Projects for computational fundamental physics in Japan and TD approaches to nuclear structure/reaction

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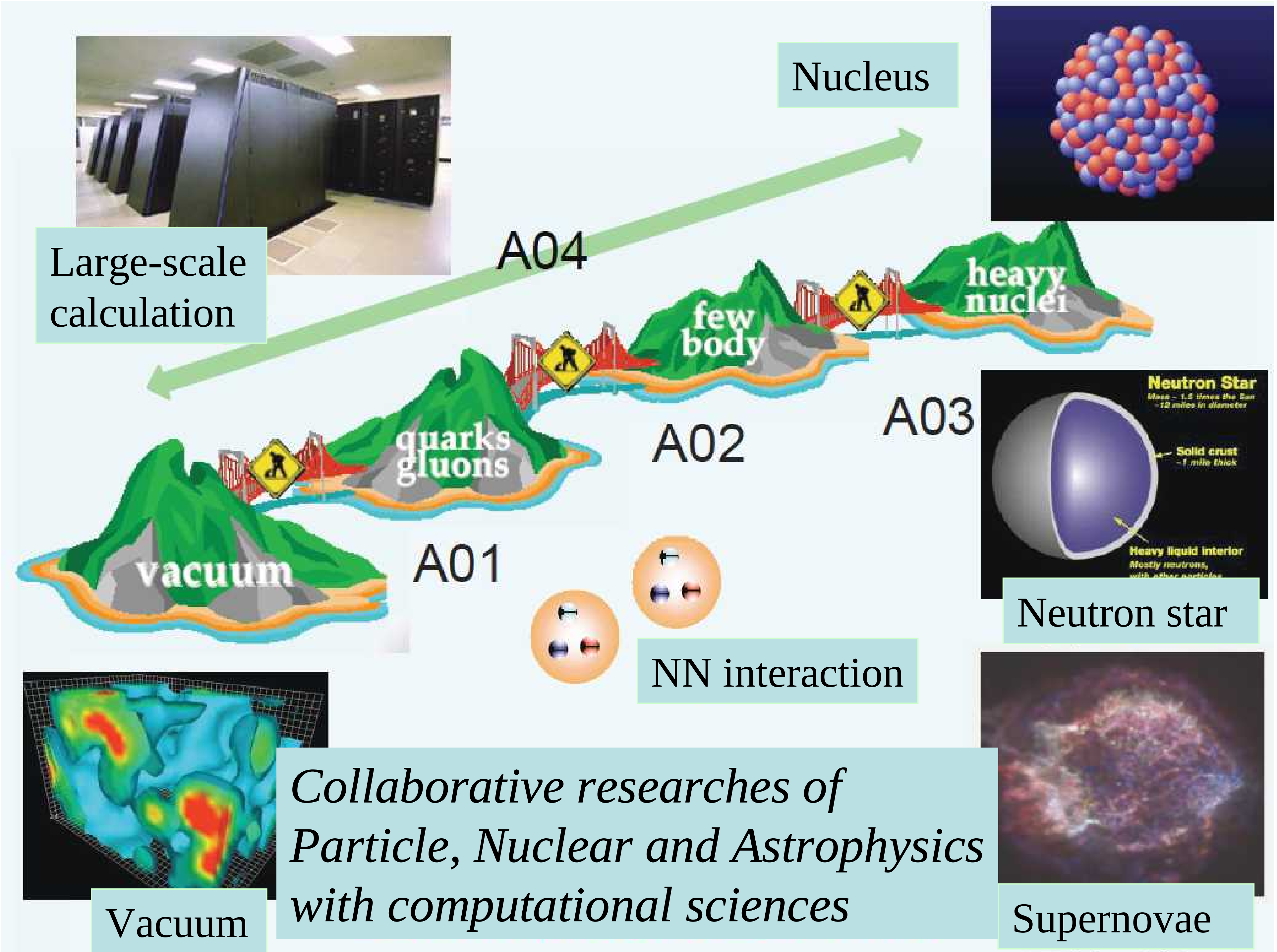
Collaborative researches of Particle, Nuclear and Astrophysics with computational sciences

URL: http://bridge.kek.jp/ (currently only in Japanese)

- JSPS Grant-in-Aid for Scientific Research on Innovative Areas (2008.12 -- 2013.3)

  Representative: S. Aoki (Univ. Tsukuba)
- A01 Particle Physics
- A02 Nuclear Physics
- A03 Astrophysics
- A04 Computer Sciences



Nucleus
Large-scale calculation
A04
heavy nuclei
few body
quarks gluons
vacuum
A01
A02
A03
Neutron Star
Solid crust
Heavy liquid interior
Neutron star
NN interaction
Vacuum
Supernovae
Collaborative researches of Particle, Nuclear and Astrophysics with computational sciences

- A01: Structure of vacuum and quark dynamics in QCD [Onogi (YITP)]
- A02: Nuclear structure from quark dynamics [Hatsuda (Tokyo)]
- A03: Explosive phenomena in universe and element synthesis from quark structure and nuclear structure [Suzuki (Tokyo Sci.)]
- A04: Universal algorithms and computer simulations [Matsufuru (KEK)]

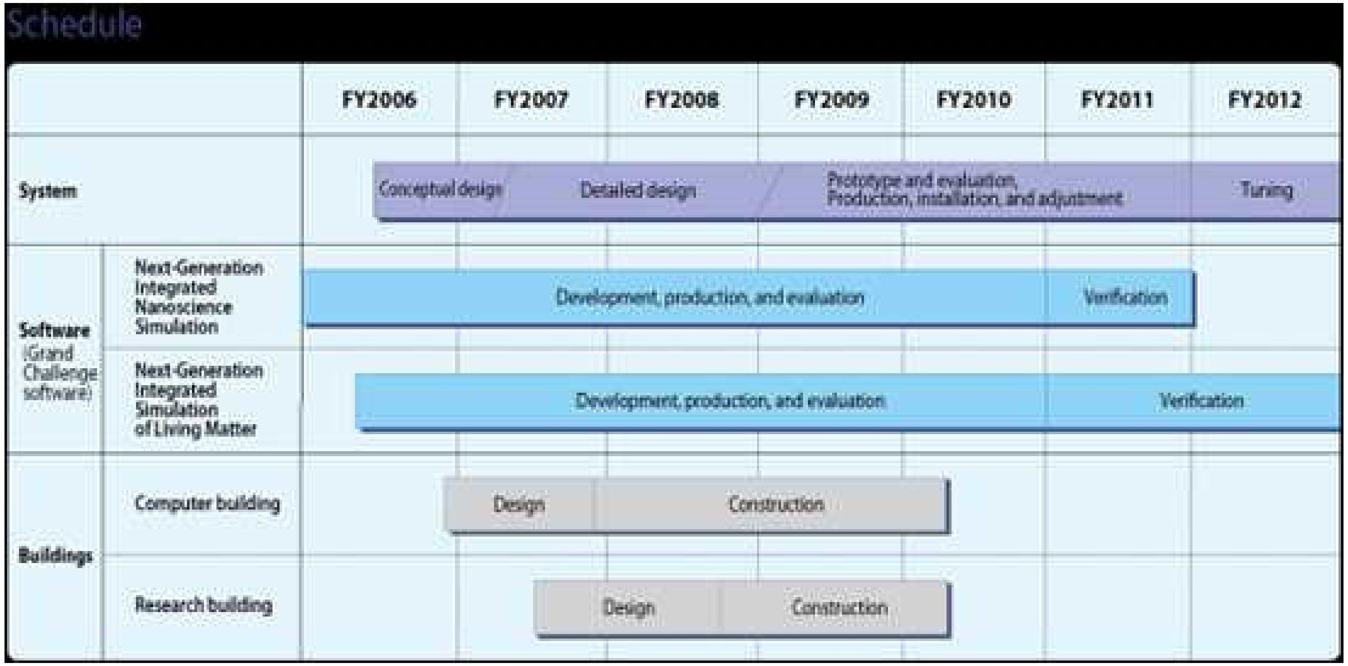
A02:
Nuclear structure from quark dynamics

- Univ. Tokyo
  - Hatsuda, Otsuka, Sasaki
- Univ. Tsukuba
  - Aoki, Ishii, Yabana
- RIKEN
  - Hiyama, Nakatsukasa
- Others
  - Nakamura (Hiroshima), Suzuki (Nihon), Takano (Waseda)
- PDs
  - Abe (Tokyo), Ikeda (RIKEN), Nagata (Hiroshima), Sasaki (Tsukuba)

New-generation supercomputer facility

Supercomputer (10 Pflops) are currently under construction in Kobe, Japan.

RIKEN is responsible for the construction.



Selected Major Fields of Applications

1. Life science and Medicine
2. New materials and energy generation
3. Climate and earthquake prediction
4. Next-generation manufacturing
5. Origin and structure of matter and universe

Ten Groups

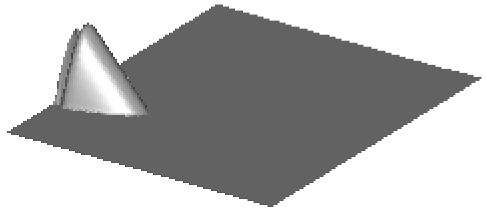
1. Models for elementary particles and phase transitions in Big Bang [Hashimoto (KEK)]
2. Unified understanding on quark dynamics using lattice QCD [Kuramashi (Tsukuba)]
3. QCD and hadron structure [Hatsuda (Tokyo)]
4. Exotic nuclei from nuclear force [Otsuka (Tokyo)]
5. Many-particle simulation for nuclear reactions and element synthesis [Nakatsukasa (RIKEN)]
6. Mechnism/Origin of supernovae, gamma-ray burst, and black holes [Shibata (Kyoto)]
7. Fundamental processes of magnetic fluid and plasma phenomena in universe [Matsumoto (Chiba)]
8. Fundamental processes of formation of stars [Makino (NAO)]
9. Fundamental processes of formation of galaxies and giant black holes [Umemura (Tsukuba)]
10. Support for massively parallel computing and data sharing management [Boku (Tsukuba)]

Nuclear Physics Applications

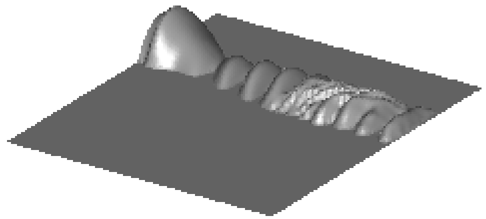
- QCD and hadron structure (Hatsuda; Tokyo)
  - Baryon interaction from lattice QCD
  - Few-body systems
  - Finite-density lattice QCD
- Exotic nuclei from nuclear force (Otsuka; Tokyo)
  - Shell model
  - NCSM calculations
  - Effective interactions
- Reaction simulation of nuclear dynamics and element synthesis (Nakatsukasa; RIKEN)
  - Large-scale simulation for many-nucleon dynamics
  - Low-energy nuclear reaction and many-nucleon resonances
  - High-density nuclear matter and explosive element synthesis

Time-dependent approaches

- Time-dependent Schroedinger equation for few-body models
  - TD wave-packet method for low-energy nuclear reaction
  - Calculation of strength function with Pauli forbidden states



- TDDFT calculation
  - Real-time TDHF (no pairing)
  - Canonical-basis TDHFB



Canonical-basis TDHFB

Full TDHFB calculation is computationally demanding.

Possible approximation: HFB → HF+BCS

Any instant of time, the state can be written in the canonical form:

$$\left|\Psi(t)\right\rangle = \prod_{k>0}\left(u_k(t) + v_k(t)c_k^+(t)c_{\bar{k}}^+(t)\right)\left|0\right\rangle \qquad \rho_k = |v_k|^2, \kappa_k = u_k v_k$$

Density matrix and pair tensor are given by

$$\rho_{\mu\nu}(t) = \sum_{k>0}\rho_k(t)\left(\left\langle\mu\middle|k(t)\right\rangle\left\langle k(t)\middle|\nu\right\rangle + \left\langle\mu\middle|\bar{k}(t)\right\rangle\left\langle\bar{k}(t)\middle|\nu\right\rangle\right)$$

$$\kappa_{\mu\nu}(t) = \sum_{k>0}\kappa_k(t)\left(\left\langle\mu\middle|k(t)\right\rangle\left\langle\nu\middle|\bar{k}(t)\right\rangle - \left\langle\mu\middle|\bar{k}(t)\right\rangle\left\langle\nu\middle|k(t)\right\rangle\right)$$

Here, $\left|k(t)\right\rangle$ and $\left|\bar{k}(t)\right\rangle$ are not related by the time reversal, in general.

Canonical-basis TDHFB

TDHFB equation in the generalized density matrix

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

$$R(t)=\begin{pmatrix}\rho(t) & \kappa(t)\\ -\kappa^{*}(t) & 1-\rho^{*}(t)\end{pmatrix},\quad H(t)=\begin{pmatrix}h(t) & \Delta(t)\\ -\Delta^{*}(t) & -h^{*}(t)\end{pmatrix}$$

Substituting the canonical expression of density and pair tensor, we can find reach a set of simple equations, if we assume that the pair potential is diagonal in the canonical basis.

$$\Delta_{\mu\nu}(t)=-\sum_{k>0}\Delta_k(t)\Big(\langle\mu|k(t)\rangle\langle\nu|\bar{k}(t)\rangle-\langle\mu|\bar{k}(t)\rangle\langle\nu|k(t)\rangle\Big)$$

$$\Delta_k(t)=-\sum_{l>0}\kappa_l(t)\bar{V}_{k\bar{k},l\bar{l}}$$

Canonical-basis TDHFB

TDHFB equations

$$i\frac{\partial}{\partial t}\left|k(t)\right\rangle = \left(h(t)-\eta_k(t)\right)\left|k(t)\right\rangle, \quad i\frac{\partial}{\partial t}\left|\bar{k}(t)\right\rangle = \left(h(t)-\eta_{\bar{k}}(t)\right)\left|\bar{k}(t)\right\rangle$$

$$i\frac{\partial}{\partial t}\rho_k(t) = \kappa_k(t)\Delta_k^*(t) - \kappa_k^*(t)\Delta_k(t)$$

$$i\frac{\partial}{\partial t}\kappa_k(t) = \left(\eta_k(t)+\eta_{\bar{k}}(t)\right)\kappa_k(t) + \Delta_k(t)\left(2\rho_k(t)-1\right)$$

The number of canonical states is similar to the particle number.

Thus, the necessary computational task is similar to that of TDHF.

(In TDHFB, the number of quasi-particle states is much larger than the particle number.)

Canonical-basis TDHFB

A schematic (simplified) pairing functional

$$E[\kappa(t)] = \sum_{k,l>0} G_{kl} \kappa_k^*(t) \kappa_l(t)$$

Blocki, Floard, NPA273 (1976) 45.

violates the gauge invariance.

In this case, we must choose the special gauge:

$$\eta_k(t) = \varepsilon_k(t) = \langle k(t)|h(t)|k(t)\rangle \Leftrightarrow \left\langle \frac{\partial k}{\partial t} \middle| k(t) \right\rangle = 0$$

$$i\frac{\partial}{\partial t}|k(t)\rangle = (h(t) - \varepsilon_k(t))|k(t)\rangle, \quad i\frac{\partial}{\partial t}|\bar{k}(t)\rangle = (h(t) - \varepsilon_{\bar{k}}(t))|\bar{k}(t)\rangle$$

$$i\frac{\partial}{\partial t}\rho_k(t) = \kappa_k(t)\Delta_k^*(t) - \kappa_k^*(t)\Delta_k(t)$$

$$i\frac{\partial}{\partial t}\kappa_k(t) = (\varepsilon_k(t) + \varepsilon_{\bar{k}}(t))\kappa_k(t) + \Delta_k(t)(2\rho_k(t) - 1)$$

Properties of CB-TDHFB

$$i\frac{\partial}{\partial t}|k(t)\rangle = \left(h(t) - \varepsilon_k(t)\right)|k(t)\rangle$$

$$i\frac{\partial}{\partial t}\rho_k(t) = \Delta^*(t)K_k(t) - \text{c.c.}$$

$$i\frac{\partial}{\partial t}K_k(t) = \left(\varepsilon_k(t) + \varepsilon_{\bar{k}}(t)\right)K_k(t) + \Delta(t)\left(2\rho_k(t) - 1\right)$$

$$\rho_k(t) \equiv |v_k(t)|^2, \quad K_k(t) \equiv u_k(t)v_k(t)$$

- Conserve the particle number and the total energy $\frac{d}{dt}\langle N\rangle = \frac{d}{dt}E_{\text{tot}} = 0$
- Conserve the orthonormality of canonical orbitals $\frac{d}{dt}\langle k(t)|k'(t)\rangle = 0$
- Reduce to TDHF for $\boldsymbol{\Delta} = 0$
- Its static limit coincides with the HF+BCS

In the small-amplitude limit,

- Nambu-Goldstone modes appear as the zero-energy modes.
- The pairing vibrations in the normal phase coincide with the pp- and hh-RPA

Skyrme Cb-TDHFB in real space

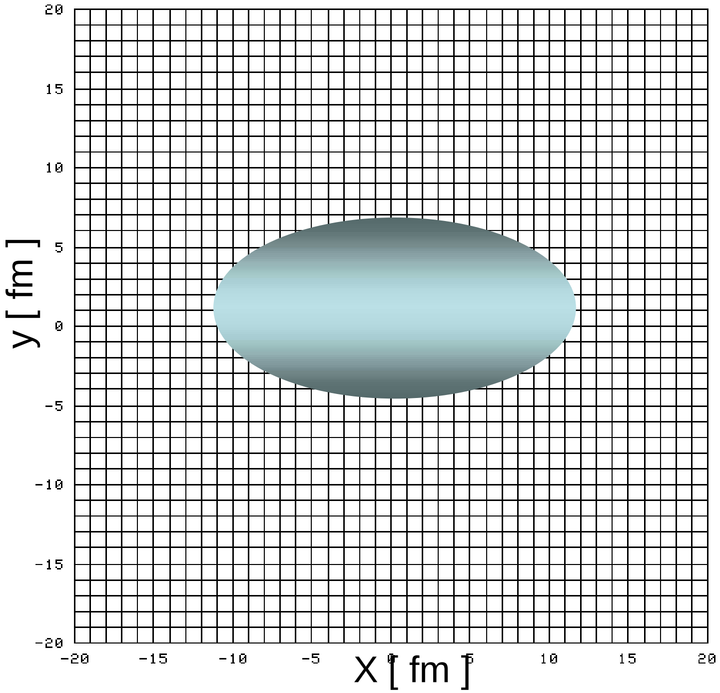
Time evolution is calculated as a simple Euler's method.

$$i\left|k(t+2dt)\right\rangle = i\left|k(t)\right\rangle + \left(h(t+dt) - \eta_k(t+dt)\right)\left|k(t+dt)\right\rangle$$

$$i\rho_k(t+2dt) = i\rho_k(t) + \left(\kappa_k(t+dt)\Delta_k(t+dt) - c.c.\right)\rho_k(t+dt)$$

$$i\kappa_k(t+2dt) = \cdots$$

3D mesh representation for canonical states



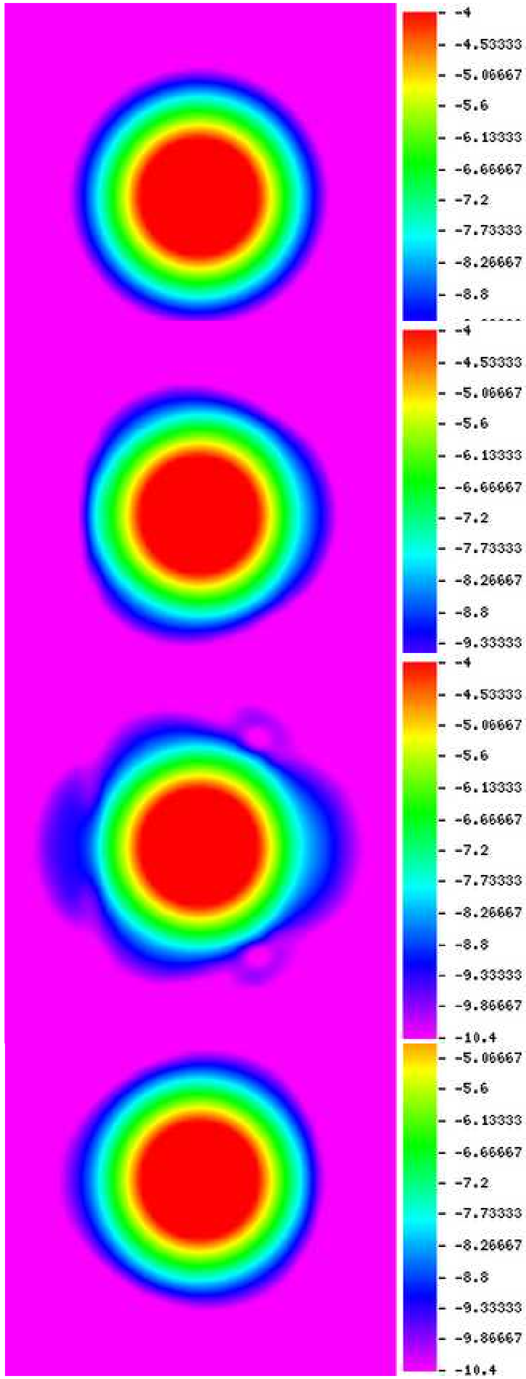
$$\left\langle \mathbf{r},\sigma;t\middle|k\right\rangle = \left\{\left\langle \mathbf{r}_i,\sigma;t_n\middle|k\right\rangle\right\}_{i=1,\cdots Mr}^{n=1,\cdots Mt}, \quad k=1,\cdots,M \geq N$$

Spatial size is a spherical box of radius of 12 fm.

Spatial mesh size is 0.8 fm.

Time step is about 0.2 fm/c

Ebata et al, to be published.



Real-time calculation

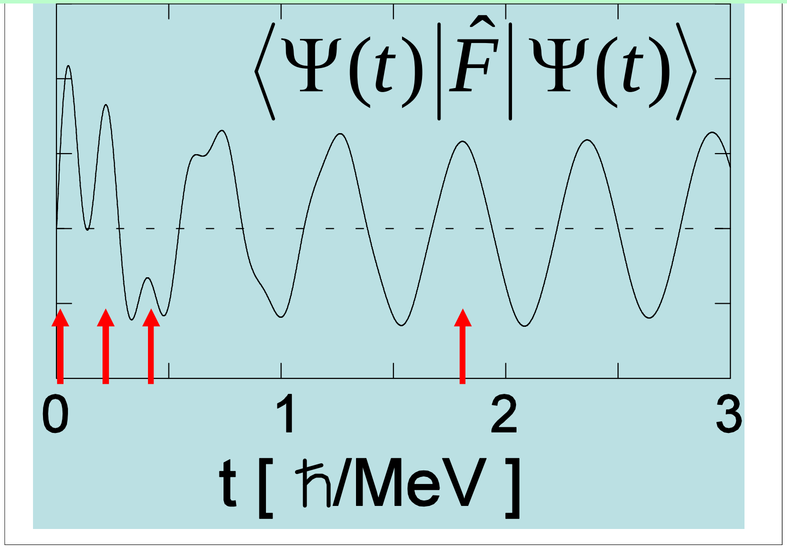
1. Weak instantaneous external perturbation

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

2. Calculate time evolution of

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

3. Fourier transform to energy domain



Real-time calculation of linear-response functions

1. Weak instantaneous external perturbation

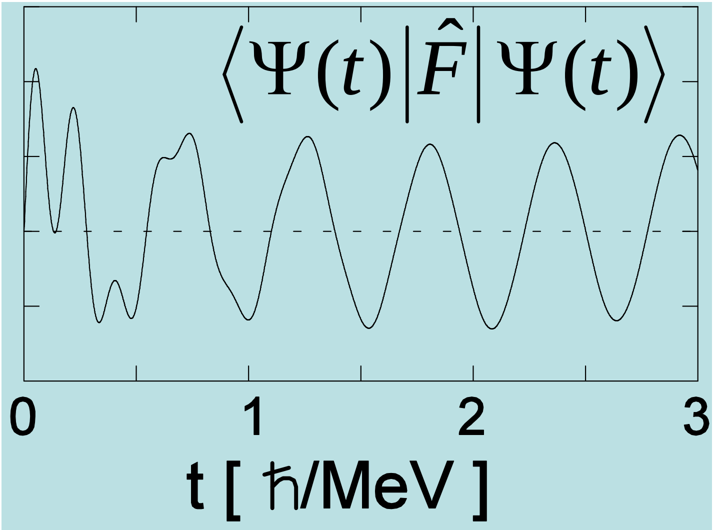
$$V_{\rm ext}(t) = \eta \hat{F} \delta(t)$$

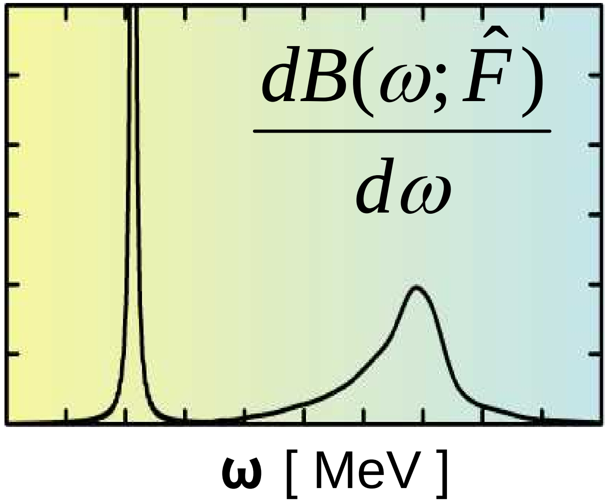
2. Calculate time evolution of

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

3. Fourier transform to energy domain

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





Ground-state properties in Ne and Mg

Skyrme functional of SkM*

Pairing functional from Tajima et al, NPA**603**, 23 (1996)

	β	γ	Δ_n	Δ_p	$-\lambda_n$	$-\lambda_p$
^{20}Ne	0.37	0°	0.0	0.0	13.07	9.19
^{22}Ne	0.37	0°	0.0	0.0	11.03	12.38
^{24}Ne	0.17	60°	0.0	0.74	10.57	13.04
^{26}Ne	0.0	–	0.0	1.00	7.17	14.92
^{28}Ne	0.0	–	0.79	1.01	3.22	17.05
^{30}Ne	0.0	–	0.0	1.01	3.79	19.09
^{32}Ne	0.36	0°	0.95	0.0	2.16	23.61
^{24}Mg	0.39	0°	0.0	0.0	14.12	9.51
^{26}Mg	0.20	54°	0.0	0.86	13.08	11.23
^{28}Mg	0.0	–	0.0	1.03	9.21	13.30
^{30}Mg	0.0	–	1.31	1.03	5.48	15.49
^{32}Mg	0.0	–	0.0	1.03	5.83	17.55
^{34}Mg	0.37	0°	1.45	0.0	4.12	20.18
^{36}Mg	0.33	0°	1.43	0.0	3.21	21.95
^{38}Mg	0.30	0°	1.47	0.0	2.38	23.69
^{40}Mg	0.29	0°	0.91	0.0	1.31	25.28

$\Delta_n = \Delta_p = 0$

$\beta > 0$

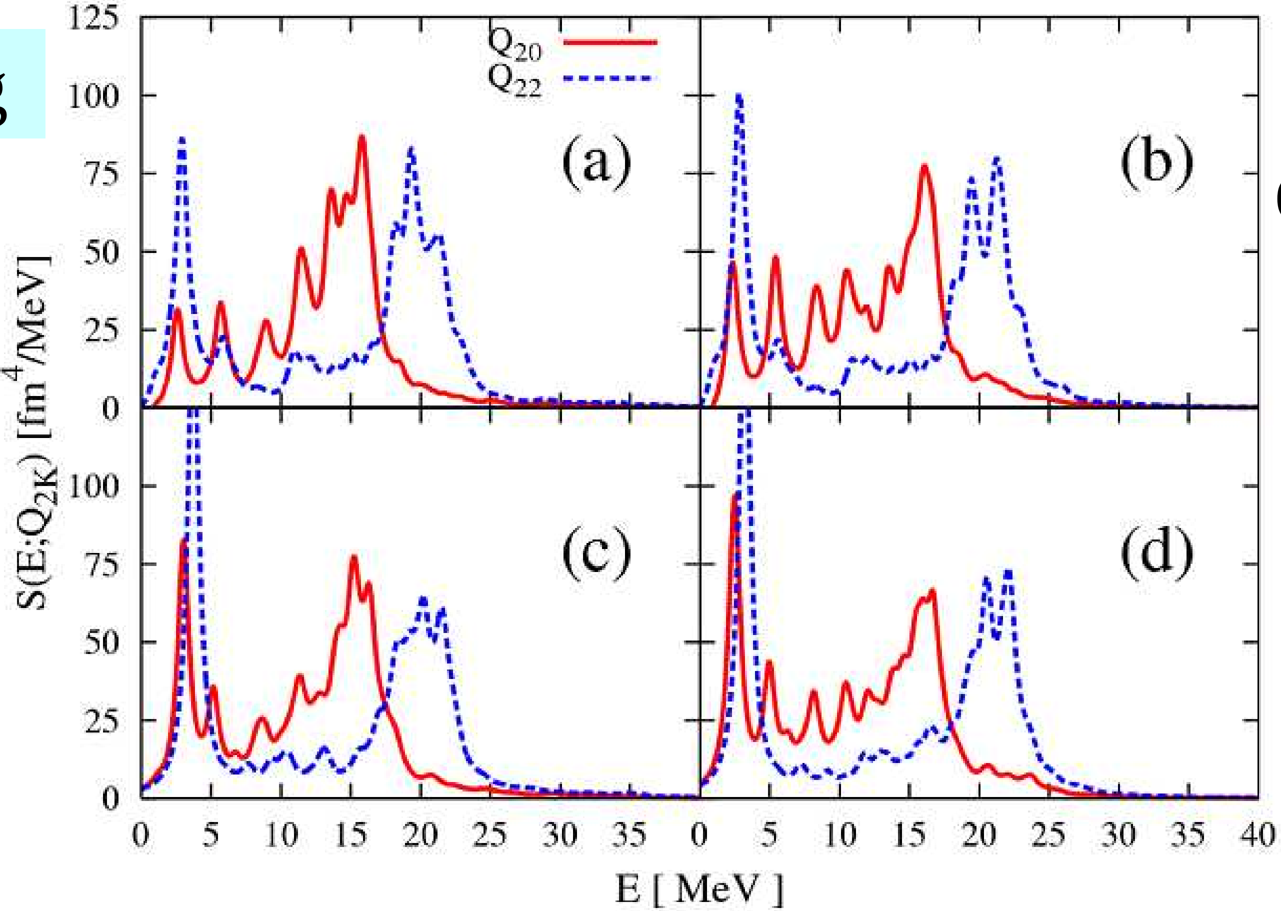
$\beta < 0$

$\beta = 0$

$\gamma \neq 0°, 60°$

Comparison with QRPA (IS quadrupole strength)

^{34}Mg



(b) Cb-TDHFB

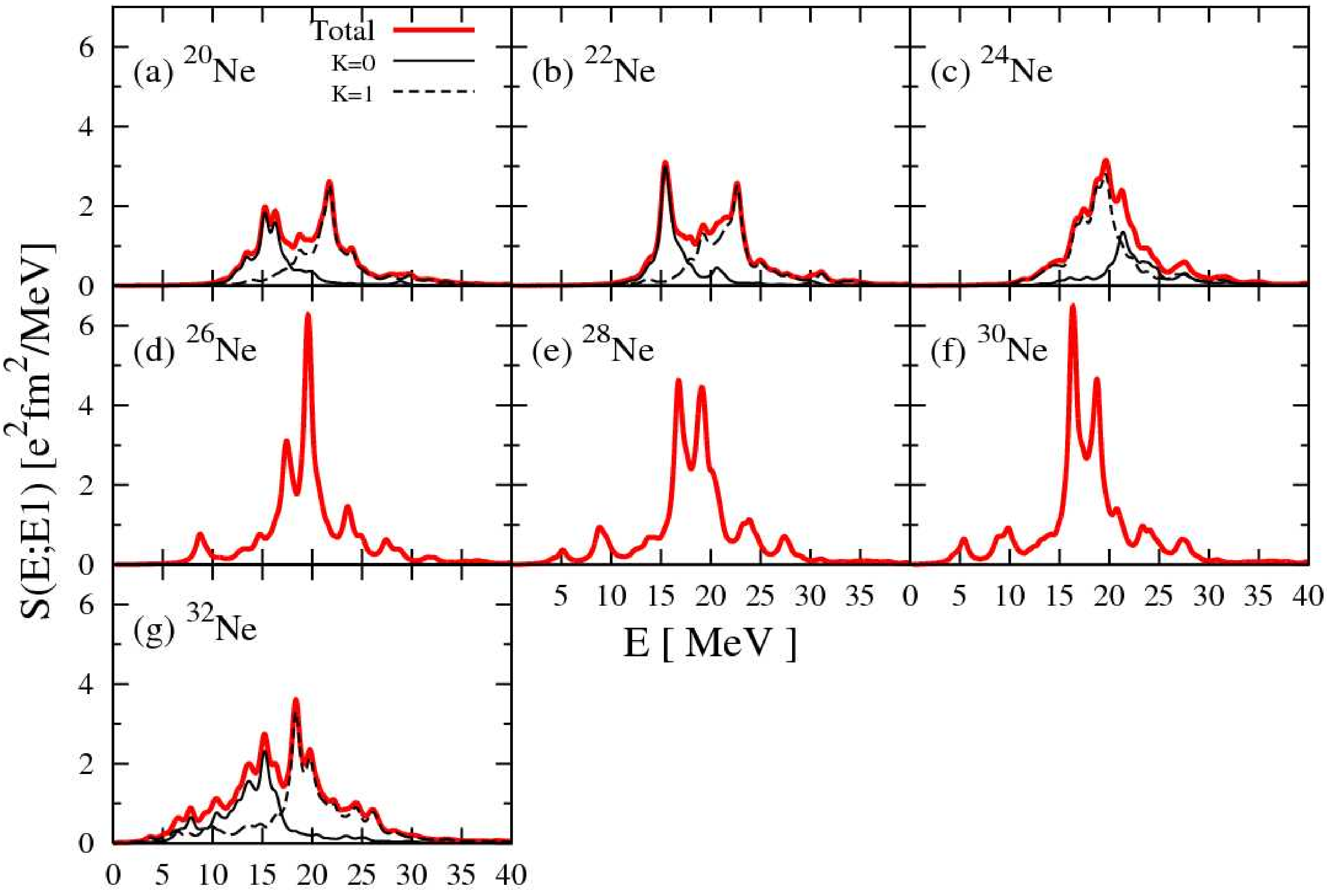
(a) Cb-TDHFB with fixed LS & Coulomb potentials

(c) QRPA without residual LS and Coulomb interactions (delta-pairing)

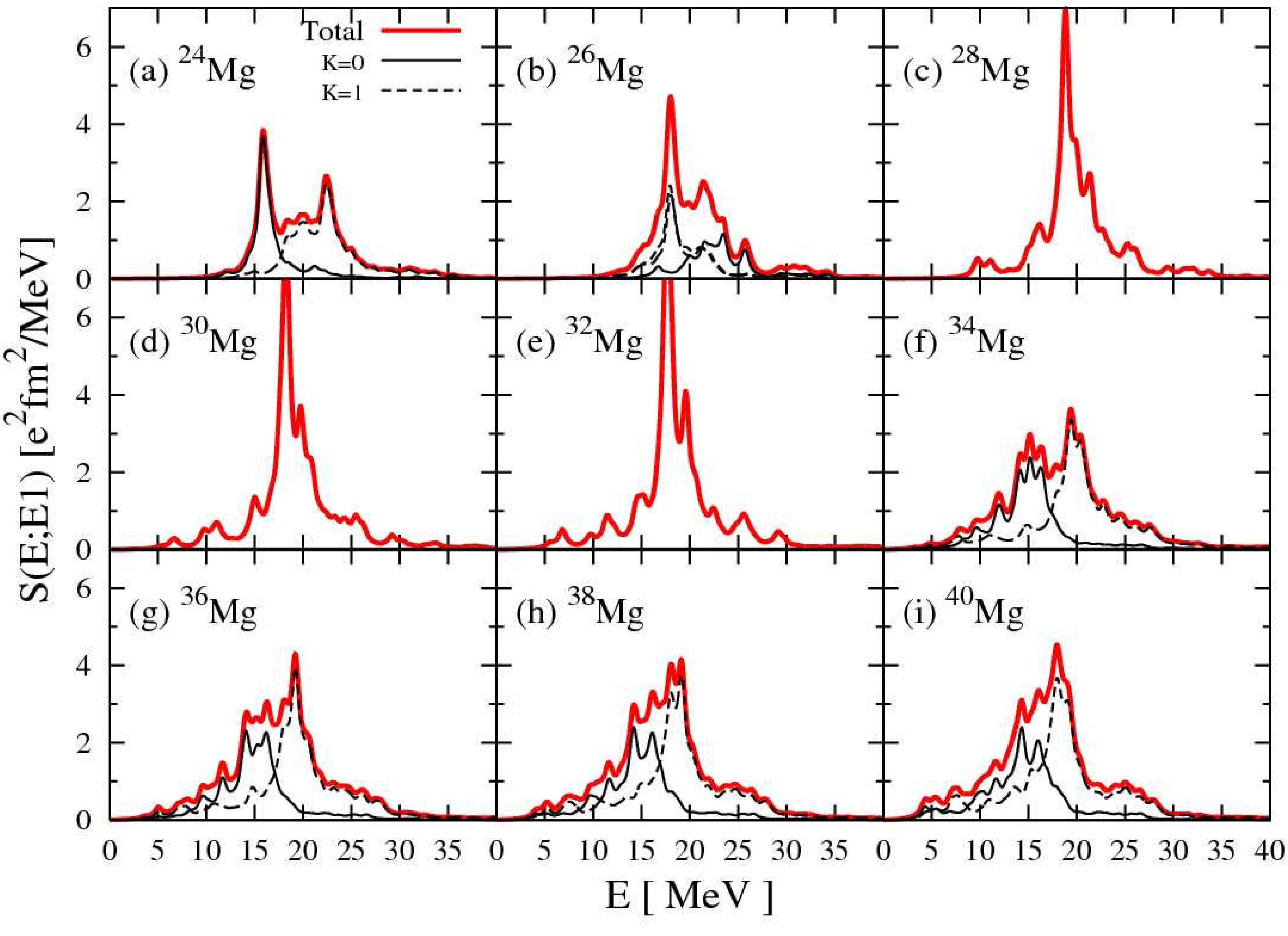
(d) QRPA (delta-pairing)
Losa et al. PRC81, 064307 (2010)

Results well agree with each other, except for height of the lowest peak.

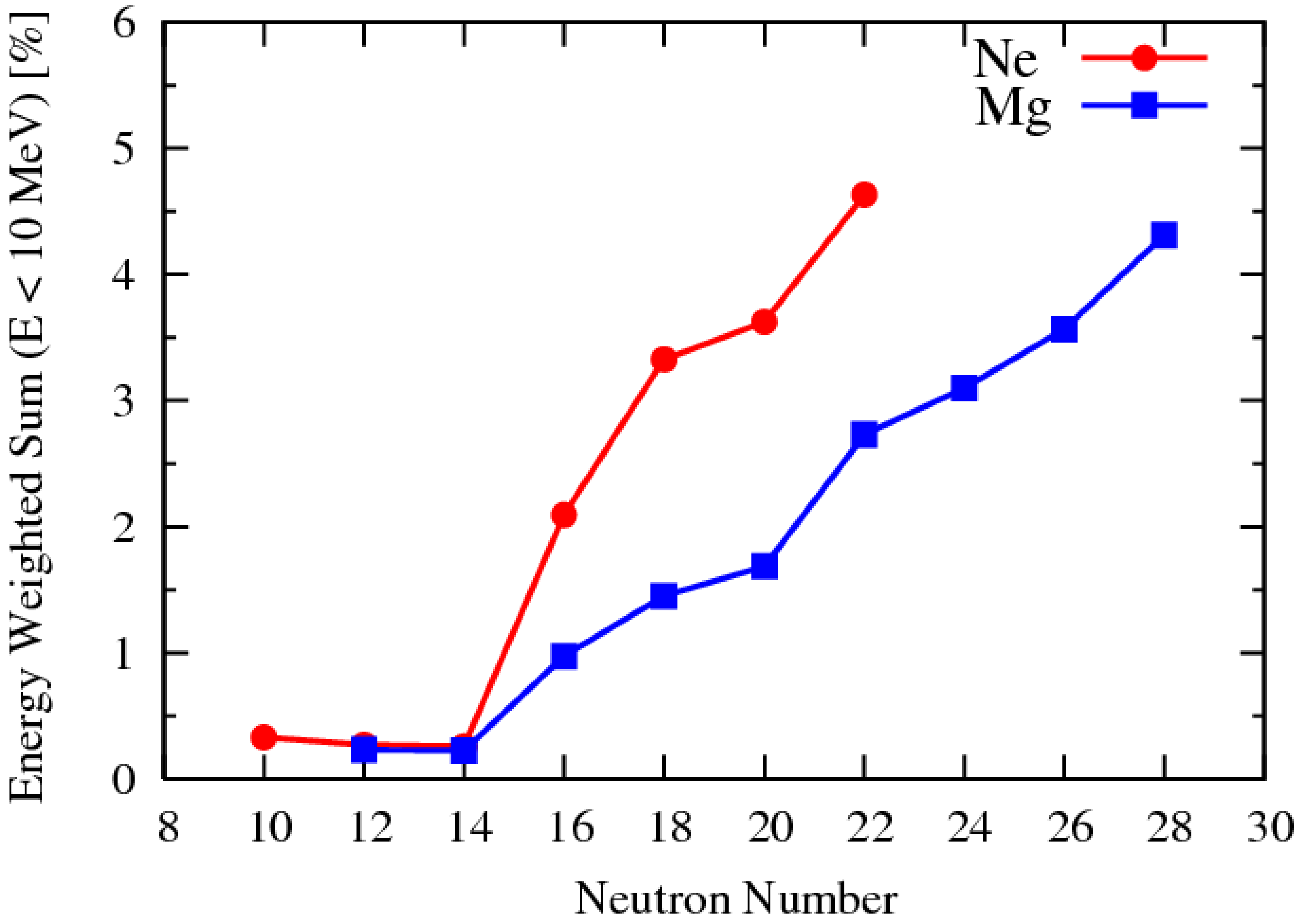
Isovector dipole responses in Ne



Isovector dipole responses in Mg



Low-energy pygmy E1 strength



Low-energy strength suddenly grows up at N=14 → 16, which may indicate effects of low-*l* neutron orbitals.

Summary

- Cb-TDHFB equations derived from TDHFB equation of motion
  - Become simple when we approximate the pair potential in a diagonal form in the TD canonical states (analogous to BCS).
  - Computational task is comparable with TDHF.
  - Need a special gauge condition for the simple pairing functional that violates the gauge invariance.
- Linear response with Cb-TDHFB using a simple pairing functional
  - Quantitatively well agree with QRPA
  - E1 strength distribution in Ne and Mg isotopes
  - Pygmy strength appear when neutron starts occupying $s_{1/2}$ orbital.