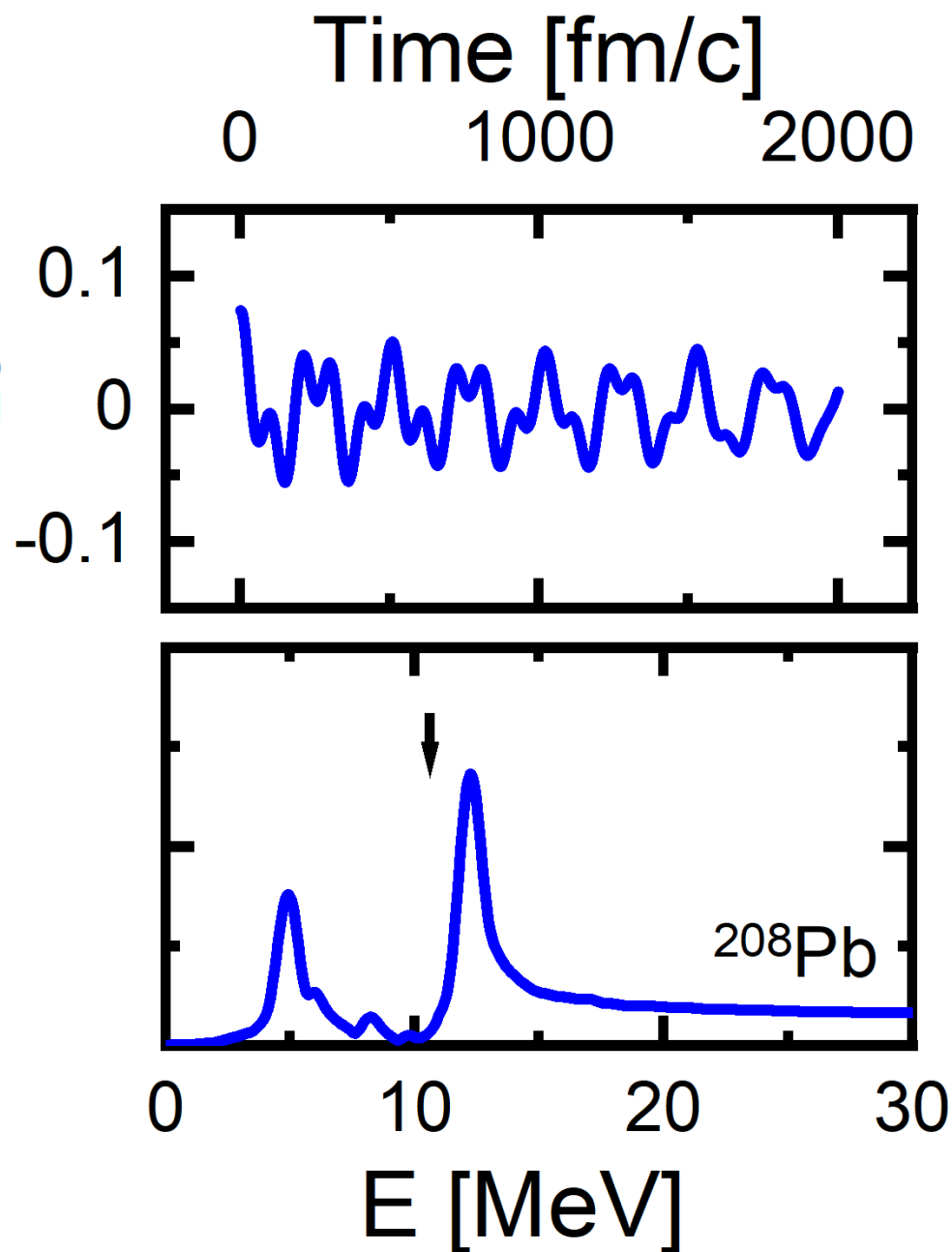


Isoscalar Quadrupole Vibrations



β_{20}

Strength



Isovector Dipole Vibrations

