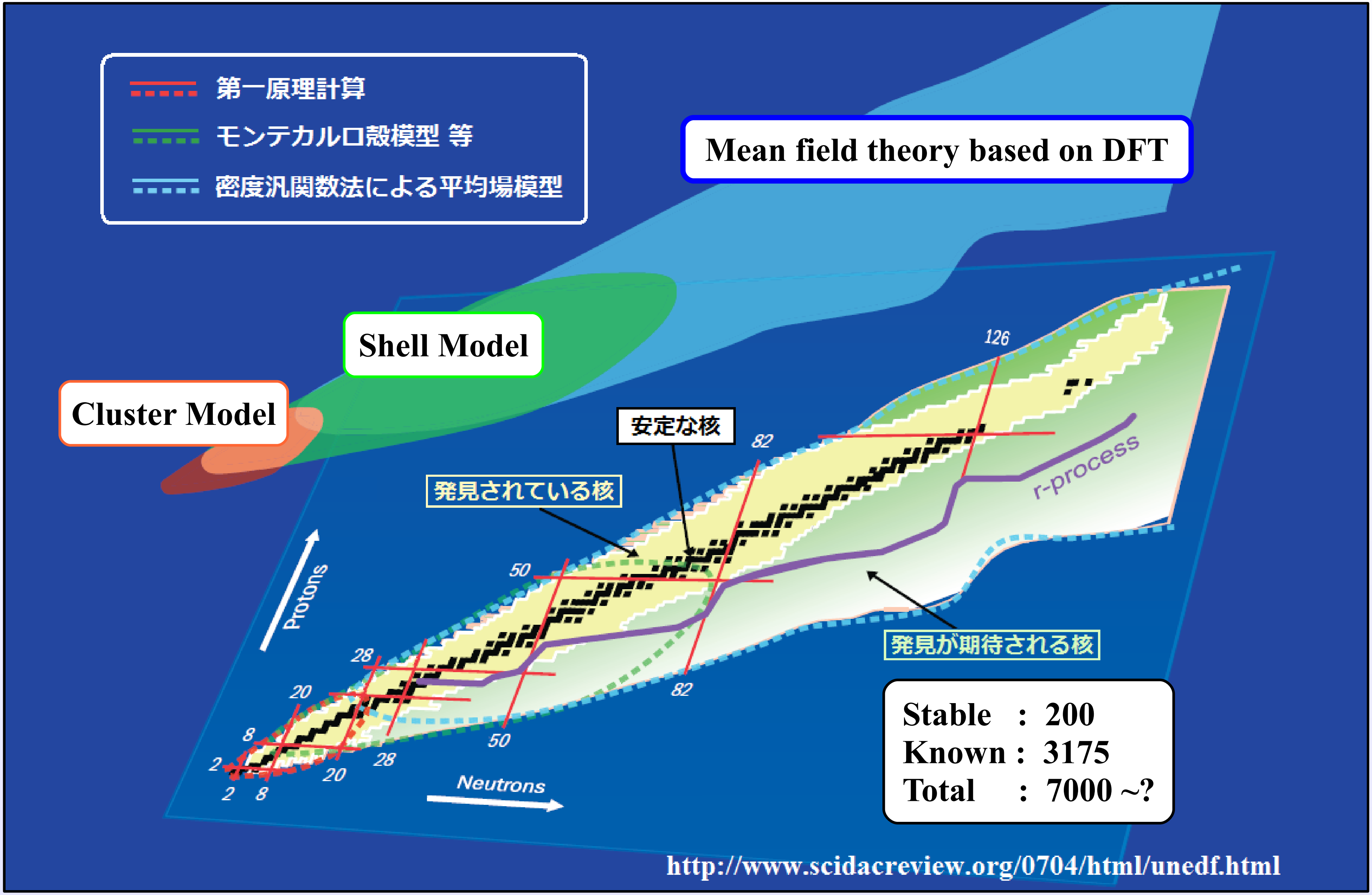
# 光核反応に対する密度汎関数理論の応用
## Application of Density Functional Theory to photo-nuclear reaction

江幡 修一郎
Ebata Shuichiro

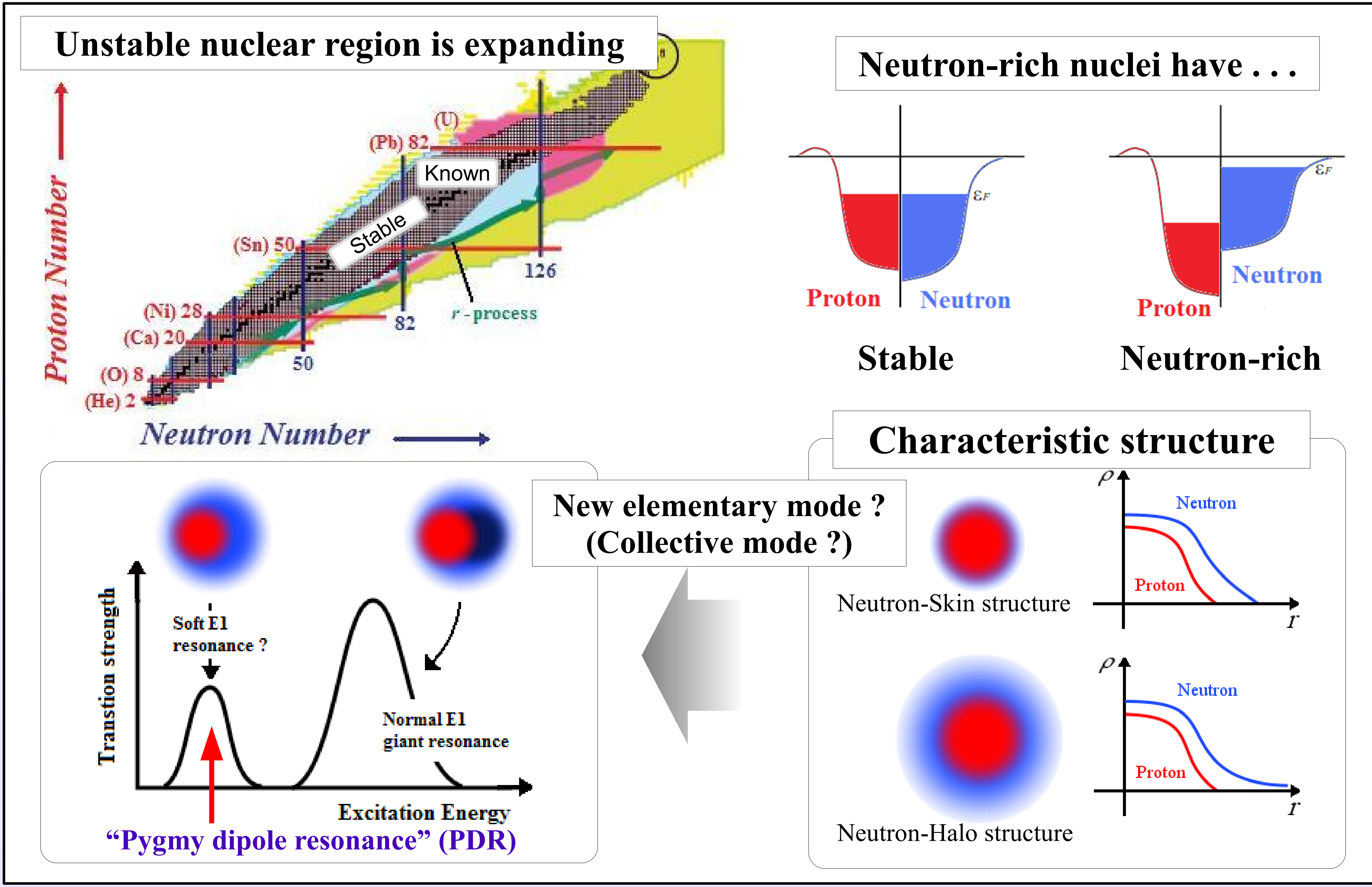
HPCI戦略分野5
研究課題2 大規模量子多体計算による核物性の解明と応用

東京大学 原子核科学研究センター
(Center for Nuclear Study, Univ. Tokyo; CNS)

# Working area of models

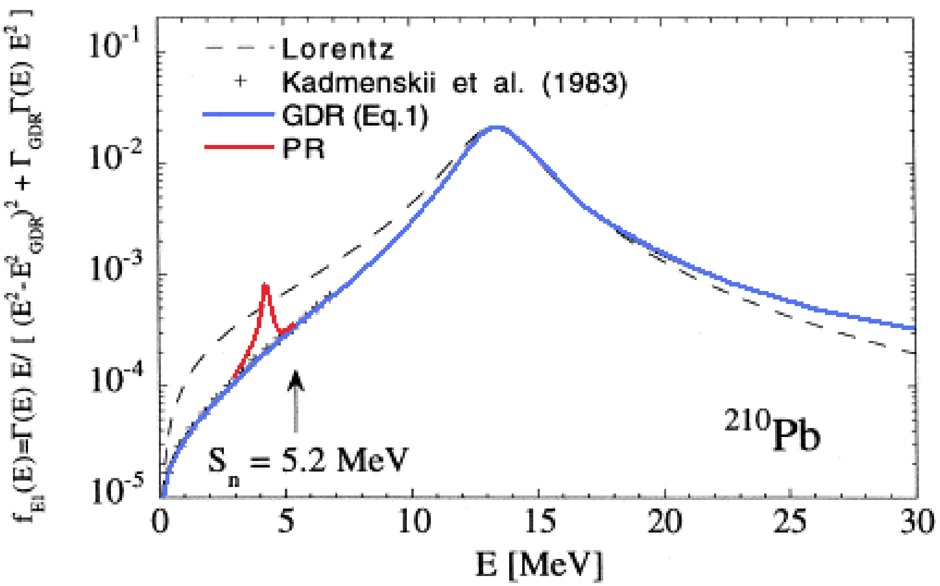


# Characteristic structure of Unstable nuclei



# Excited states of unstable nuclei have a important role on the *r*-process neucleosynthesis.

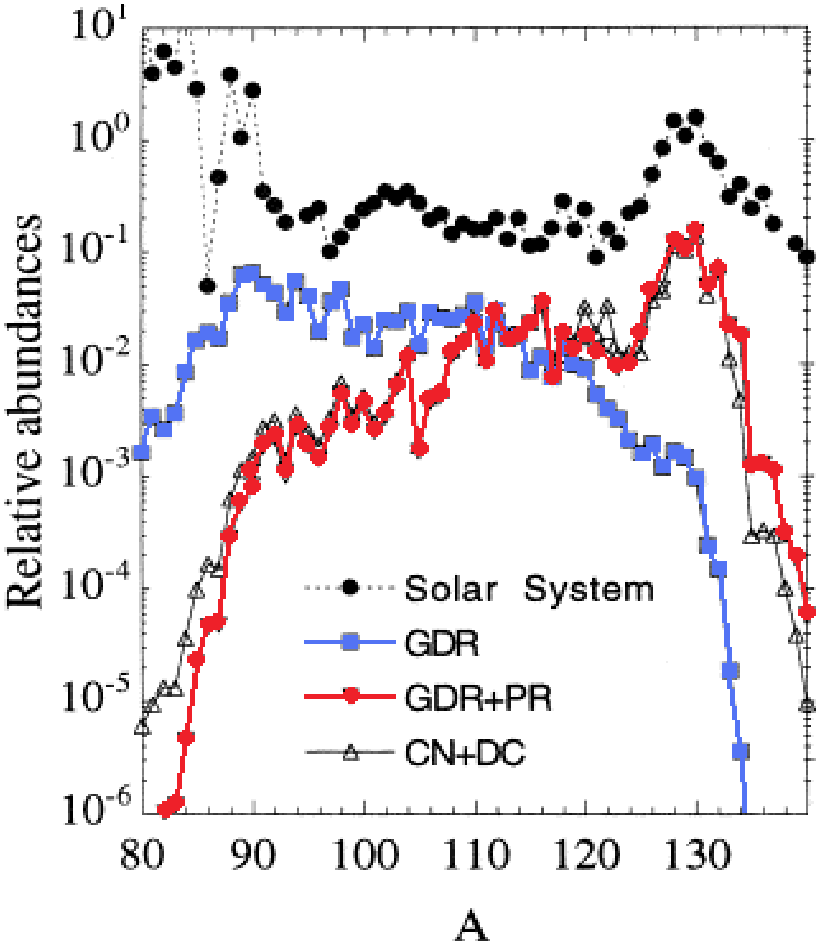
Example for $^{210}$Pb,
*E1* strength function expressed in Lorentzian




S. Goriely, Phys. Lett. B **436**, 10 (1998)

**PDR is a small part** of Total strength
**but,** the effect **for the abundance** is **large.**

Solar abundance calculated with the Lorentzian *E1* strengths



As the first step,
**Photo-nuclear** reaction (***E1* mode**)

To describe and understand
**Excited modes** and **Dynamics** of
**Various nuclei (stable, unstable)**

# Contents

**Introduction**
Models and working area,
Unstable nuclei and *E1* mode

**Formulation** of Cb-TDHFB

**Example** of linear response cal.
for *E1* mode ($^{172}$Yb)

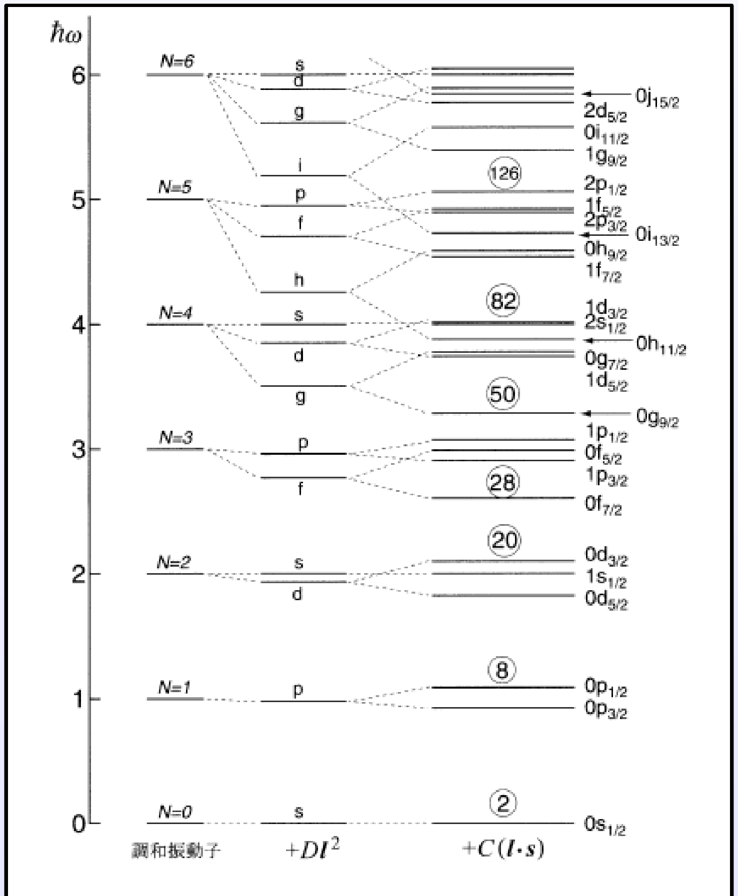
**Results** of low-lying *E1* strength
for heavy nuclei (A > 100)

**Summary** and **Future work**

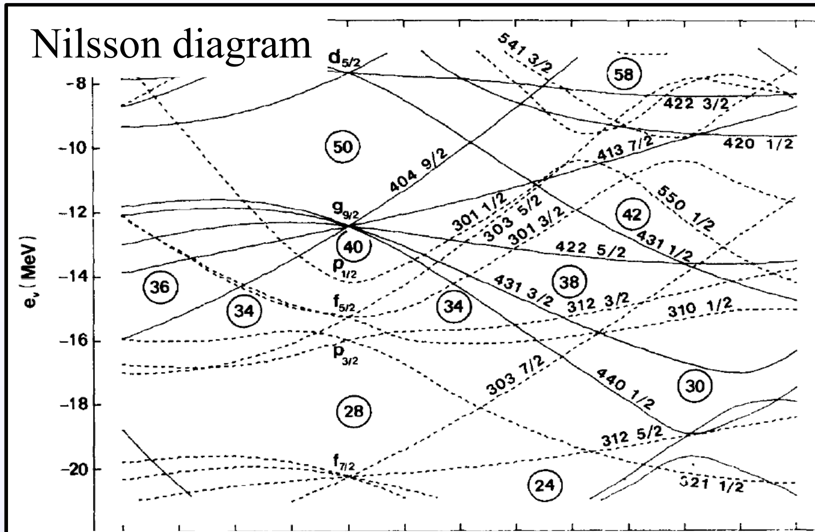
# Important points for nuclear structure

## Nucleus have mean-field

Nucleon in the mean-field
→ shell structure (magic number)
→ single-particle states

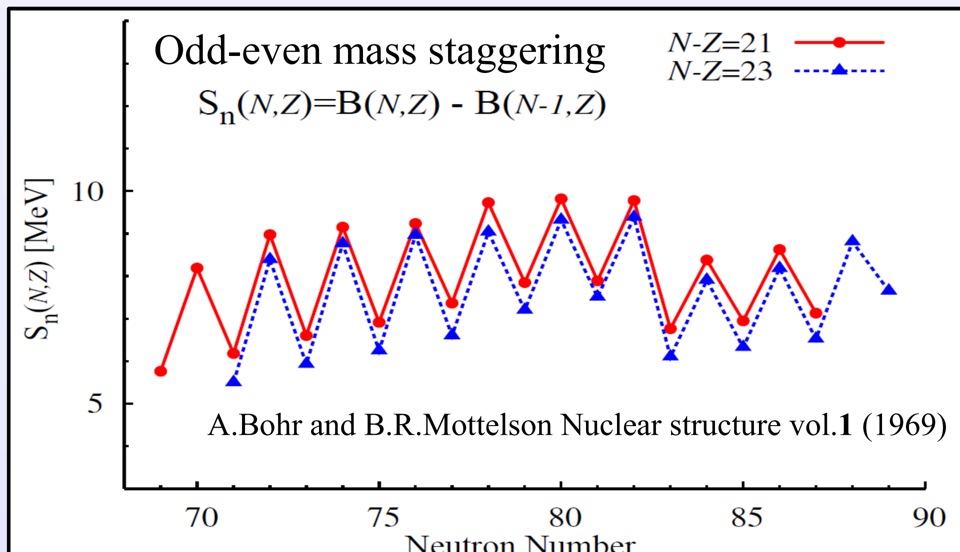



## Deformation of mean-field




W.Nazarawicz, *et. al.* Nucl. Phys. A**435** (1985) 397.

## Pairing correlation



# Several Mean-field models based on DFT

| | Statics | Dynamics |
|---|---|---|
| No Pairing | Hartree-Fock(HF) | Time-Dependent HF (TDHF, RPA) |
| BCS Pairing | HF+BCS | --- |
| With Pairing | Hartree-Fock-Bogoliubov (HFB) | TDHFB (QRPA) |

※ RPA: Random-Phase Approximation
※ QRPA: Quasi-particle RPA

# Nuclear dynamics described by TDHF theory

H.Flocard, S.E.Koonin and M.S.Weiss Phys. Rev. **C17** (1978) 1682

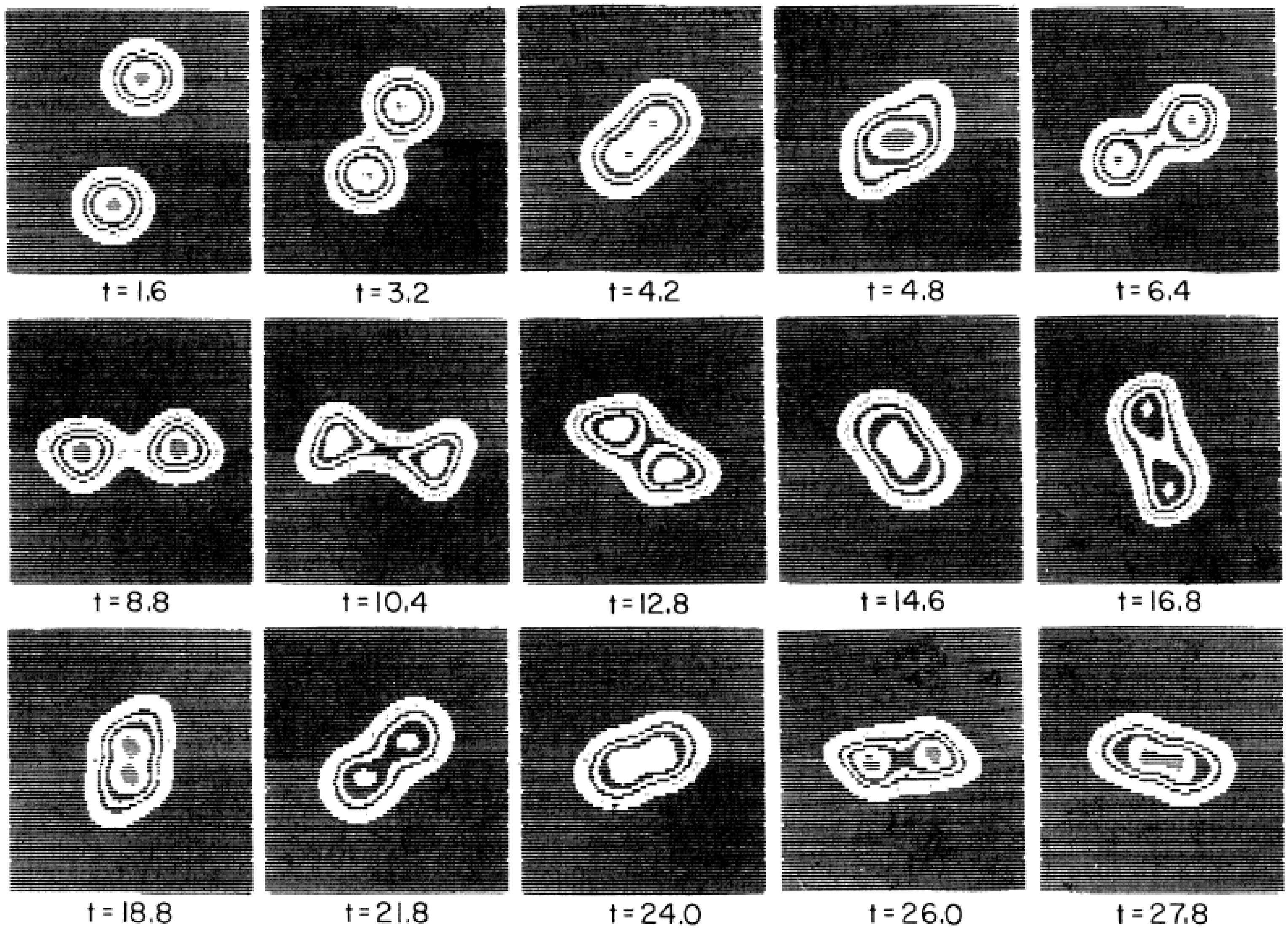



FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O+^{16}O$ collision at $E_{1ab}=105$ MeV and incident angular momentum $L=13\hbar$ . The times $t$ are given in units of $10^{-22}$ sec.

# Several Mean-field models based on DFT

| | **Statics** | **Dynamics** |
| --- | --- | --- |
| **No Pairing** | Hartree-Fock(HF) | Time-Dependent HF (TDHF, RPA) |
| **BCS Pairing** | HF+BCS | **Cb-TDHFB** |
| **With Pairing** | Hartree-Fock-Bogoliubov (HFB) | TDHFB (QRPA) |

※ RPA: Random-Phase Approximation
※ QRPA: Quasi-particle RPA

# What is Cb-TDHFB ?

More detail ... **S. Ebata et al., PRC82, 034306**

**Cb-TDHFB** can be derived from **TDHFB** represented in **canonical basis***, with an **approximation** of pairing potential which is **diagonal** as like **BCS**.

$$|\Psi(t)\rangle \equiv \prod_{k>0}\left(u_k(t) + v_k(t)\hat{c}_k^\dagger(t)\hat{c}_{\bar{k}}^\dagger(t)\right)|0\rangle$$

$\bar{k}$ **: Pair of *k*-state**
(**no restriction of time-reversal**)

*Canonical basis diagonalize density matrix.

$\rho_k(t) \equiv |v_k(t)|^2$ **: Occupation probability**

$\kappa_k(t) \equiv u_k(t)v_k(t)$ **: Pair probability**

**Cb-TDHFB** is a time-dependent scheme including pairing correlations as in the BCS approximation.

## Cb-TDHFB equations

$$i\hbar\frac{\partial}{\partial t}|\phi_k(t)\rangle = \left(h(t) - \eta_k(t)\right)|\phi_k(t)\rangle$$

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

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

$$\eta_k(t) \equiv \langle\phi_k(t)|\, h(t)\, |\phi_k(t)\rangle + i\hbar\left\langle\frac{\partial\phi_k}{\partial t}\middle|\phi_k(t)\right\rangle$$

**Properties of Cb-TDHFB**

$d/dt\langle\phi_k(t)|\phi_{k'}(t)\rangle = 0,$

$d/dt\langle\hat{N}\rangle = 0,\ d/dtE_{\mathrm{Total}} = 0$

In the limit of $\Delta = 0$, → **TDHF**

In the static limit, → **HF+BCS**

# Linear response calculation with TD scheme (procedure)

**Calculate HF or HF+BCS ground state** $|\Psi(0)\rangle$

A **instantaneous** external field

$\hat{V}_{\rm ext}(t) \equiv -k\hat{F}\delta(t) \quad k \ll 1 \qquad |\Psi(0_+)\rangle \equiv e^{i\hbar k\hat{F}}|\Psi(0)\rangle \quad \hat{F}$ : one-body operator

**Calculate the time-evolution with TDHF or Cb-TDHFB**

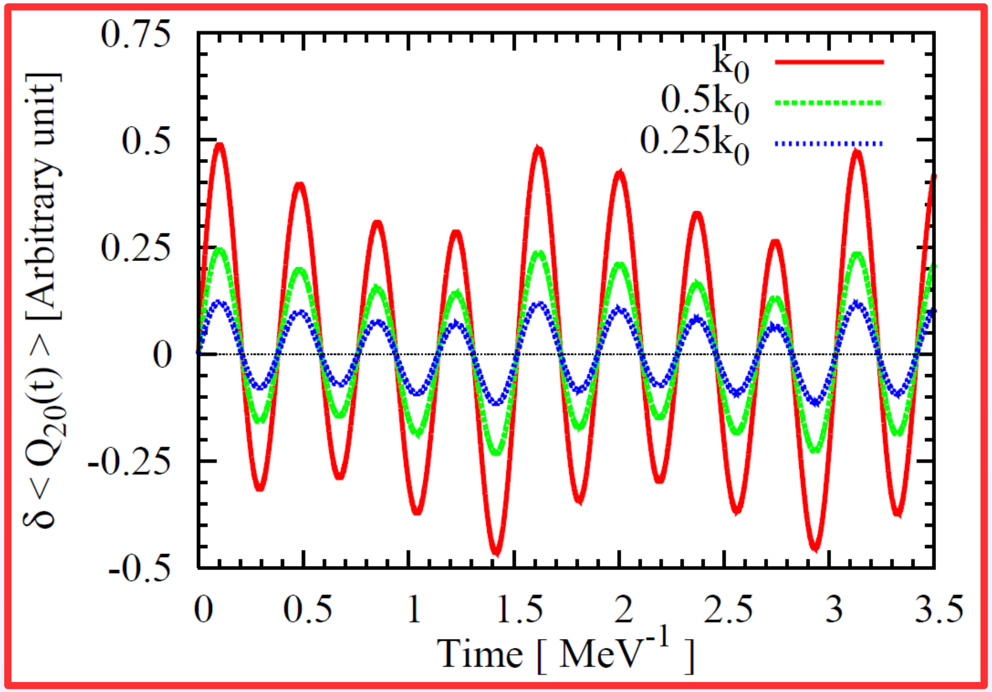
Strength function *S(E;F)* is obtained with Fourier transformation.

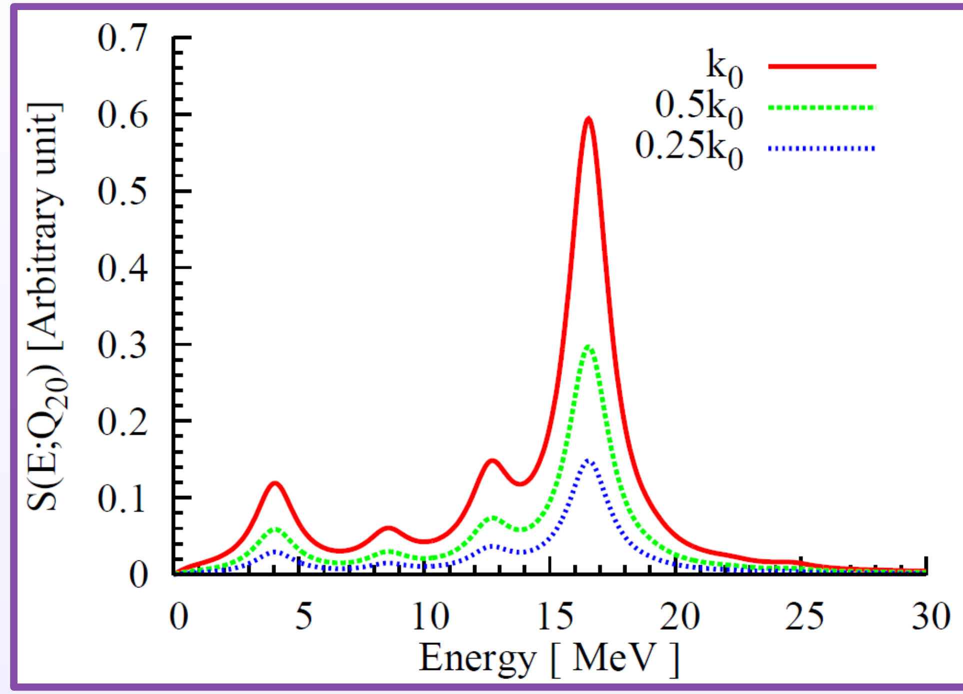
$$S(E;\hat{F}) = \sum_n \left|\langle n|\hat{F}|0\rangle\right|^2 \delta(E-\tilde{E}_n) \qquad \tilde{E}_n \equiv E_n - E_0, \quad E_n > E_0$$

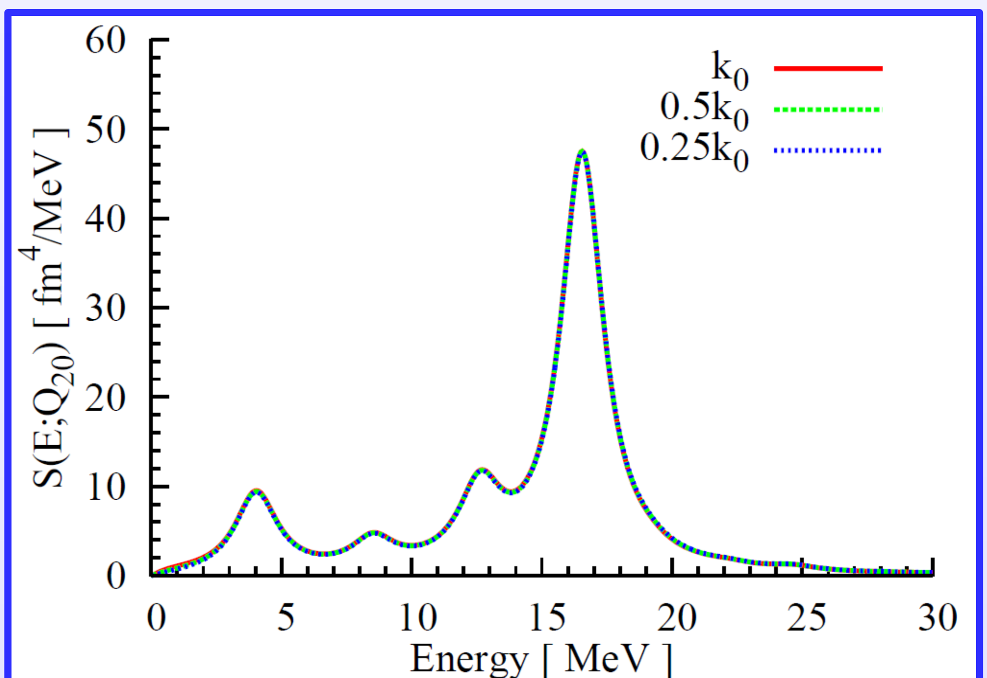
$$= -\frac{1}{k\pi}\lim_{\Gamma\to 0} \mathrm{Im}\int_0^\infty dt\; e^{(iE-\Gamma/2)t/\hbar}\left(f(t)-f(0)\right) \qquad f(t) \equiv \langle\Psi(t)|\,\hat{F}\,|\Psi(t)\rangle$$

$\Gamma$: Smoothing parameter (~1 MeV)

# Linear response calculation with TD scheme ( for $^{20}$Ne )




$$-\frac{1}{k\pi}\mathrm{Im}\int_0^T dt\; e^{(iE-\Gamma/2)t/\hbar}\left(f(t)-f(0)\right)$$

$$=\sum_n \left|\langle n|\hat{F}|0\rangle\right|^2 \delta(E-\tilde{E}_n)$$

If we chose the suitable $k$ ,
we can get the results of linear response.

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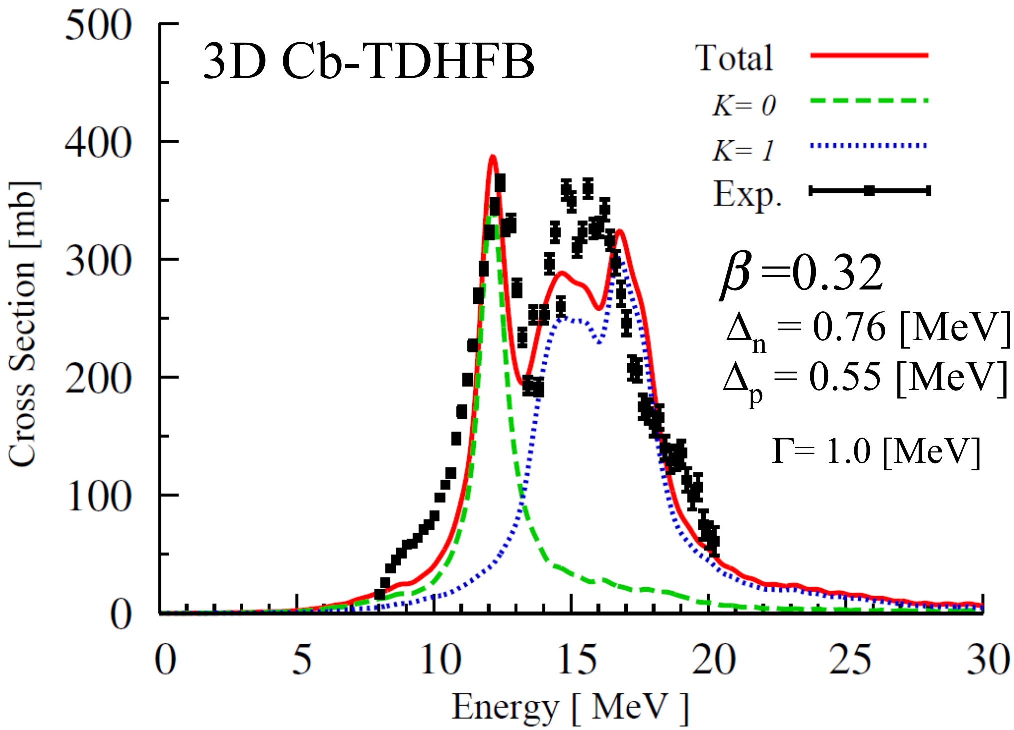
# Example : Photo-absorption cross section of $^{172}$Yb



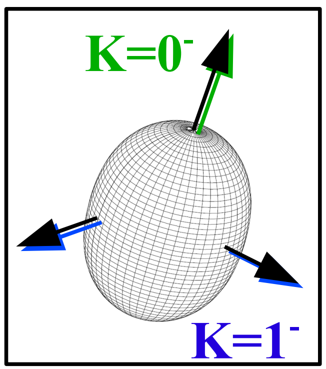

Cb-TDHFB can reproduce the photo-absorption cross section of $^{172}$Yb.

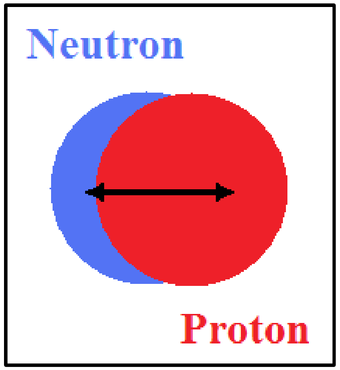
- **Heavy nucleus**
- **Deformed nucleus**
- Including pairing

Total cal. cost : **300 CPU hours**
(with **a Single processor**; Intel Core i7 3.0 GHz)

Box size : R=15[fm], mesh=1[fm] (3D-Spherical)
Canonical-basis space (HF+BCS g.s.) :
146 states for neutron,
98 states for proton

Experimental data:
A.M.Goryachev and G.N.Zalesnyy Vopr. Teor. Yad. Fiz. 5, 42 (1976).




$$\hat{F}^N = -(Ze/A)(\hat{z} + \hat{x} + \hat{y}) \ ,$$
$$\hat{F}^P = (Ne/A)(\hat{z} + \hat{x} + \hat{y})$$

# Dimension : HF vs. HF+BCS vs. HFB

HF → **Pairing correlation** → HF+BCS → **Generalize** → HFB

$$|\Phi_{\rm HF}\rangle \equiv \prod_{l=1}^{A} a_l^\dagger |-\rangle$$

$$a_l^\dagger = \sum_\mu D_{\mu l} c_\mu^\dagger$$

: Canonical basis

$$DD^\dagger = D^\dagger D = 1$$

$$|\Phi_{\rm BCS}\rangle \equiv \prod_{k>0} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle$$

$$\propto \prod_k \alpha_k |-\rangle$$

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}}, \quad \alpha_{\bar{k}}^\dagger = u_k a_{\bar{k}}^\dagger + v_k a_k$$

: BCS quasi-particle state

$$|\Phi_{\rm HFB}\rangle \equiv \prod_k \beta_k^\dagger |-\rangle$$

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$$

: Generalized quasi-particle state

*One body density matrix is diagonalized in ***Canonical basis***. $\rho_{ll'} \equiv \langle \Phi | c_{l'}^\dagger c_l | \Phi \rangle$

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| | $N$ : nucleon # | $N'$ : canonical basis # | $M$ : basis # |
|---|---|---|---|
| Dimension | $NM$ | $N'M$ | $2M^2$ |
| | $N = N'$ | $N < N'$ | |

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TDHFB $\quad i\hbar\dot{\mathcal{R}} = [\mathcal{H}, \mathcal{R}]$

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa & 1-\rho^* \end{pmatrix}$$ : Generalized density matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$ : Generalized Hamiltonian

$$\Delta_{\alpha\beta} \equiv \frac{1}{2}\sum_{\mu,\nu} \bar{\mathcal{V}}_{\alpha\beta\mu\nu}\kappa_{\mu\nu}$$ : Pair potential

# Dimension : HF+BCS vs. HFB in coordinate space representation

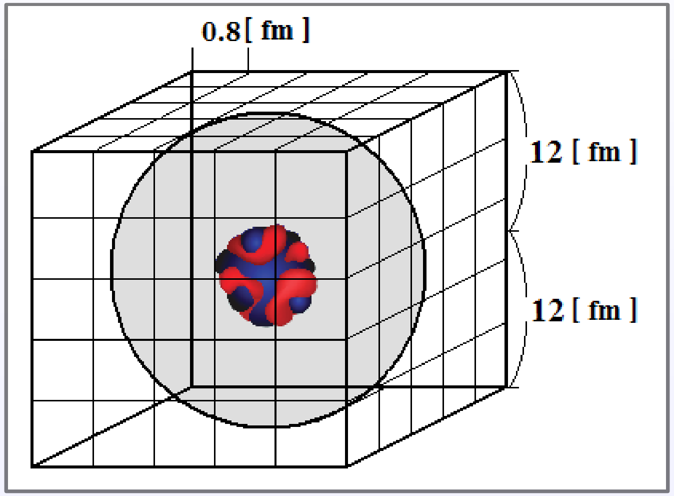
Wave function in 3D-Cartesian coordinate space

Example )

$(24/0.8)^3 = 27{,}000$ points

$$\phi_l(\vec{r},\sigma;t) = \langle \vec{r},\sigma|\phi_l(t)\rangle$$

$$\rightarrow \phi_l(i,j,k,\sigma;t) \quad M \simeq 27,000$$




| | HF+BCS | HFB |
|---|---|---|
| | $\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}},$ | $\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$ |
| Dimension | $N'M$ ($N' \sim 300$ for $^{238}$U) | $2M^2$ |

Difference of matrix elements

$$\left(\frac{M}{N'}\right)^2 \sim 10,000$$

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## Heavy ion collision ($^{238}$U to $^{238}$U)

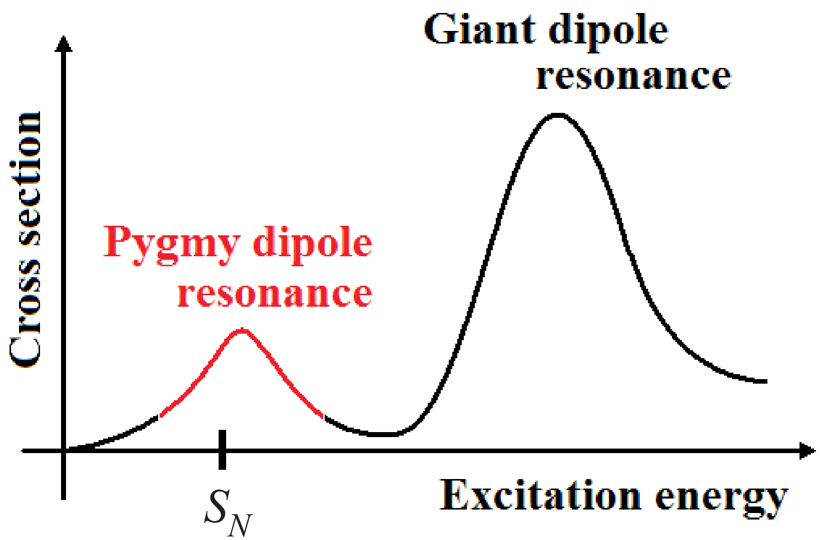
Cb-TDHFB : 500 – 600 canonical basis

→ Parallelization for canonical basis

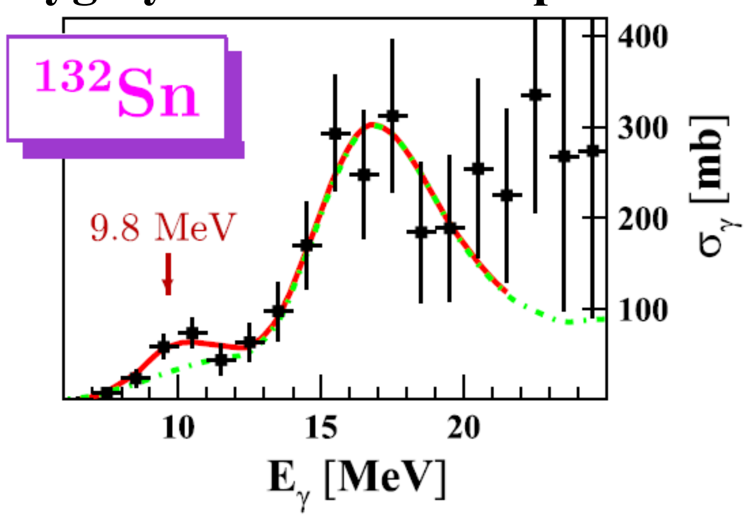
(Cb-TDHFB can conserve the orthogonality between canonical-basis)

# Contents

# Low-lying *E1* strength : Pygmy dipole resonance




**Pygmy resonance in experiment**




P. Adrich, et al.,Phys. Rev Lett. **95**, 132501 (2005)

**Common sense of PDR ?**

The peak of PDR appears lower than one of GDR.

PDR peaks appear around separation energy.

**Experiments**

$^{26}$Ne; J. Gibelin et al., Phys. Rev. Lett. **101**, 212503(2008).

$^{68}$Ni; O. Wieland et al., Phys. Rev. Lett. **102**, 092502(2009).

$^{130,132}$Sn; P. Adrich et al., Phys. Rev. Lett. **95**, 132501(2005).

$^{208}$Pb; N. Ryezayavaet al.,Phys. Rev. Lett. **89**, 272502(2002).

etc.

# Setup

**External filed :**

**Isovector dipole mode** (for ***E1*** **strength**)

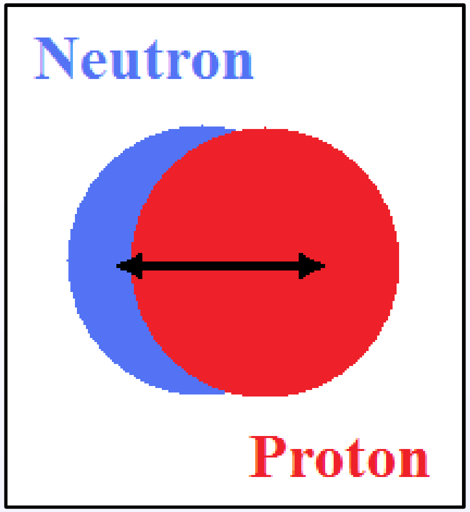
$$\hat{F}_i^{\mathrm{N}} = -(Ze/A)\hat{\boldsymbol{r}}_i \ ,\hat{F}_i^{\mathrm{P}} = (Ne/A)\hat{\boldsymbol{r}}_i$$

**Effective Interaction : Skyrme force (SkM*),**

Smoothed Pairing strength $G$ (ref. N. Tajima *et al.* NPA**603**(1996)23)

$$\Delta(t) = \sum G_l \kappa_l(t) \qquad G_l = f(\varepsilon_l)G \qquad f(\varepsilon_l)$$ : cutoff function

**Isovector** Dipole




Neutron and Proton vibrate **in anti-phase**.

**Nucleus :** **$^{14\text{-}28}$O, $^{18\text{-}32}$Ne, $^{18\text{-}40}$Mg, $^{24\text{-}46}$Si, $^{28\text{-}50}$S, $^{32\text{-}58}$Ar, $^{34\text{-}64}$Ca, $^{56\text{-}80}$Ni, $^{78\text{-}86}$Zn, $^{80\text{-}96}$Ge, $^{82\text{-}100}$Se, $^{84\text{-}106}$Kr, $^{86\text{-}124}$Sr, $^{88\text{-}132}$Zr, $^{100\text{-}132}$Mo, $^{120\text{-}134}$Ru, $^{122\text{-}136}$Pd, $^{124\text{-}138}$Cd, $^{98\text{-}140}$Sn, $^{128\text{-}142}$Te, $^{130\text{-}142}$Xe, etc.** ( about **250** kinds of Nucleus )

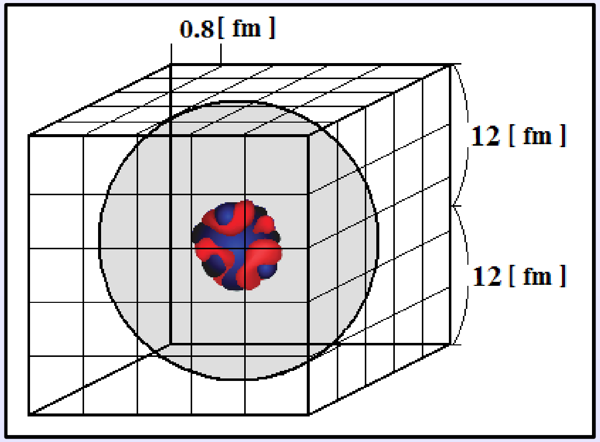
**Calculation space (**3D-Spherical meshed box**):**

For heavy nuclei ($A$ > 70),

we use the box has radius **15** [fm] and meshed by **1.0** [fm].

$$\phi_l(\vec{r},\sigma;t) \to \phi_l(i,j,k,\sigma;t)$$

Lattice points $i+j+k \simeq 15,000$



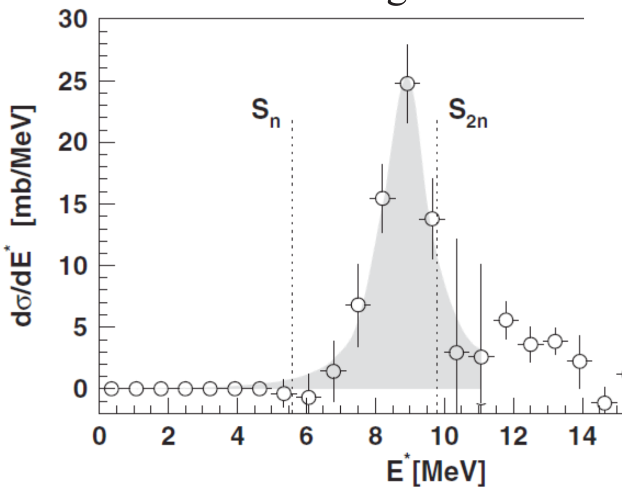
# To quantify **the low-lying *E1* strength systematically,**

$$\frac{m_1(E_c = 10)}{m_1} \equiv \frac{\int_0^{10[\mathrm{MeV}]} E\ S(E; E1) dE}{\int E\ S(E; E1) dE}$$

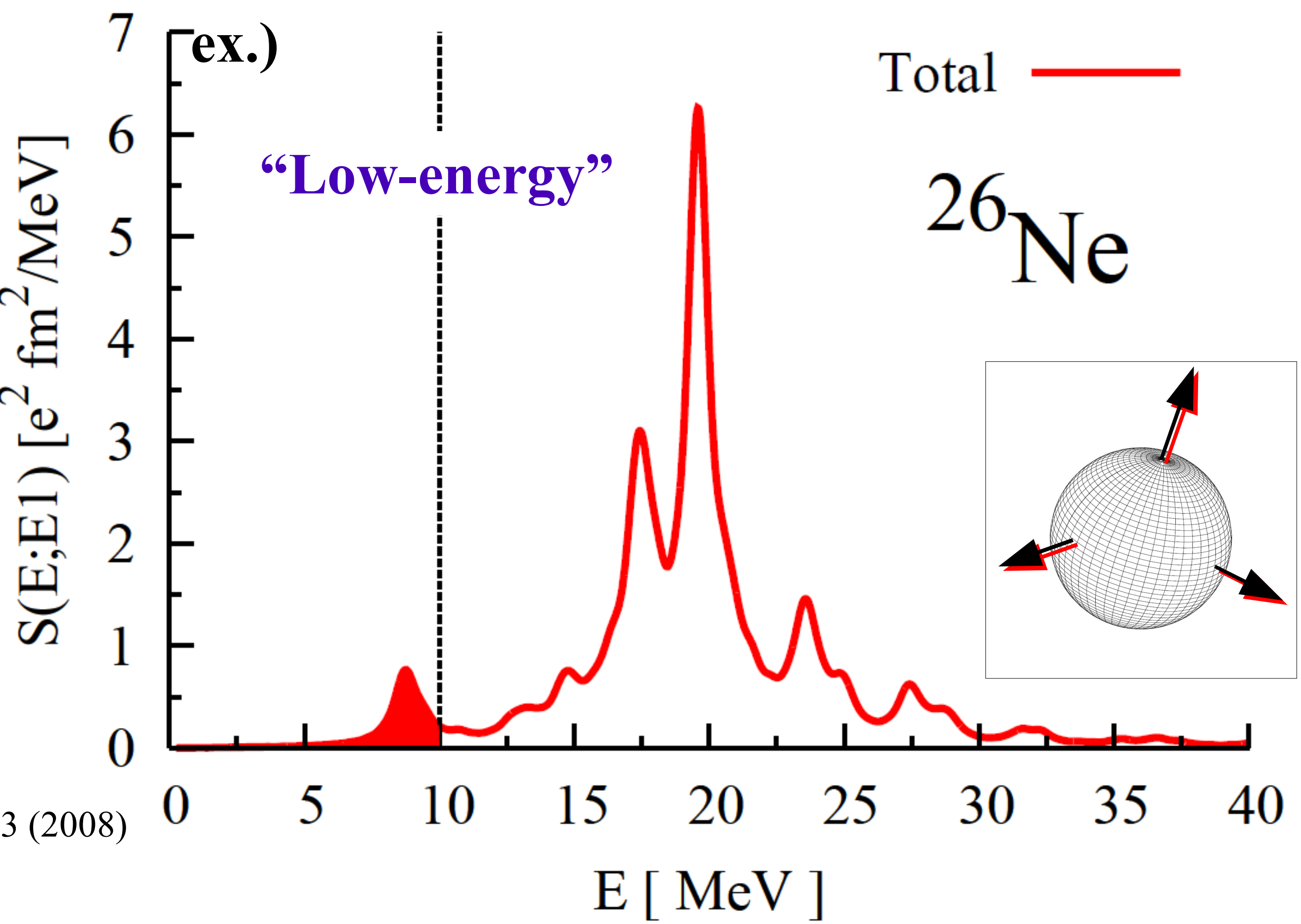
The ratio of low-lying *E1* strength in Total *E1* strength (sum rule).

We use the ratio to analyze the low-lying *E1* strength for ***all*** calculated nuclei.

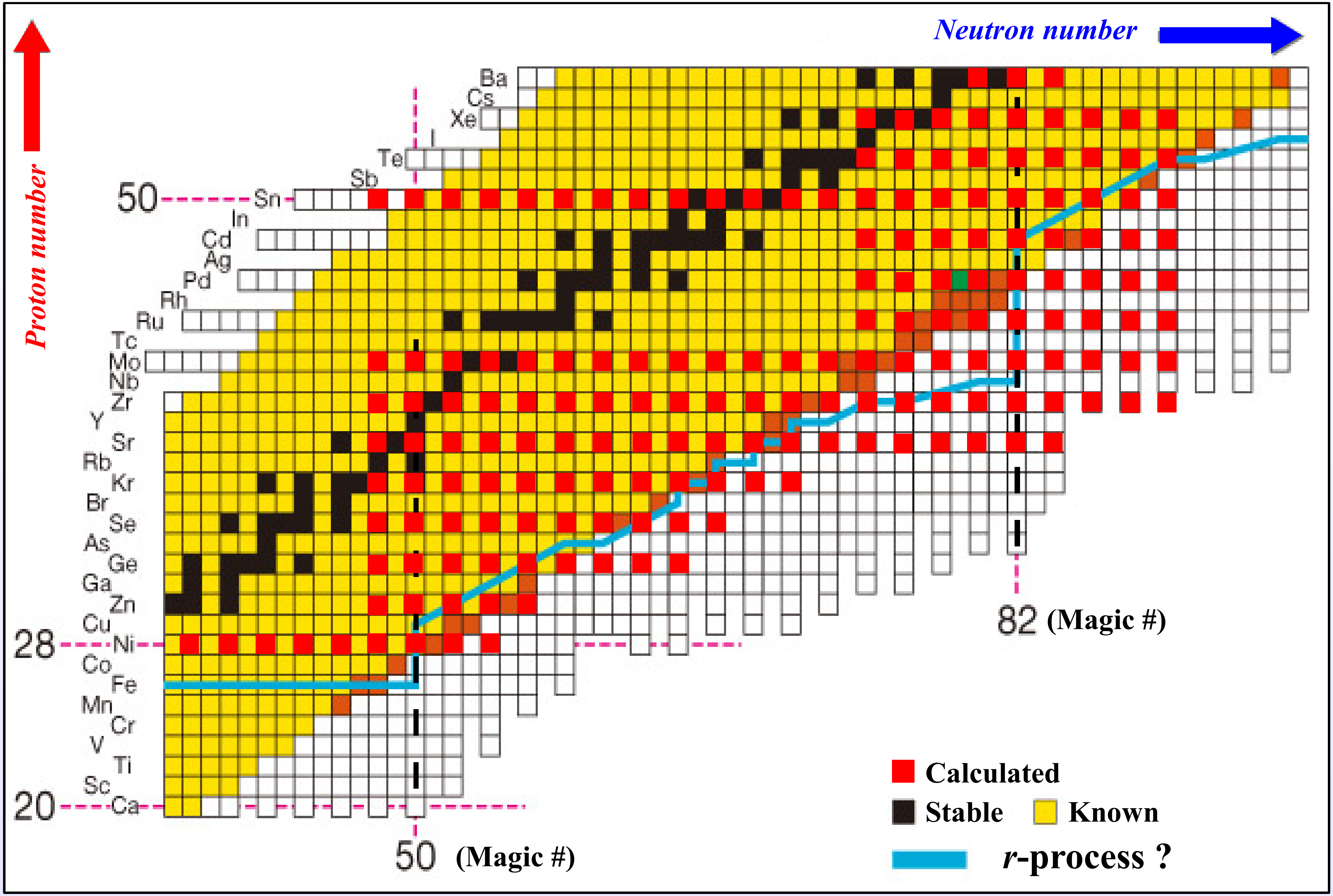
$^{26}$Ne on a $^{208}$Pb target



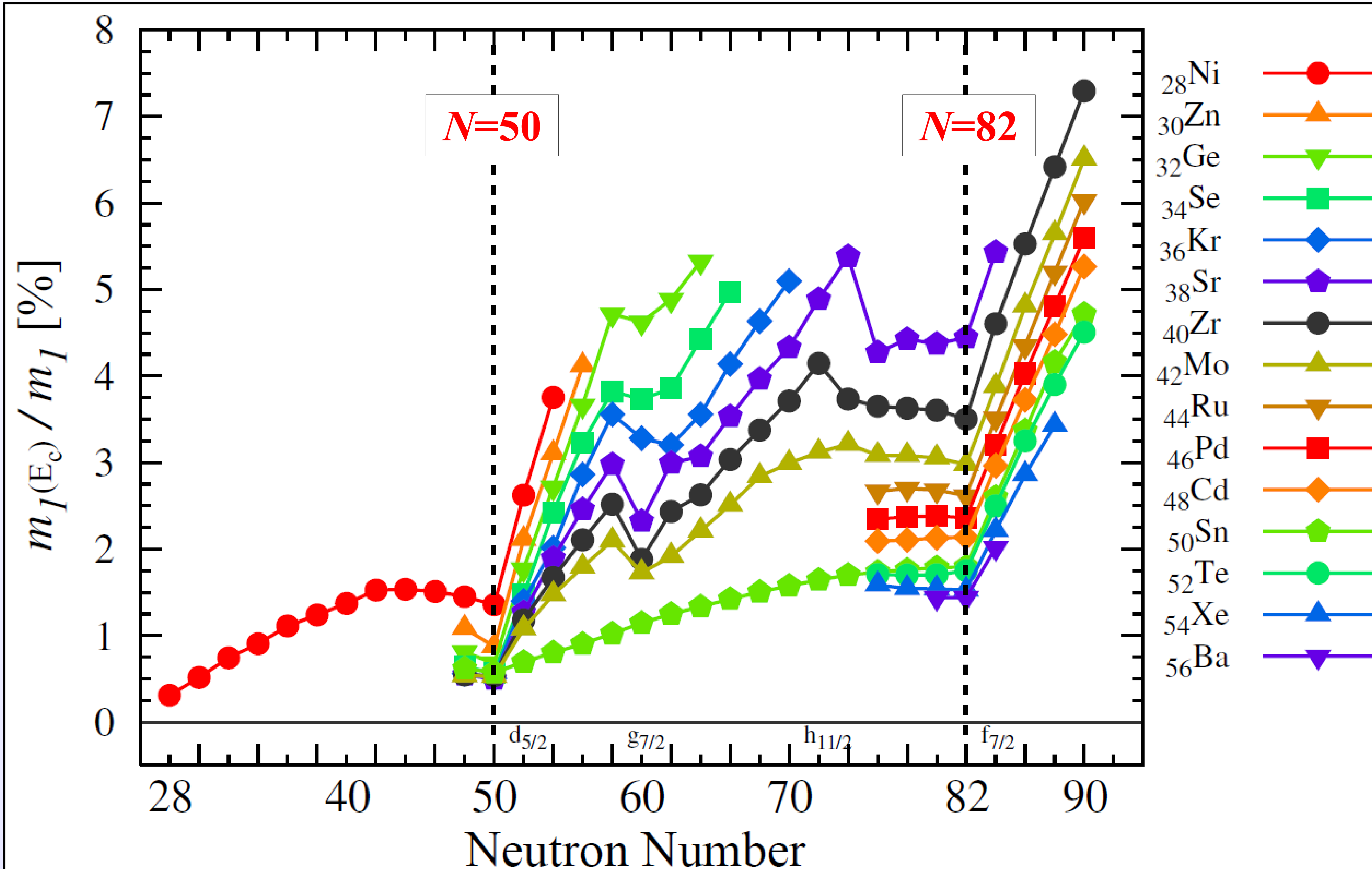

J. Gibelin, et al., Phys. Rev Lett. **101**, 212503 (2008)



# Results of Low-lying *E1* strength **for heavy nuclei (A > 100)**



# *N*#-dependence of the **Low-lying *E1* strength** for heavy nuclei



# Contents

# Summary & Future work

## Development of Cb-TDHFB method in 3D

- We develop Cb-TDHFB which can investigate the excited state of heavy nuclei with small numerical cost.
- Cb-TDHFB is suitable to the parallelization for canonical-basis.

## Systematic study of *E1* mode with Cb-TDHFB

- We investigate the **low-lying *E1*** strength **systematically** (for 250 kinds of nuclei) including the effects of **deformation** and **pairing**.
- We can see a very characteristic neutron number dependence of low-lying *E1* modes for heavy nuclei.

## Apply the Cb-TDHFB to ...

**Pygmy dipole resonance for more heavy nuclei,**

**Other modes (ISQ, ISM, IVM, scissors, etc.) systematically,**

**Reaction (Heavy ion collision, Fusion, Fission, etc.)**