HPCI戦略プログラム分野５
全体シンポジウム

2013.3.6 (Wed.)
於 富士ソフトアキバプラザ

時間依存密度汎関数法を用いた 核ダイナミクスの研究

課題2 大規模量子多体計算による核物性解明とその応用

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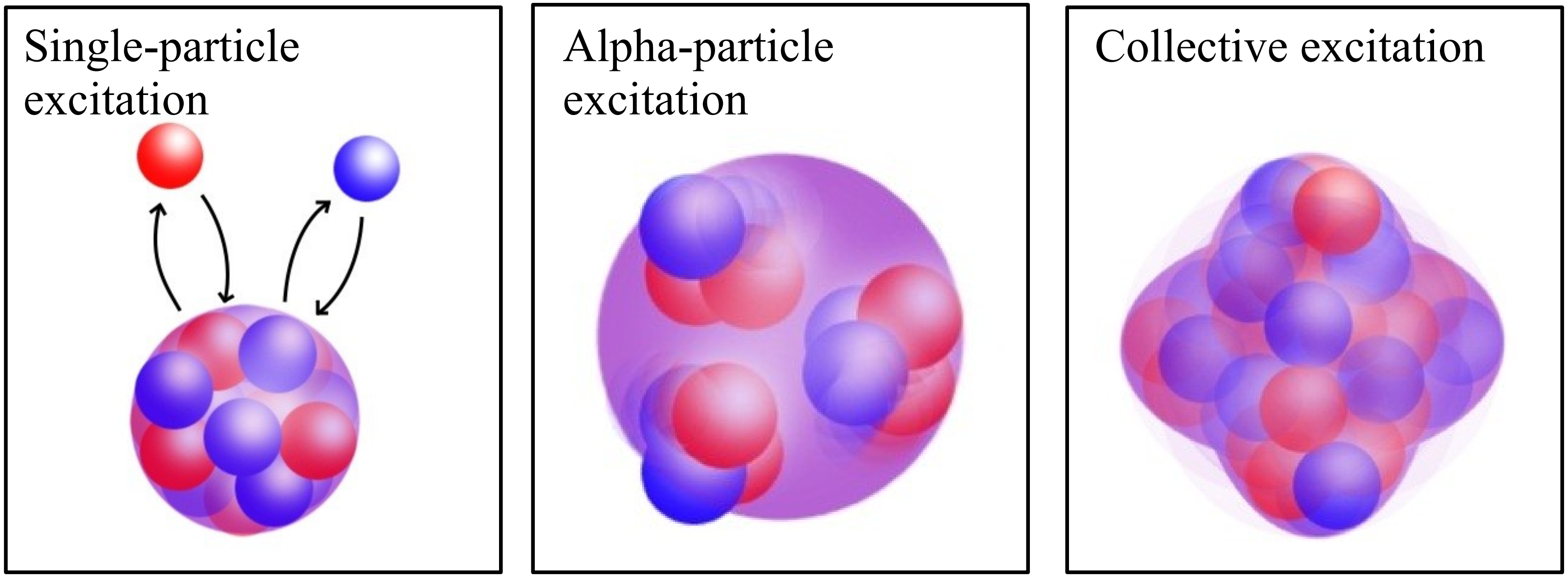
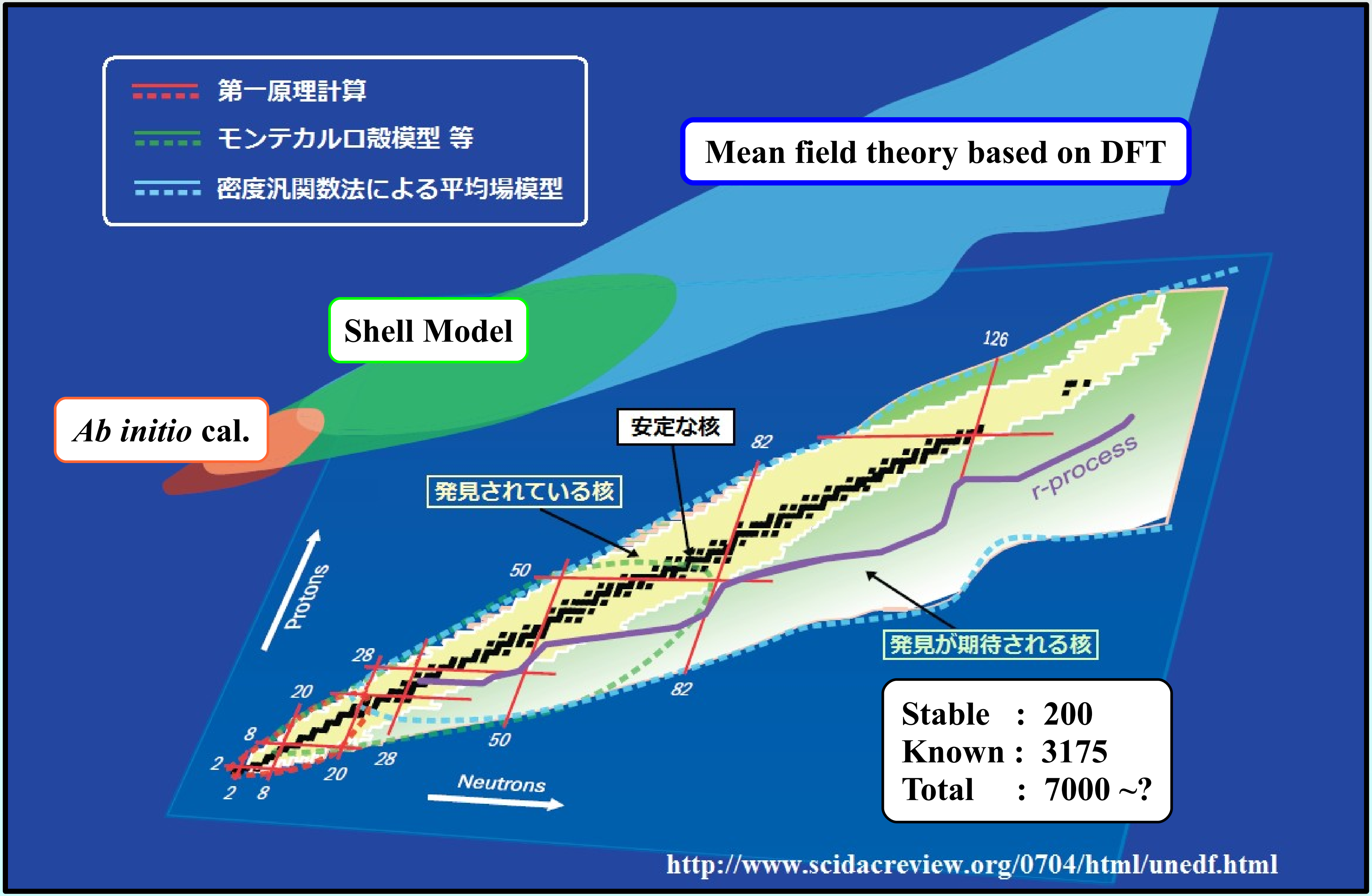
原子核研究について

有限量子多体系に現われる秩序を統一的に理解する

← 多様な原子核の性質を研究



模型の適用範囲



第一原理計算
モンテカルロ殻模型 等
密度汎関数法による平均場模型
Mean field theory based on DFT
Shell Model
Ab initio cal.
安定な核
発見されている核
発見が期待される核
r-process
Protons
Neutrons
126
82
50
28
20
8
2
Stable : 200
Known : 3175
Total : 7000 ~?
http://www.scidacreview.org/0704/html/unedf.html

密度汎関数法を基礎とする様々な理論

	For static	For dynamics
No Pairing	Hartree-Fock(HF)	Time-Dependent HF (TDHF, RPA)
With BCS Pairing	HF+BCS	TDHF+BCS
		Cb-TDHFB
With Pairing	Hartree-Fock-Bogoliubov (HFB)	TDHFB (QRPA)

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

多体波動関数の次元：HF vs. HF+BCS vs. HFB

HF → (Pairing correlation) → HF+BCS → (Generalize) → HFB

HF

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

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

: Canonical basis

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

HF+BCS

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

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

: BCS quasi-particle state

HFB

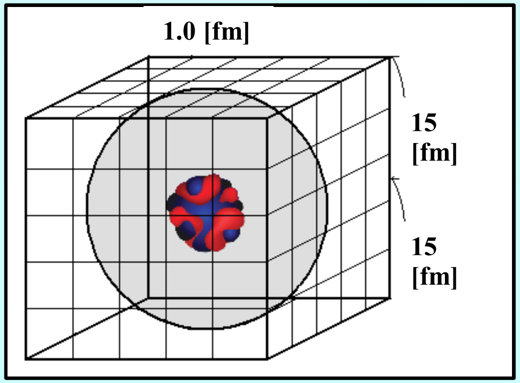
$$|\Phi_{\mathrm{HFB}}\rangle \equiv \prod_k \beta_k^\dagger |-\rangle$$

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

: Generalized quasi-particle state

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

Dimension	NM	$N'M$	$2M^2$
	$N = N'$	$N' > N$	
	N : nucleon #	N' : canonical basis #	M : basis #



Example

$\phi_l(\vec{r}, \sigma; t) \rightarrow \phi_l(x, y, z, \sigma; t)$

Lattice points $x + y + z \simeq 15{,}000$

N' ~ 300 for 238U

Difference of matrix elements

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

Canonical-basis TDHFB (Cb-TDHFB)

Ebata *et al*, Phys. Rev. C**82**, 034306

$$\rho_{\mu\nu} = \langle\Psi|\, \hat{c}_\nu^\dagger \hat{c}_\mu \,|\Psi\rangle$$: Density matrix

$$\kappa_{\mu\nu} = \langle\Psi|\, \hat{c}_\nu \hat{c}_\mu \,|\Psi\rangle$$: Pair tensor

μ, ν : Arbitrary complete set

TDHFB

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

$$\mathcal{R}(t) = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa(t) & 1-\rho^*(t) \end{pmatrix}$$

$$\mathcal{H}(t) = \begin{pmatrix} h(t) & \Delta(t) \\ -\Delta^*(t) & -h^*(t) \end{pmatrix}$$

Canonical basis diagonalize Density matrix.

$$\hat{a}_k^\dagger \equiv \sum_\mu D_{\mu k}\hat{c}_\mu^\dagger$$ **: Canonical basis**

$$\Rightarrow (D^\dagger \rho D)_{kk'} = \rho_k \delta_{kk'}, \quad \langle\Psi|\, \hat{a}_k^\dagger \hat{a}_k \,|\Psi\rangle = \rho_k, \quad 0 \le \rho_k \le 1$$

In this Canonical-basis,
the number of matrix elements can be compressed to diagonal components.

The computational cost of TDHFB may be reduced also in Canonical-basis representation !?

$$\hat{a}_k^\dagger(t) \equiv \sum_\mu \langle\mu|\phi_k(t)\rangle\, \hat{c}_\mu^\dagger$$ **: Time-dependent Canonical basis**

$\{|\phi_k(t)\rangle\}$: Time-dependent Canonical single-particle basis

This set is assumed to be orthonormal. $\langle\phi_k(t)|\phi_l(t)\rangle = \delta_{kl}$

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**.

$$|\Psi(t)\rangle_{\rm BCS} = \prod_{k>0} (u_k(t) + v_k(t)\hat{c}_k^\dagger \hat{c}_{\bar{k}}^\dagger)|0\rangle$$

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

*Canonical basis diagonalize density matrix.

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

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

Cb-TDHFB is a time-dependent scheme including pairing correlations as in the BCS approximation. $\Delta_{k\bar{l}}(t) = -\Delta_k \delta_{kl}$

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

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

$d/dt\langle\hat{N}\rangle = 0,\ d/dt E_{\rm Total} = 0$

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

In the static limit, → **HF+BCS**

時間依存した方法による線形応答計算

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

Adding
a **instantaneous** external field
to ground state

$$\hat{V}_{\rm ext}(t) \equiv -k\hat{F}\delta(t) \qquad k \ll 1$$

$$|\Psi(0_+)\rangle \equiv e^{i\hbar k\hat{F}}|\Psi(0)\rangle$$

$\hat{F}$: one-body operator

Calculate the time-evolution with TDHF or Cb-TDHFB

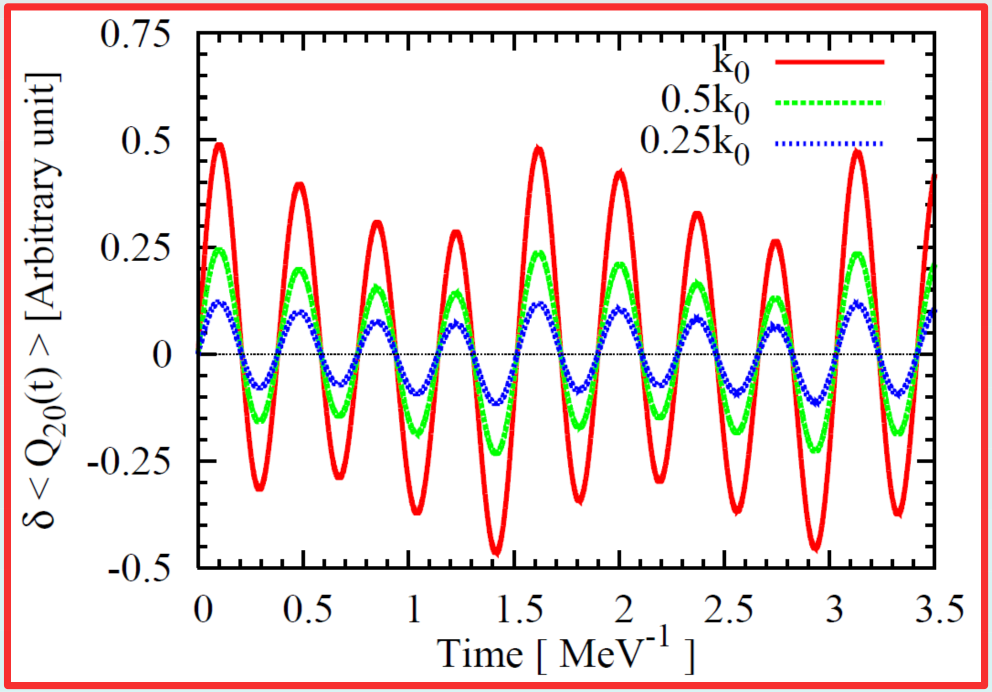
Strength function *S(E;F)* is gotten as Fourier transformed TD- $\langle\hat{F}\rangle$.

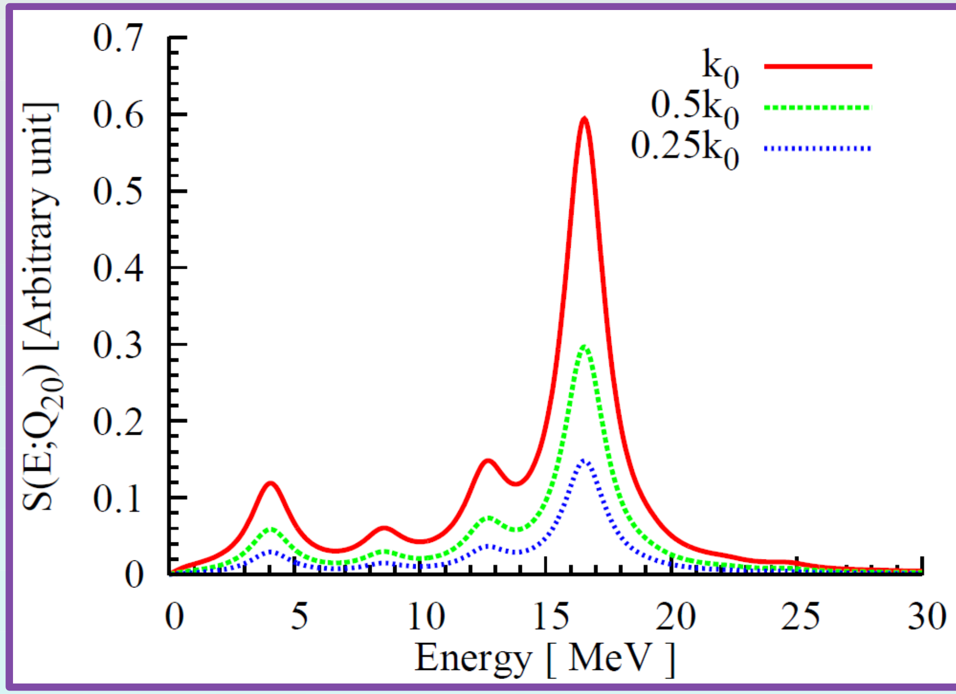
$$S(E;\hat{F}) = \sum_n \left|\langle n|\hat{F}|0\rangle\right|^2 \delta(E-\tilde{E}_n) \qquad \tilde{E}_n \equiv E_n - E_0, \quad E_n > E_0$$

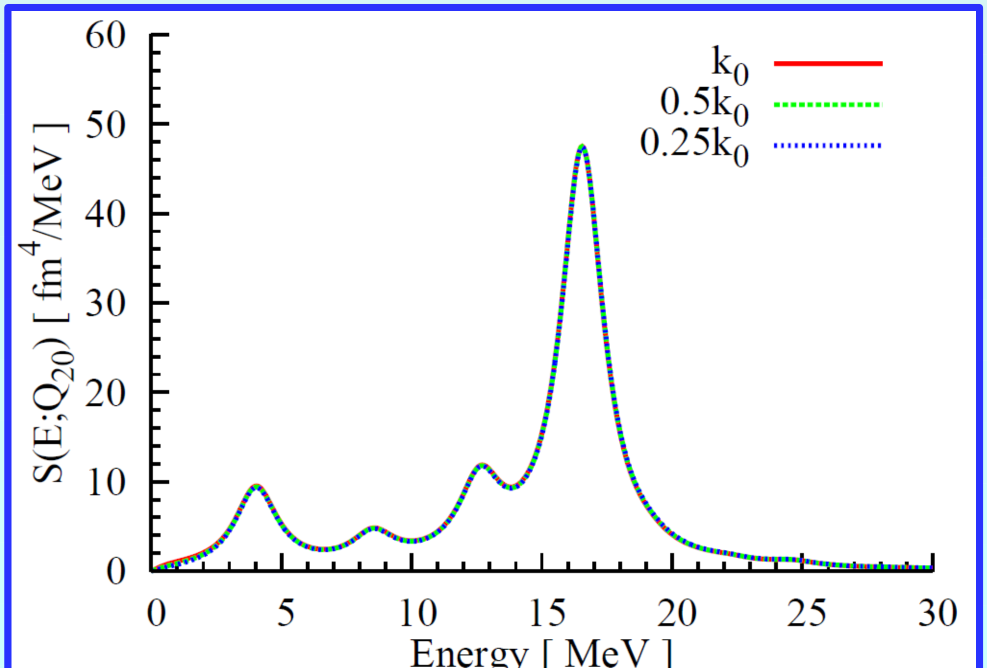
$$= -\frac{1}{k\pi}\lim_{\Gamma\to 0} \mathrm{Im}\int_0^\infty dt\; e^{(iE-\Gamma/2)t/\hbar}(f(t)-f(0)) \qquad f(t) \equiv \langle\Psi(t)|\,\hat{F}\,|\Psi(t)\rangle$$

Γ: Smoothing parameter

時間依存した方法による線形応答計算 (ex. ^{20}Ne)



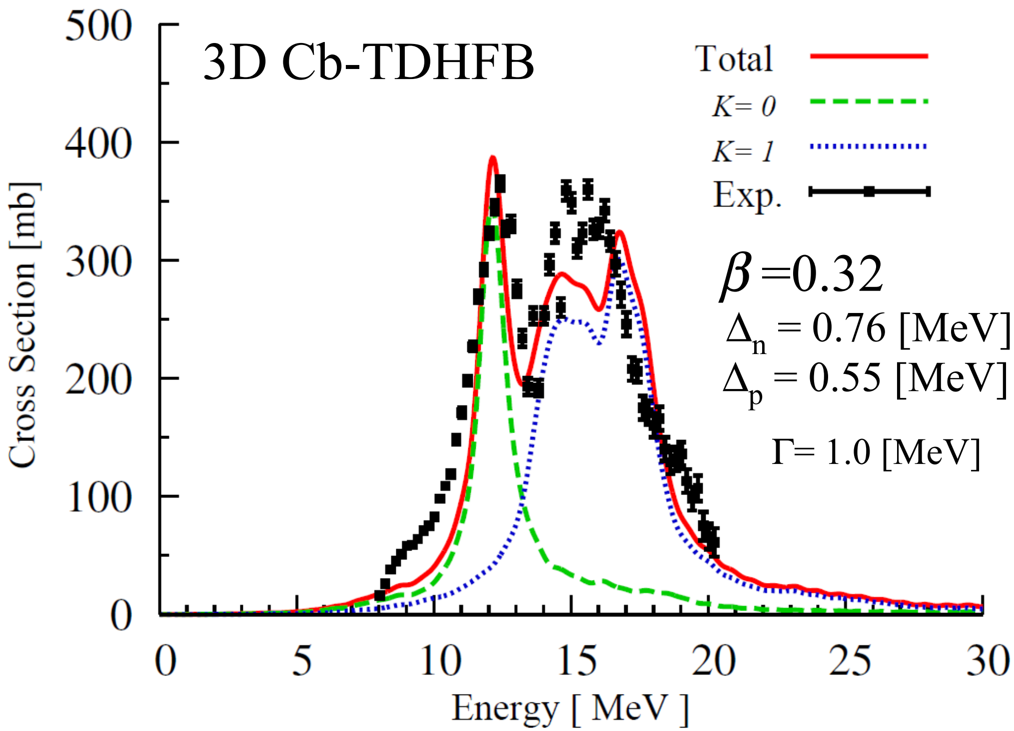




$$-\frac{1}{k\pi}\mathrm{Im}\int_0^T dt\, e^{(iE-\Gamma/2)t/\hbar}(f(t)-f(0))$$

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

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



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

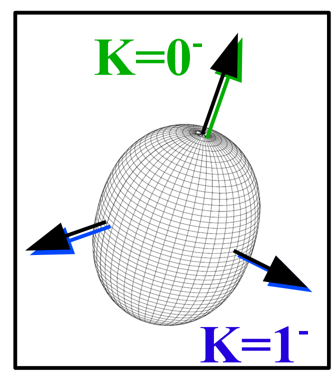
- **Heavy nucleus**
- **Deformed nucleus**
- Including pairing

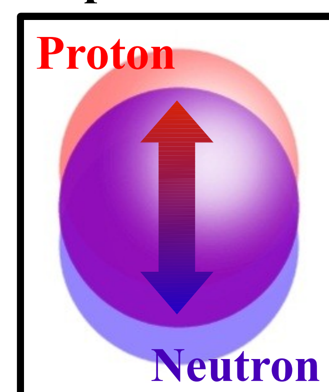
Total cal. cost : **300 CPU hours**
(with **a Single processor**; Intel Core i7 3.0 GHz)

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).

Dipole mode





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

Today's contents

- 原子核研究について
- 研究方法について

  密度汎関数法を基礎とする方法

  線形応答計算
- **系統的な*E1*モードの研究**
- 反応現象のシミュレーション

不安定核研究について

統一的に核物性を知りたい

“一般的”な原子核の性質

安定核は“一般的”か？

不安定核を含めた統一的理解

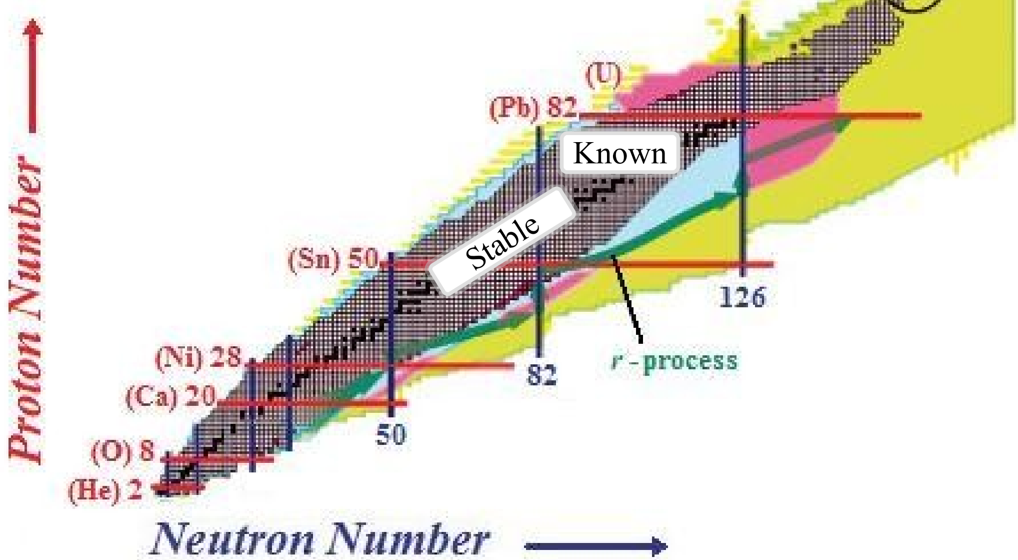
原子核を調べる為の自由度

核子数、エネルギー、スピン　＋ **密度**

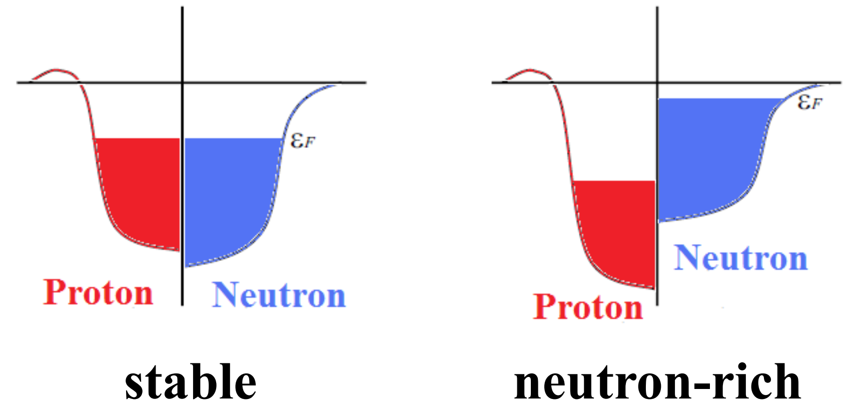
核物質を調べる
新たな自由度を得た。

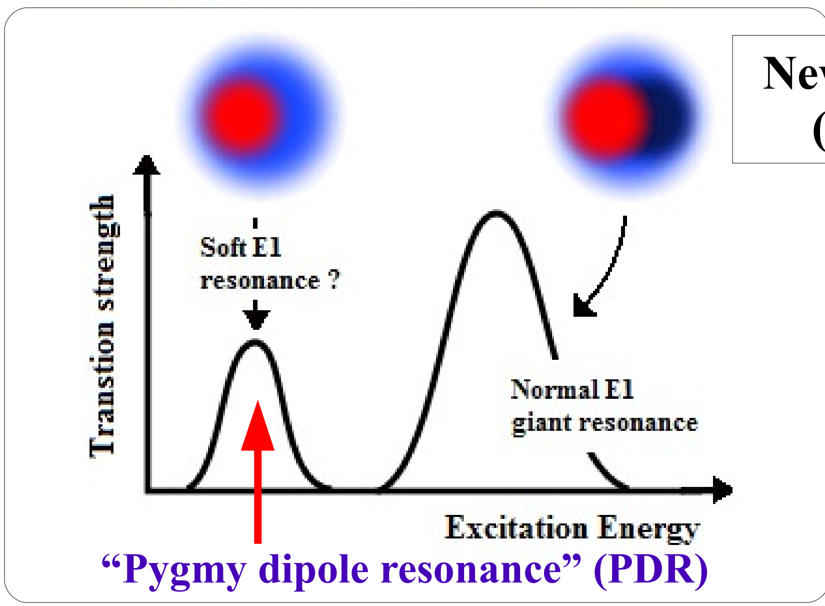
不安定核で現れる特徴的な密度分布

Unstable nuclear region is expanding



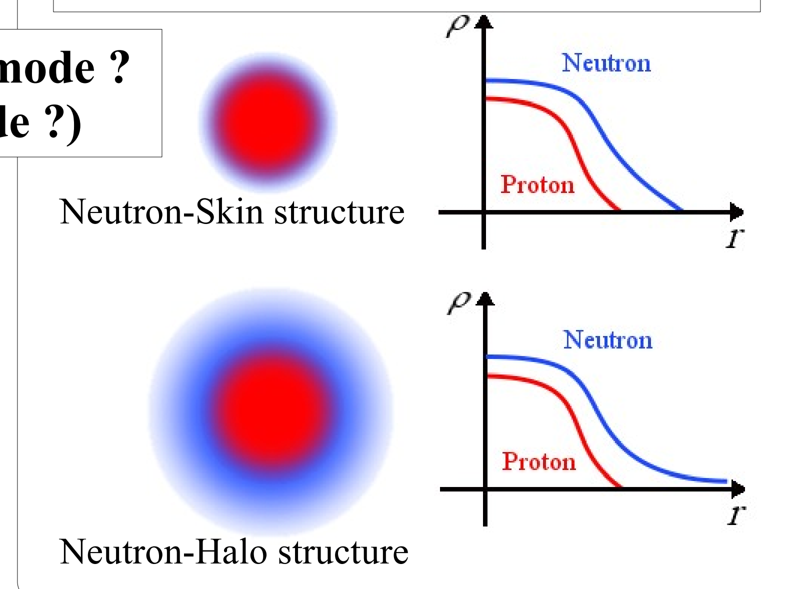
Neutron-rich nuclei have . . .





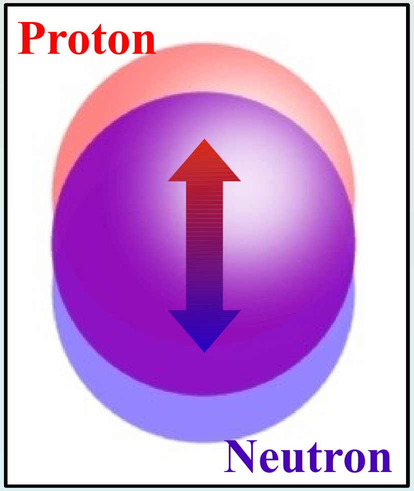
New elementary mode ? (Collective mode ?)

Characteristic structure



Calculation Setup

Isovector Dipole



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

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)

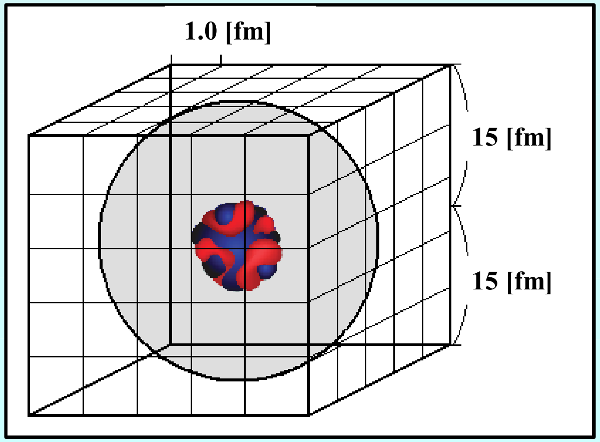
$$\Delta(t) = \sum G_l \kappa_l(t) \qquad G_l = f(\varepsilon_l)G \qquad f(\varepsilon_l)$$: cutoff function

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, $^{56\text{-}84}$Ni, $^{60\text{-}88}$Zn, $^{64\text{-}98}$Ge, $^{68\text{-}104}$Se, $^{72\text{-}118}$Kr, $^{76\text{-}118}$Sr, $^{80\text{-}122}$Zr, $^{84\text{-}124}$Mo, $^{88\text{-}130}$Ru, $^{92\text{-}134}$Pd, $^{96\text{-}138}$Cd, $^{100\text{-}140}$Sn, $^{128\text{-}142}$Te, $^{130\text{-}142}$Xe, etc. (about **350** kinds of Nucleus **)**

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

For heavy nuclei ($Z > 28$),

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

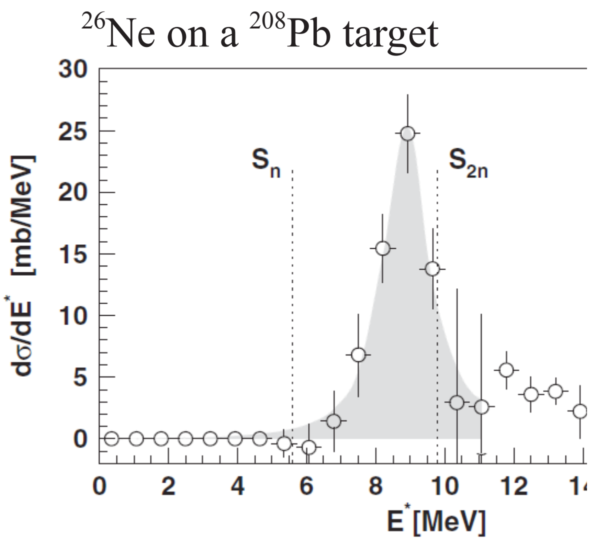


Neutron number dependence of PDR

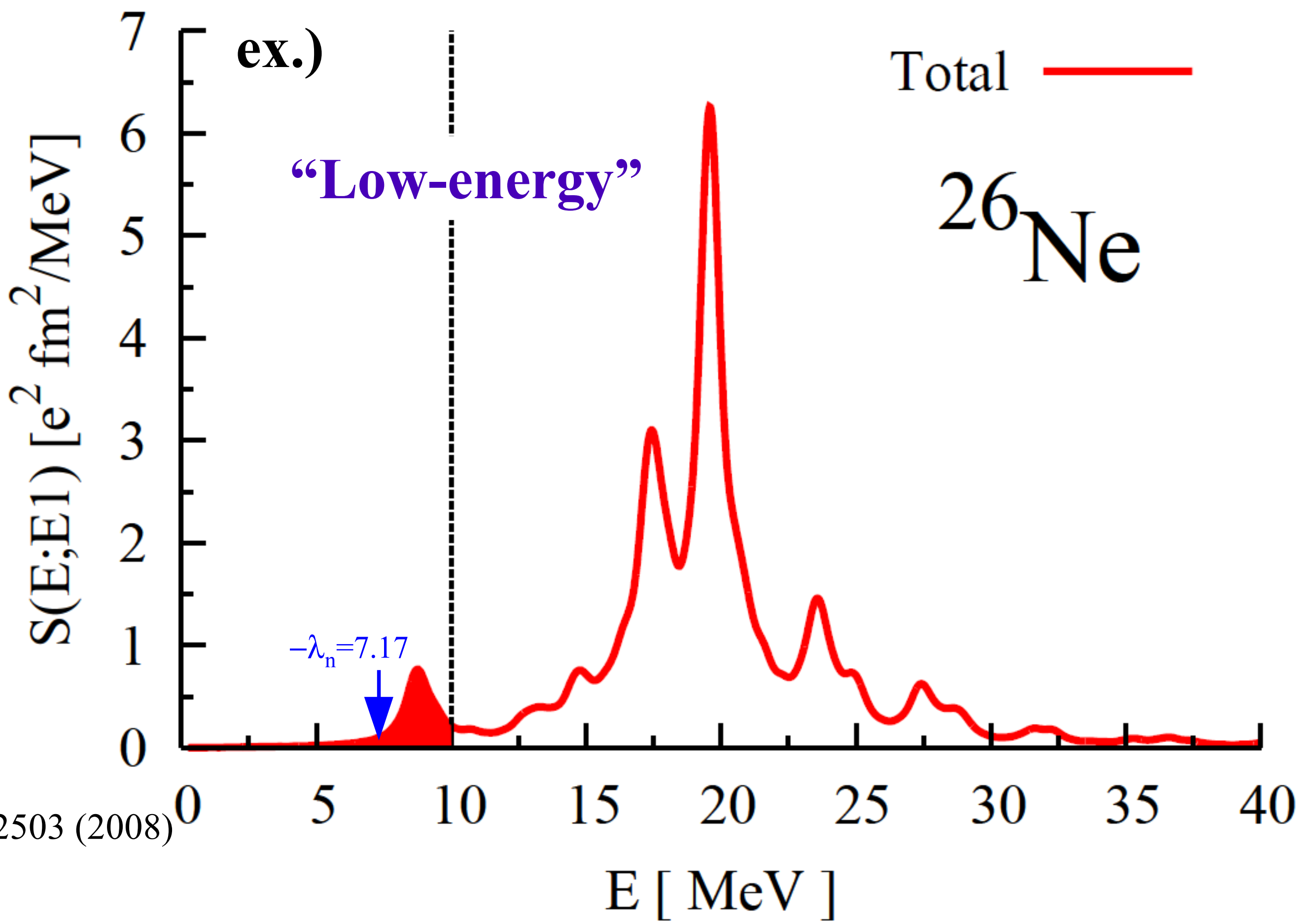
$$\frac{m_1(E_c=10)}{m_1} \equiv \frac{\int_0^{10[\mathrm{MeV}]} E\ S(E;E1)dE}{\int E\ S(E;E1)dE}$$

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

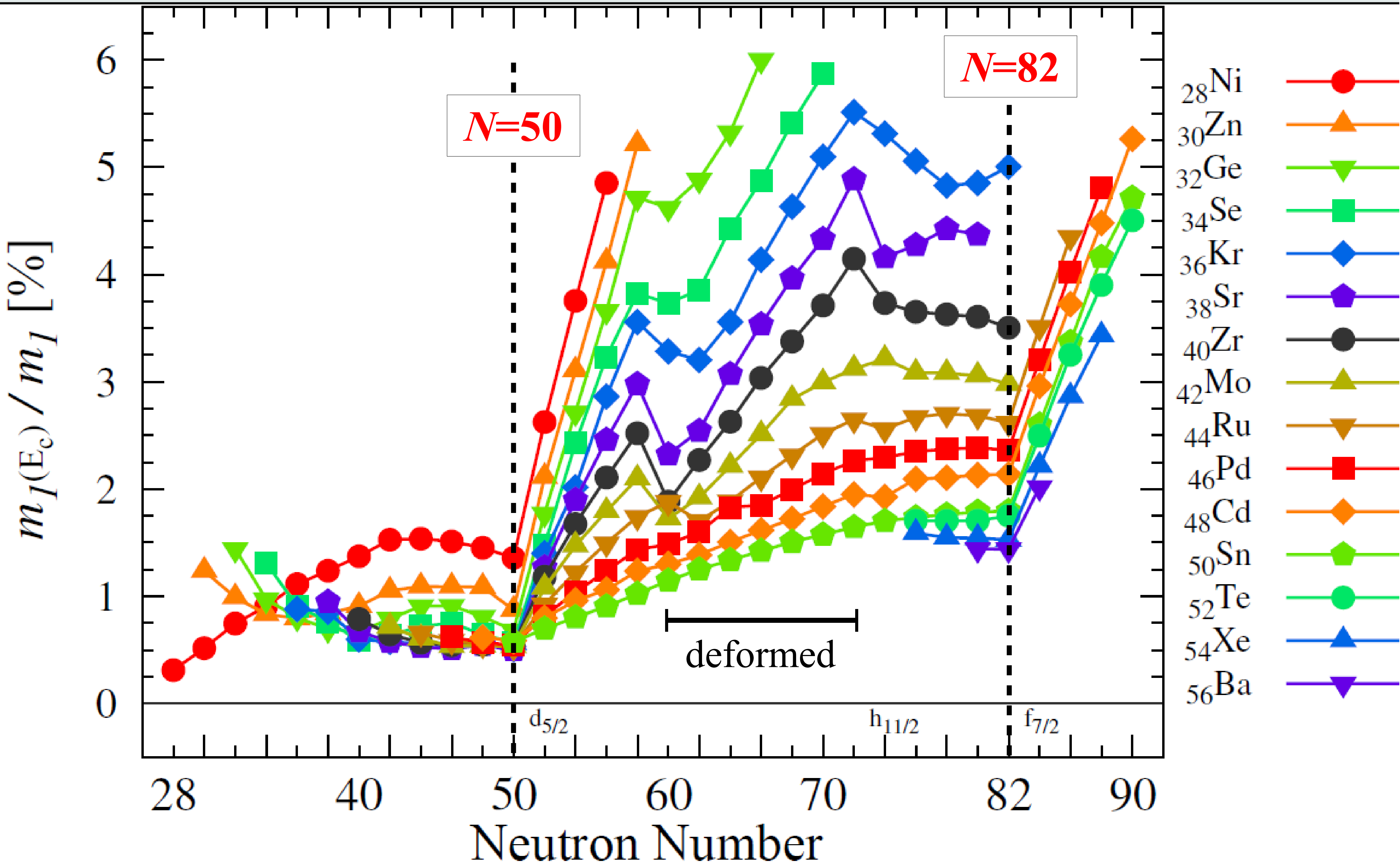
We use the ratio to analyze the low-lying *E1* strength for ***all*** calculated nuclei.



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



N-# dependence of PDR (heavy isotopes (272 items): $Z \geq 28$)



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- **反応現象のシミュレーション**

Nuclear Collision using Time-dependent DFT (TDHF)

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

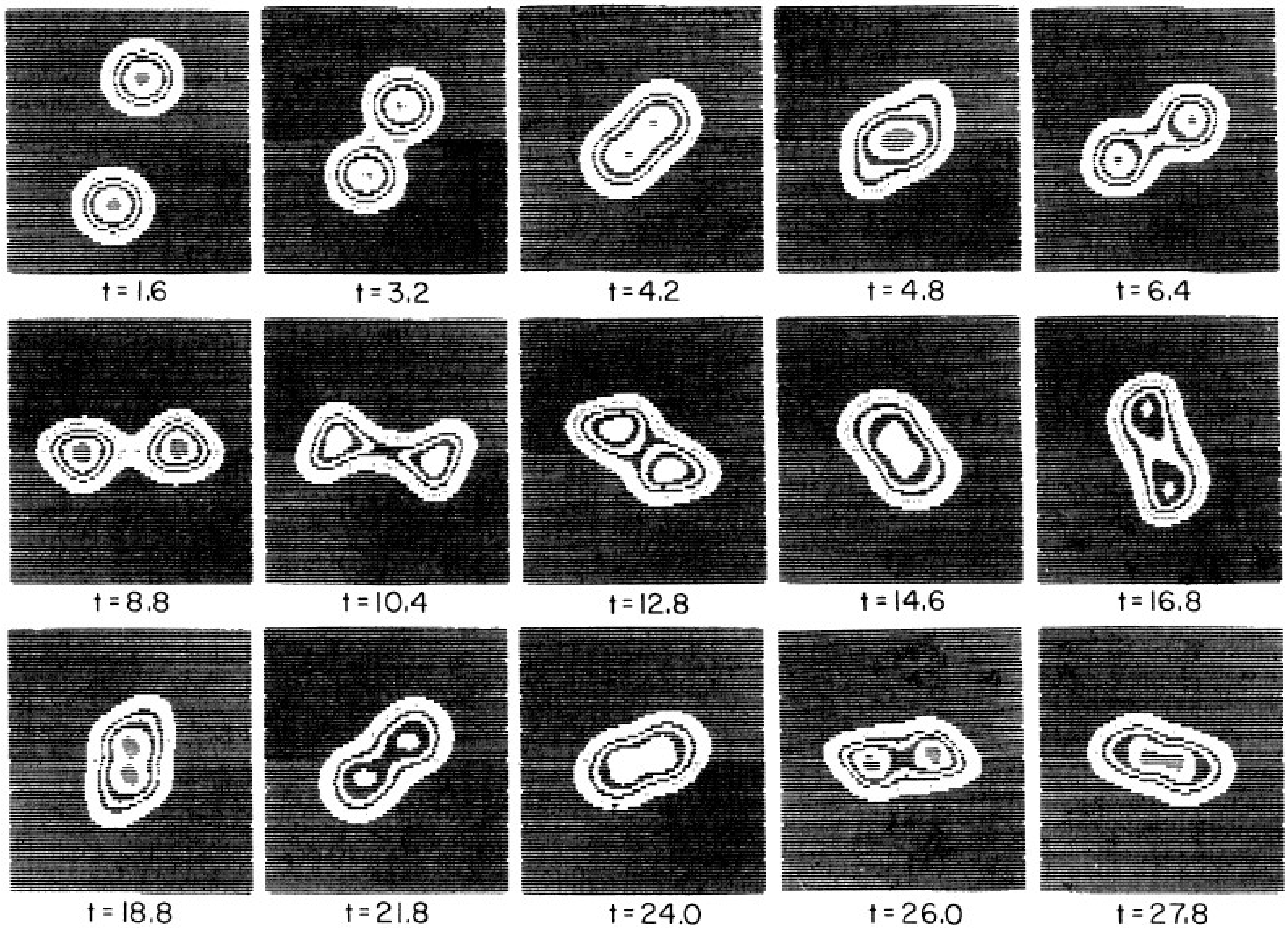
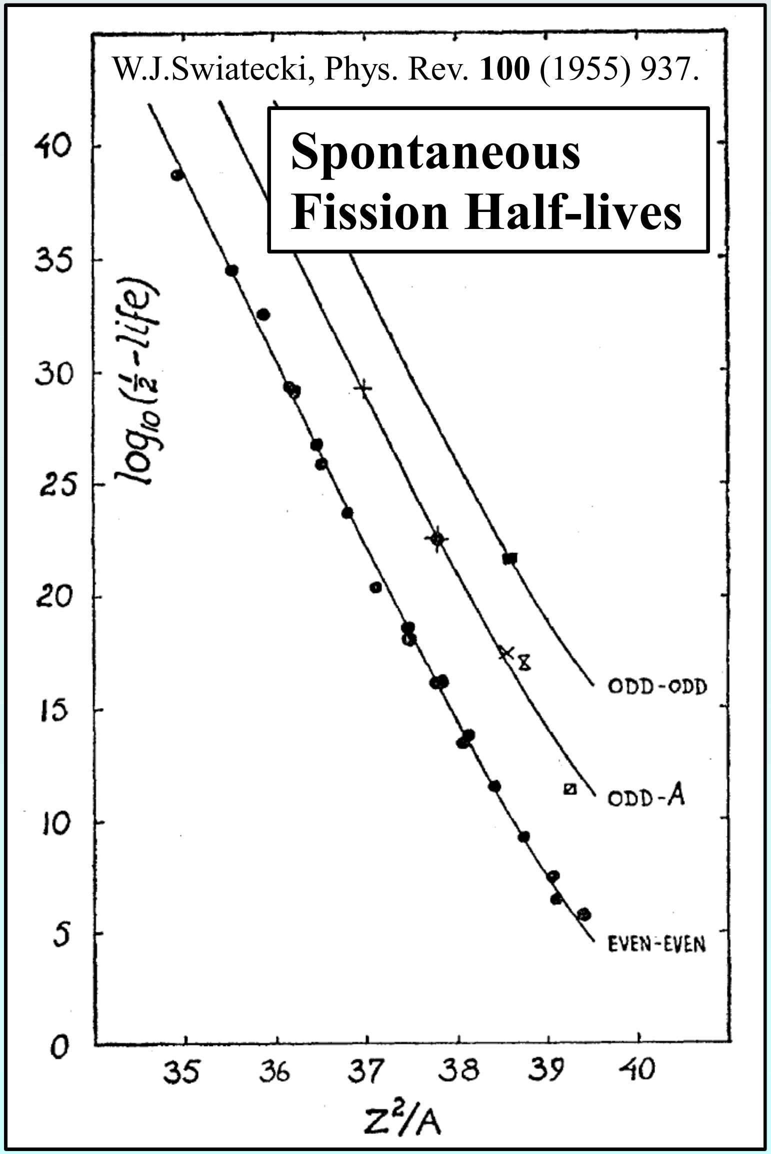


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O + ^{16}O$ collision at $E_{1ab} = 105$ MeV and incident angular momentum $L = 13\hbar$. The times t are given in units of 10^{-22} sec.

Expected pairing correlation effects in Heavy ion collision ?

- **Level crossing**
  - Energy Dissipation
  - Neck formation
  - Odd-even effects
    for spontaneous fission half-lives ?
- **Fusion *or* Fission cross section**
- **Pair transfer reaction**
- **Nuclear Josephson effect**



Setup for collision

Incident Energy : 18 - 20 [MeV] (E_{cm} = 9.0 – 10 [MeV], V_{FD} ~ 9 MeV)

Impact parameter : 0.0, 2.8 - 3.1 [fm]

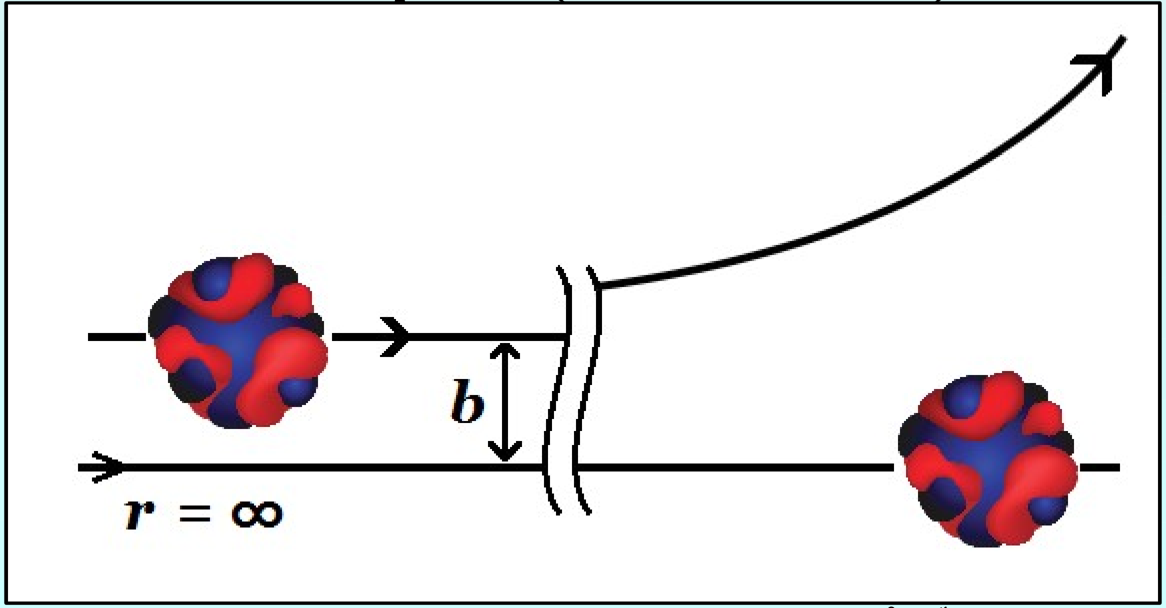
Effective Interaction : Skyrme force (SkM*), Contact pairing

Projectile : ^{22}O, Target : ^{22}O (HF g.s. has also spherical shape)

# of canonical-basis for HF+BCS g.s. ; (N, Z) = (32 (16+16) , 16 (8+8))

Average of gap energy ; $\bar{\Delta}_n = 2.066$ [MeV] $V_0^{\rm n} = -412.5$ [MeV]

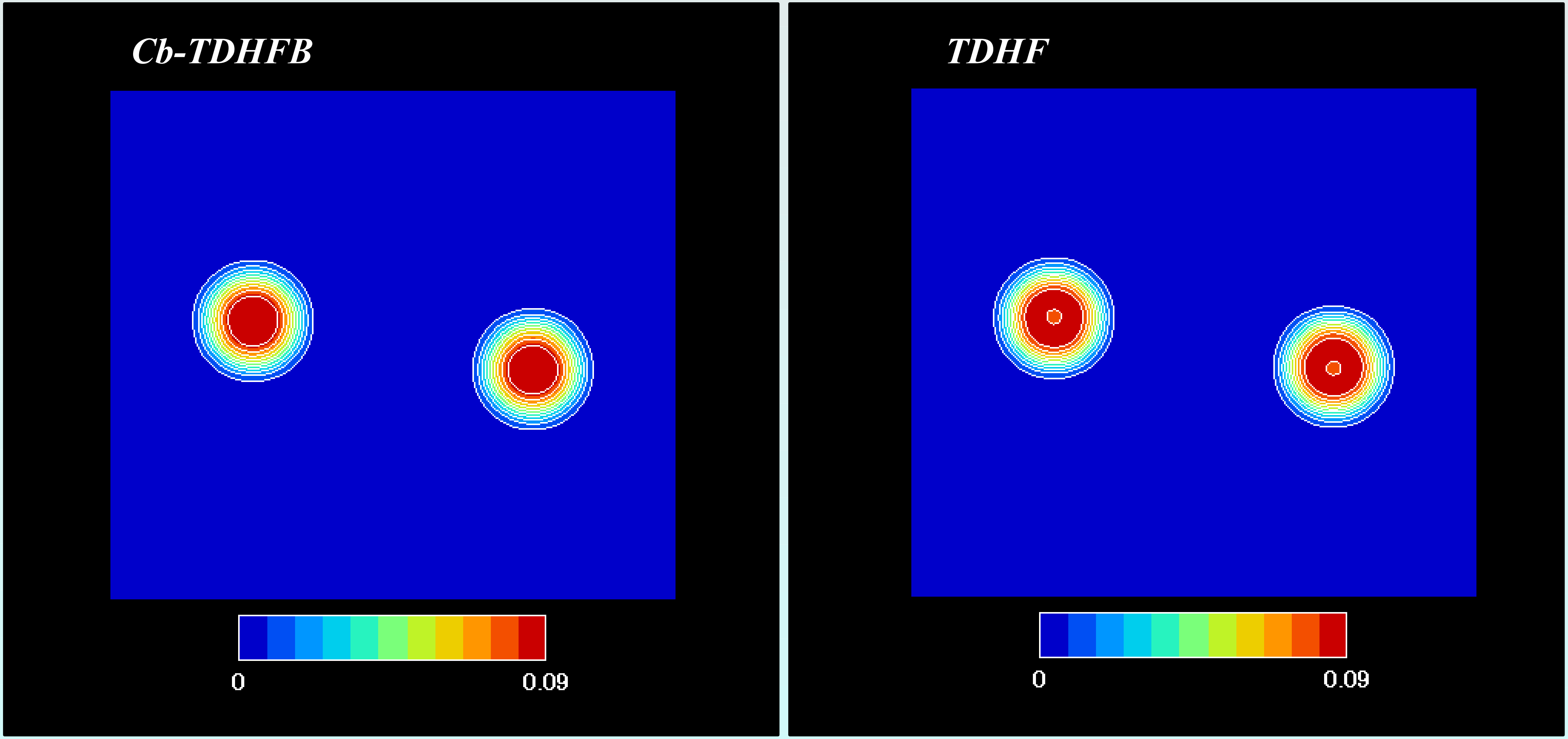
Calculation space (3D meshed box**):**



Length of box for (***x***, ***y***, ***z***) is **36, 20, 40**[fm] meshed by **1.0** [fm]

Simulation of ^{22}O + ^{22}O collision with b = 3.0 [fm] and E_{cm}=10 [MeV]

Time-evolution of Neutron density distribution



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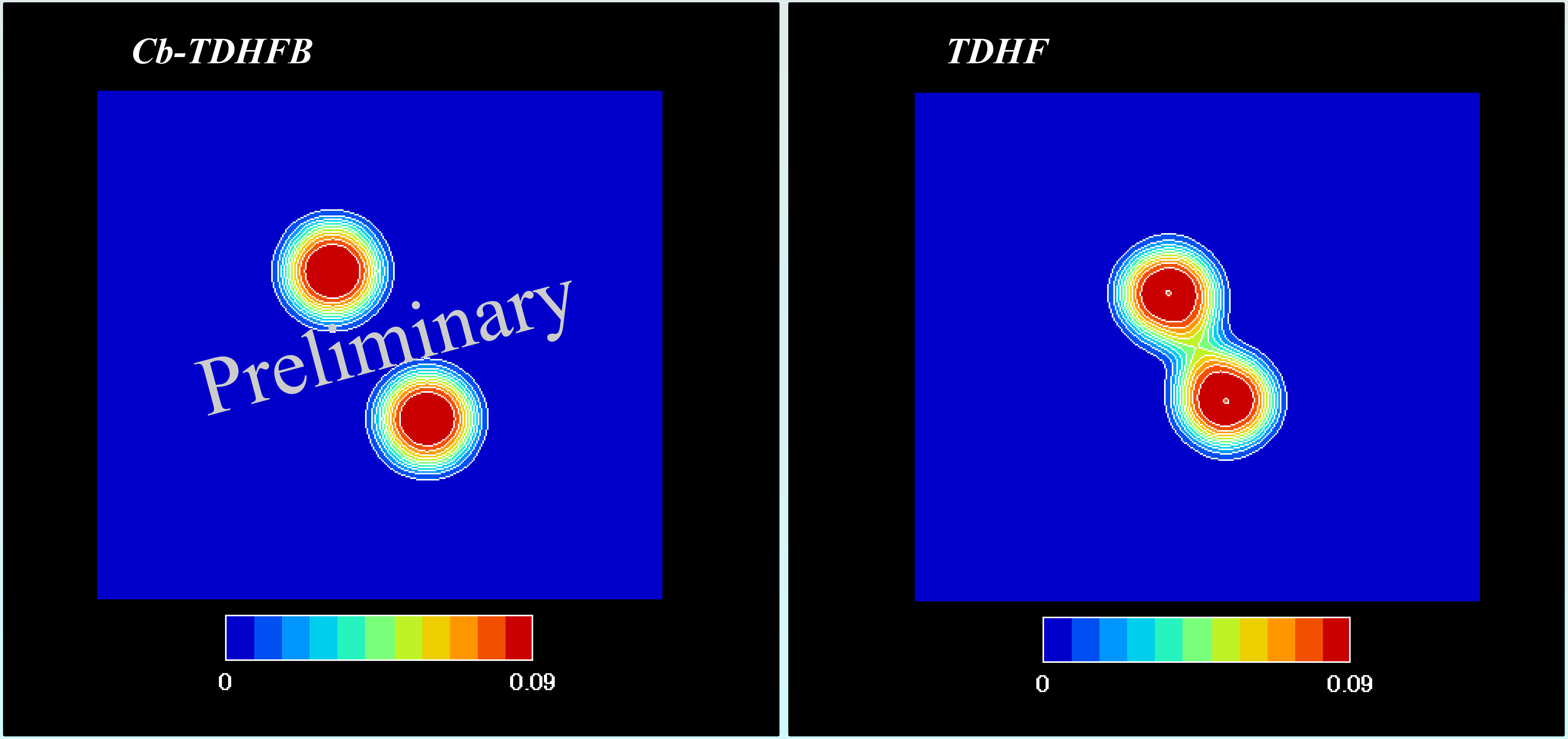


$$\sigma_F = 2\pi \int_0^{b_f} db\ b \qquad \sigma_F^{\mathrm{BCS}} < \sigma_F^{\mathrm{HF}}$$

!?

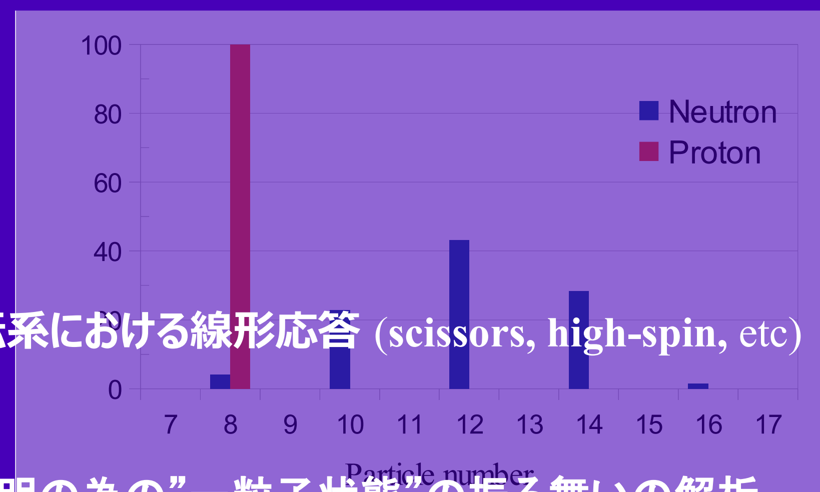
Summary & Perspective

時間依存平均場模型を用いた核ダイナミクスの研究

- 三次元座標空間上でCb-TDHFB計算を実行し、
  変形と対相関の効果を含めた**線形応答の系統的な計算が可能**となった。
- 対相関を含んだ**原子核反応**計算にCb-TDHFBを応用する事が出来た。

Perspective

★ **系統的計算の為の MPI＋OpenMP cording**



★ **線形応答計算**

- **他の励起状態の系統的研究** (ISM, ISQ, ISO, etc)
- **多スレーター行列式による線形応答**
  ← 多体の**量子揺らぎ**を考慮した励起状態
- **回転系における線形応答** (scissors, high-spin, etc)

★ **核反応答計算**

- **系統的な研究による対相関の具体的な効果、散逸機構解明の為の”一粒子状態”の振る舞いの解析**
  - **Fusion cross section**
  - **Level crossing**
- **多核子移行反応の為の粒子数射影**
  - **Nucleon transfer (Pair transfer), Nuclear Josephson effects**