Theoretical issues in physics of SHE
: nuclear reaction perspectives

Kouichi Hagino
Kyoto University

2019 IYPT
International Year
of the Periodic Table
of Chemical Elements

1. Introduction-1: periodic tables
2. Introduction-2: superheavy elements
3. Formation reactions
4. Theoretical issues
5. Physics of neutron-rich nuclei
6. Summary

Periodic table of elemetns (1869)

2019
IYPT

International Year
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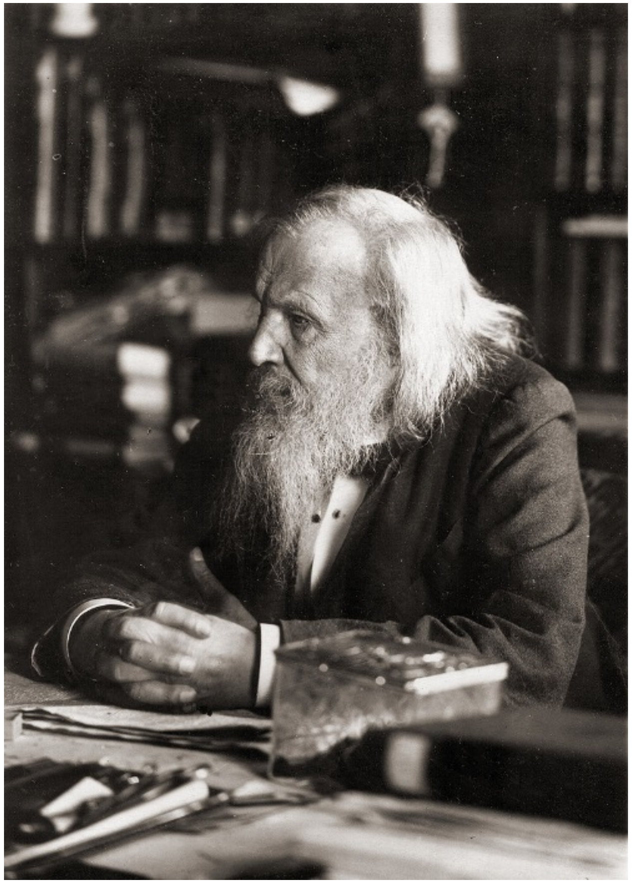
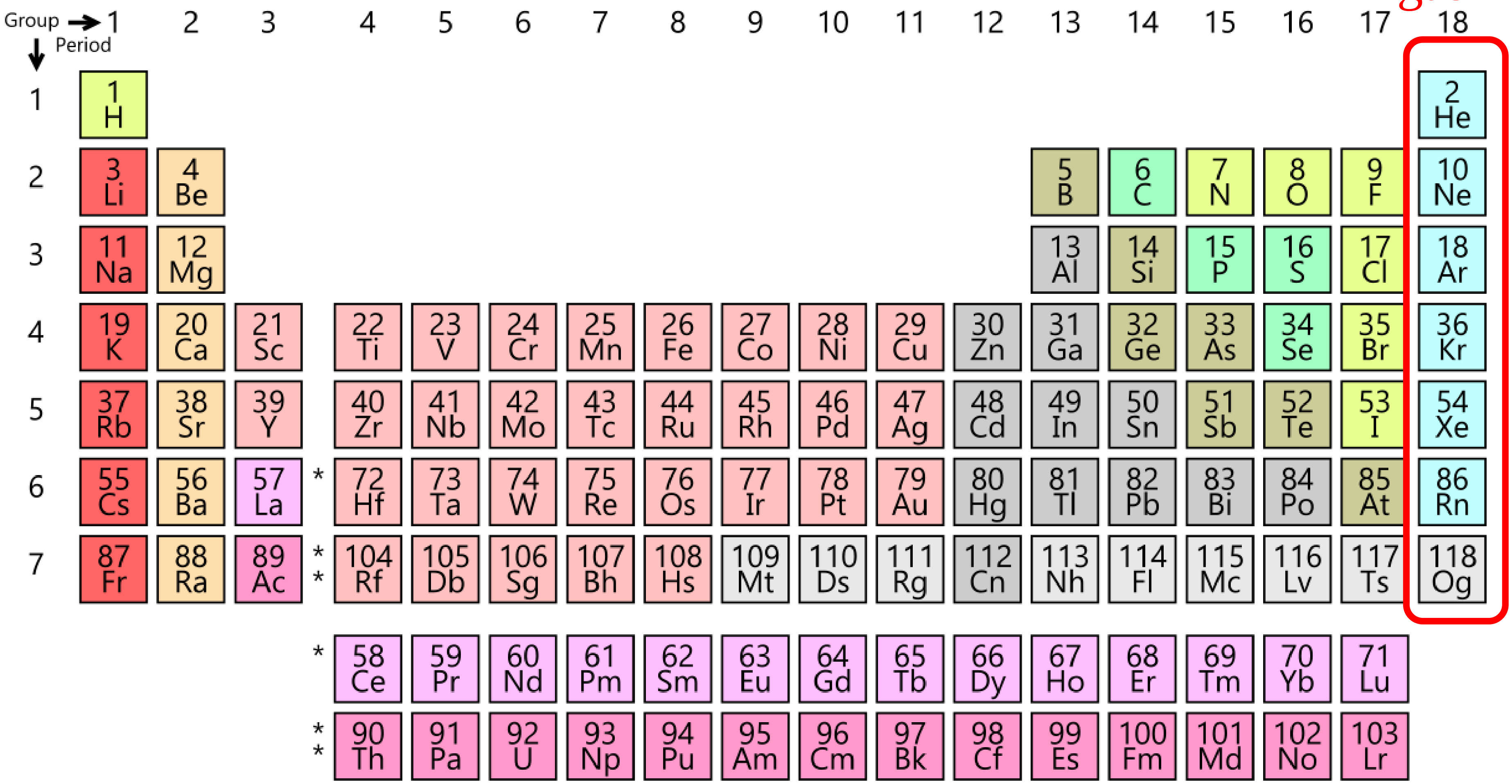
of Chemical Elements



Mendereev
(1834-1907)

periodic table of elements



Group → Period ↓	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
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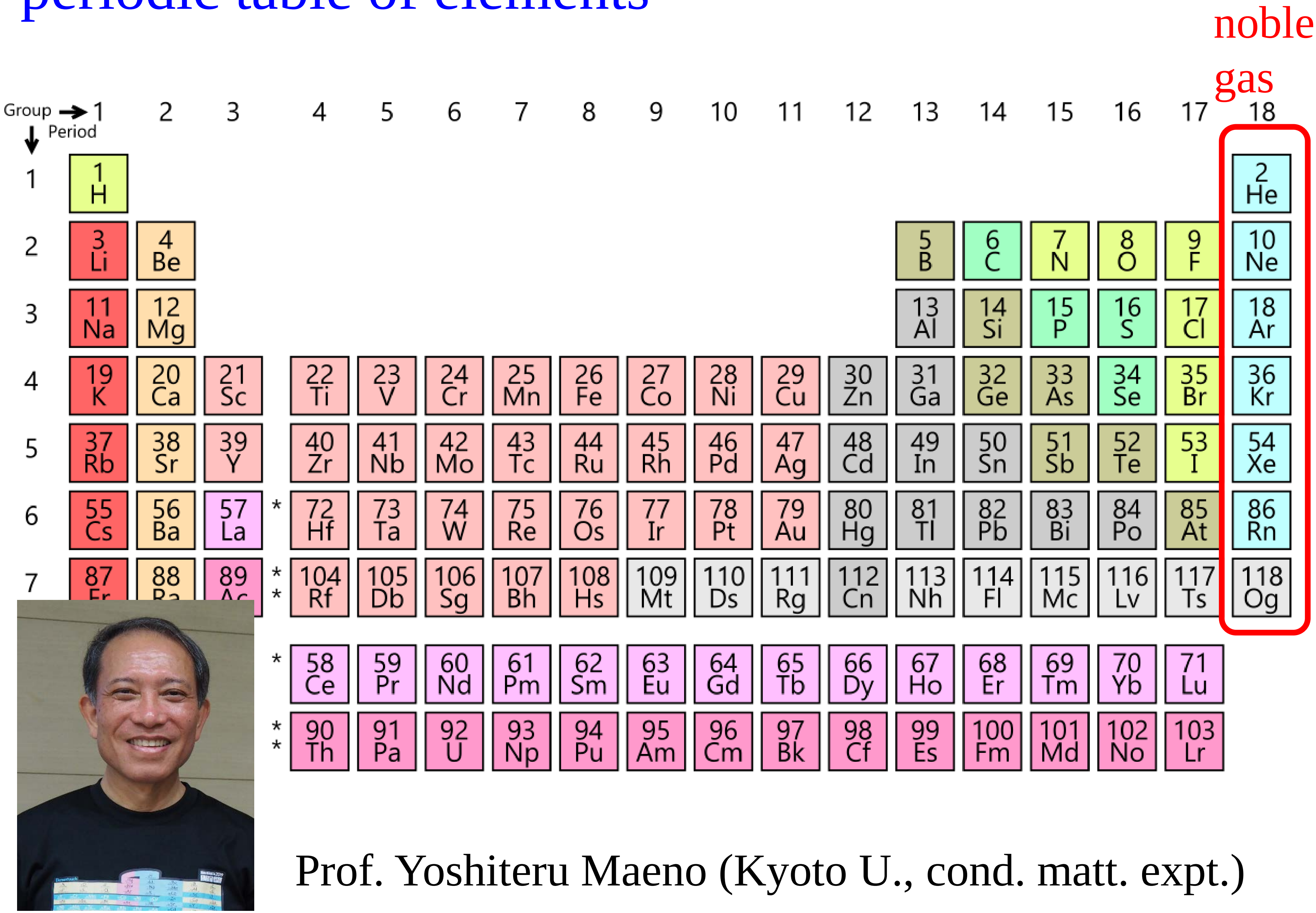
noble gas

periodic table of elements



noble gas

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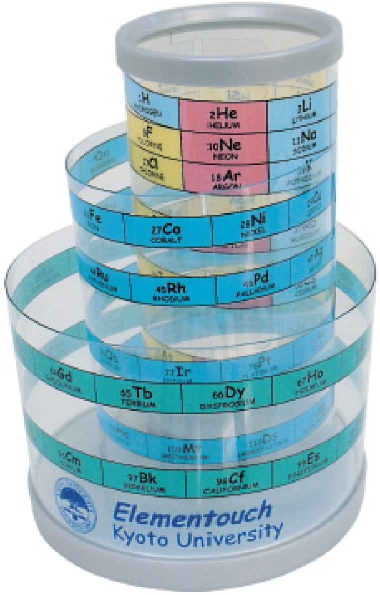
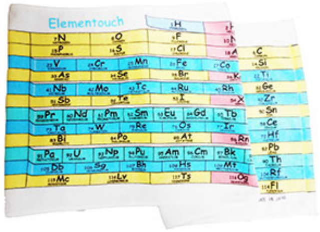
Prof. Yoshiteru Maeno (Kyoto U., cond. matt. expt.)

periodic table of elements



3D periodic table “elementouch”
(Y. Maeno, 2001)

mug cup



towel

T-shirt
(Kyoto-U. coop)

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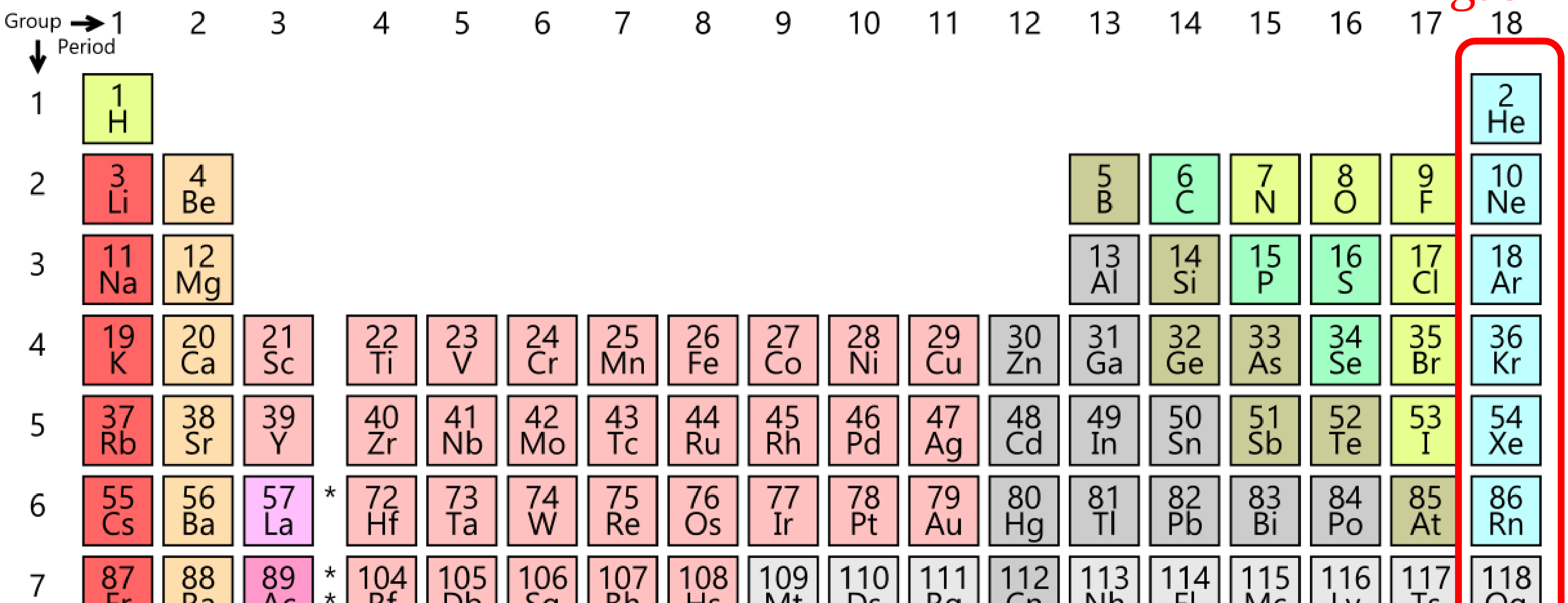
periodic table of ~~elements~~ nuclei?

proton
magic # ← noble
gas



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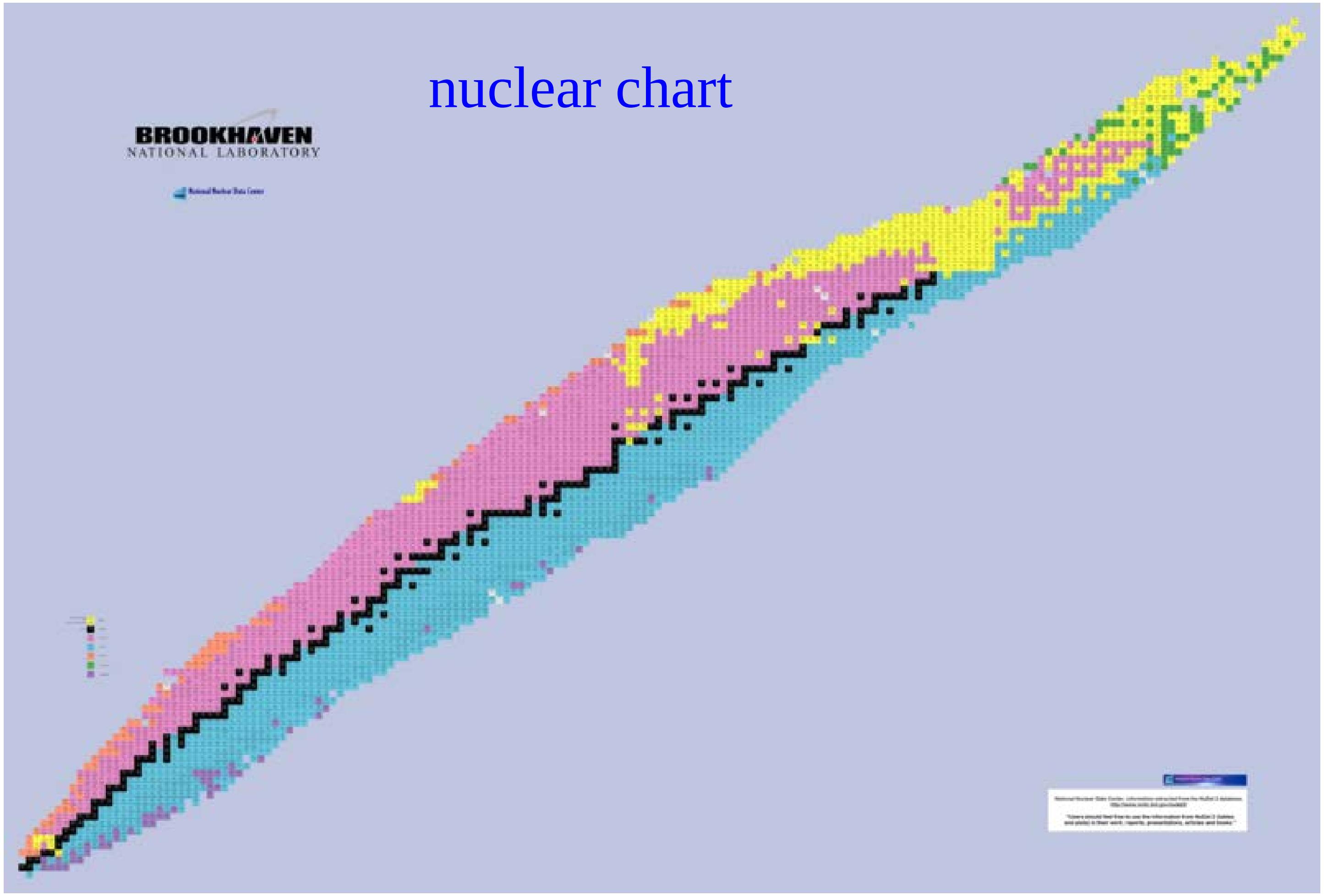
Nuclear periodic table

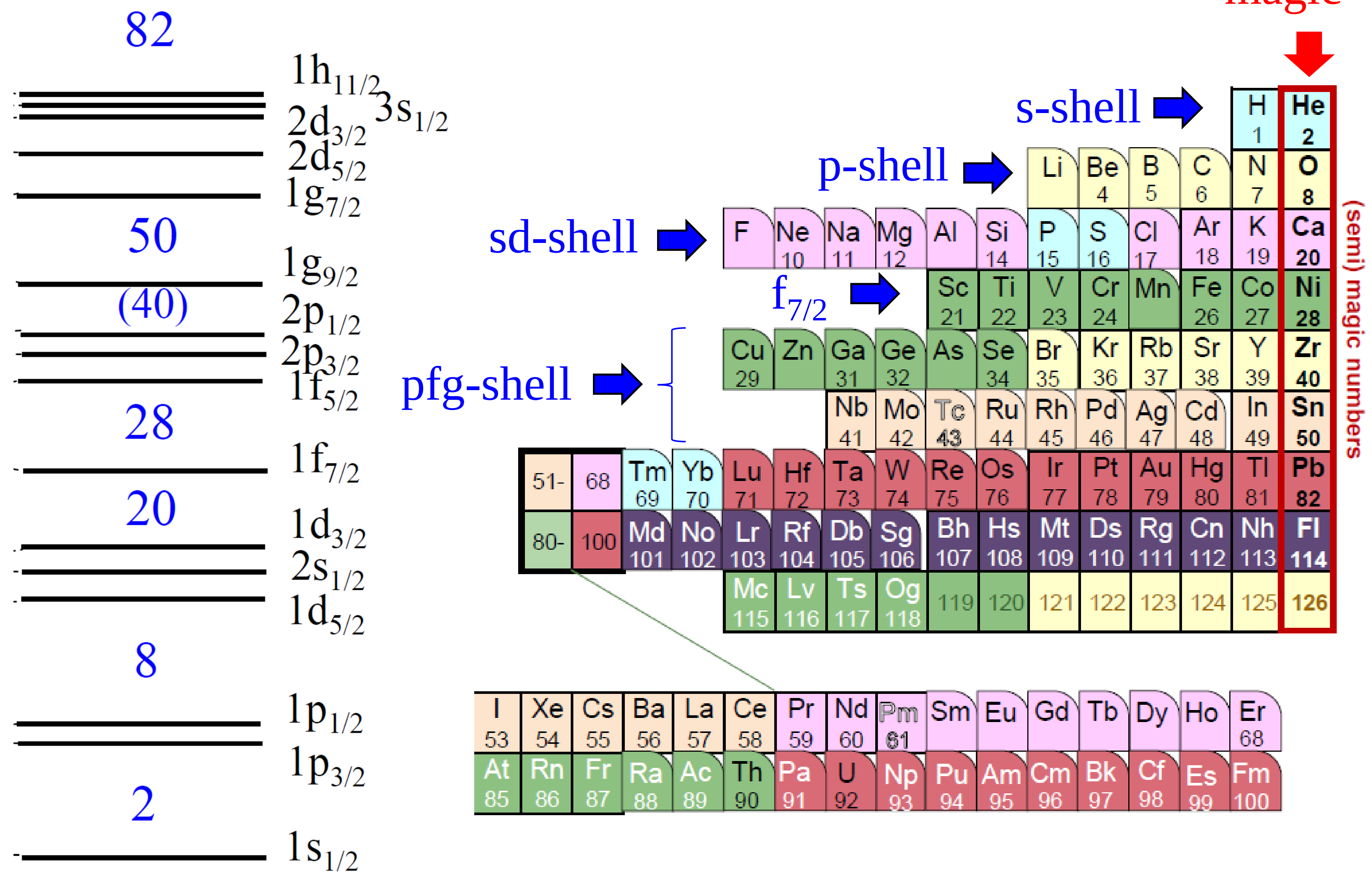


nuclear chart

Yet, a pedagogical significance
(to familiarize nuclear physics)

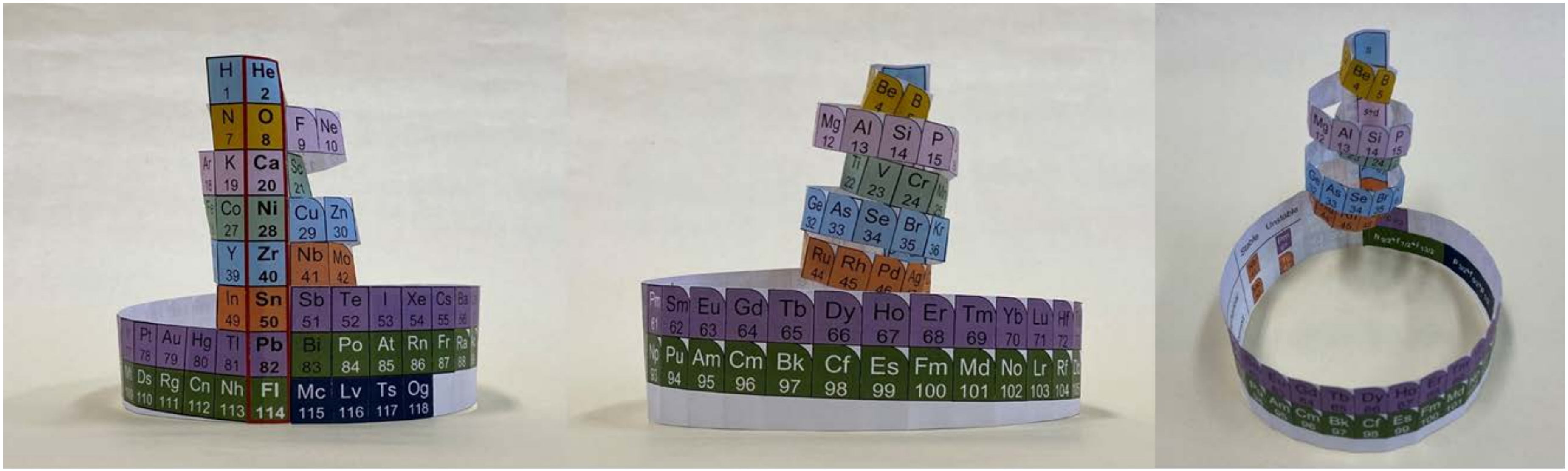
Nuclear periodic table

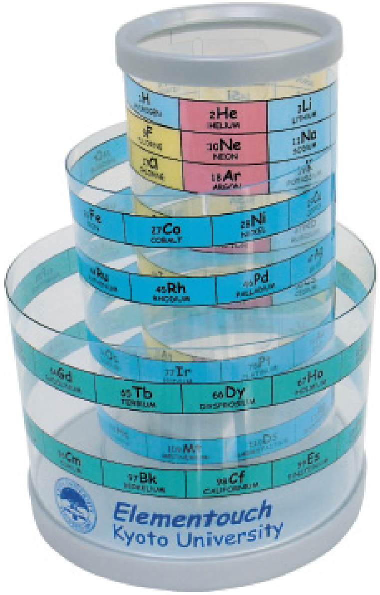
K. Hagino and Y. Maeno,
Found. of Chem. 22, 267 (2020).



Nuclear periodic table

“nucletouch” (a 3D model)





cf. “elementouch”
(Y. Maeno, 2001)

mug cup

towel

T-shirt
(Kyoto-U. coop)

掌握元素性质的新工具！京都大学创建原子核周期表

2020年05月11日 化学材料

新しい周期表を考案 京大、原子核の性質を表現

2020/5/3付 | 日本経済新聞 朝刊

京都大学の前野悦輝教授と萩野浩一教授は、原子核の性質をわかりやすく
い周期表を考案した。従来の周期表が元素の化学的な性質を知るのに役立
て、新しい周期表は元素の原子核の性質を知るのに使える。

NEWS RELEASE 27-MAY-2020

A special elemental magic

Kyoto scientists announce a 'nuclear' periodic table

KYOTO UNIVERSITY

Японские физики представили новую периодическую таблицу элементов

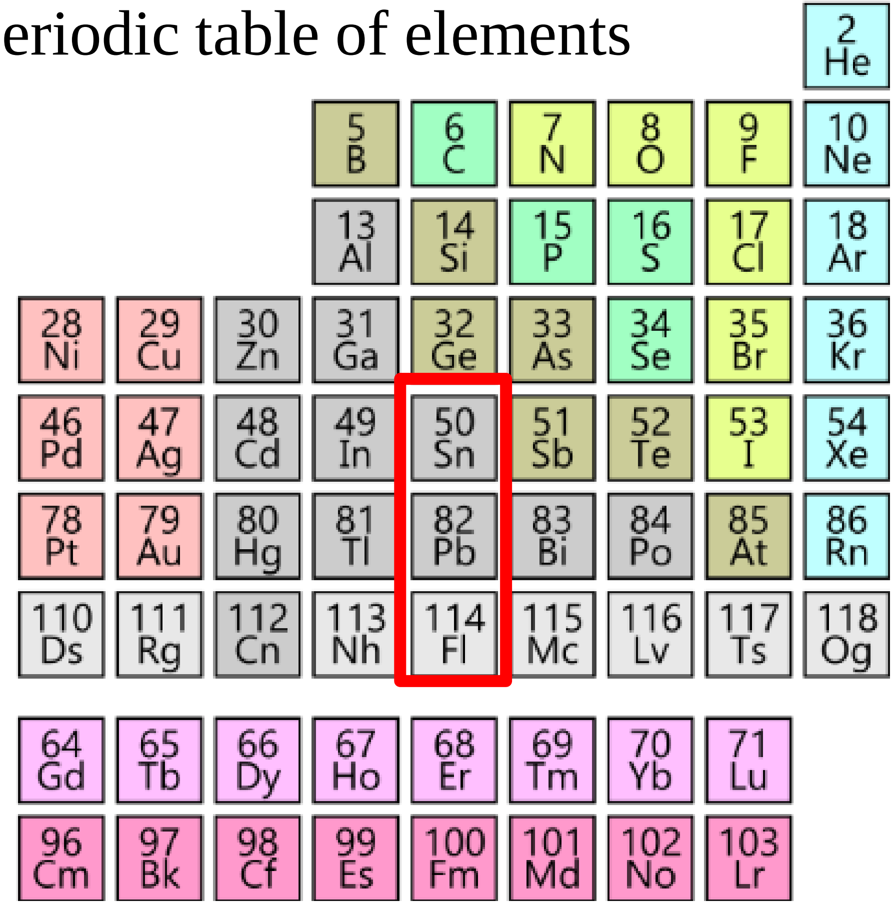
19:34 27.05.2020 58122

© Фото : Kyoto University/Yoshiteru Maeno/Kouichi Hagino

МОСКВА, 27 мая — РИА Новости. Ученые из Киотского университета представили периодическую таблицу элементов, которая в отличие от таблицы Менделеева, где за основу взяты электроны в атоме, основана на a magical coincidence

Y. Maeno, K. Hagino, and T. Ishiguro,
Found. of Chem., in press.

periodic table of elements



								2 He
			5 B	6 C	7 N	8 O	9 F	10 Ne
			13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
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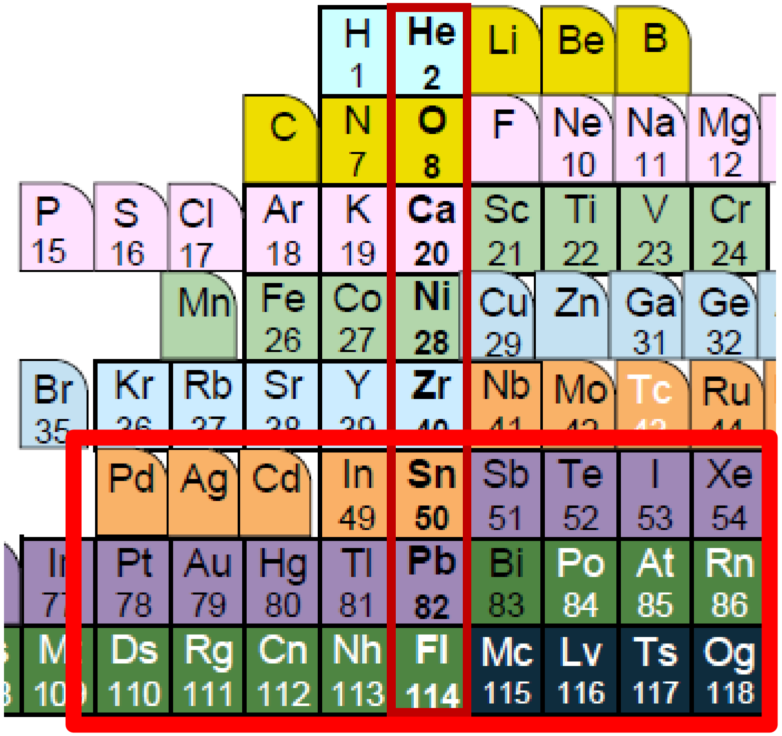
nuclear periodic table



				H 1	**He 2**	Li	Be	B	
			C	N 7	**O 8**	F	Ne 10	Na 11	Mg 12
P 15	S 16	Cl 17	Ar 18	K 19	**Ca 20**	Sc 21	Ti 22	V 23	Cr 24
		Mn	Fe 26	Co 27	**Ni 28**	Cu 29	Zn	Ga 31	Ge 32
Br 35	Kr 36	Rb 37	Sr 38	Y 39	**Zr 40**	Nb 41	Mo 42	Tc 43	Ru 44
	Pd	Ag	Cd	In 49	**Sn 50**	Sb 51	Te 52	I 53	Xe 54
Ir 77	Pt 78	Au 79	Hg 80	Tl 81	**Pb 82**	Bi 83	Po 84	At 85	Rn 86
M 10	Ds 110	Rg 111	Cn 112	Nh 113	**Fl 114**	Mc 115	Lv 116	Ts 117	Og 118

the nuclear magic numbers are there in the same column!
(the same elements around them)

a magical coincidence which can be recognized only after making a nuclear periodic table

Superheavy elements and Neutron-rich Nuclei

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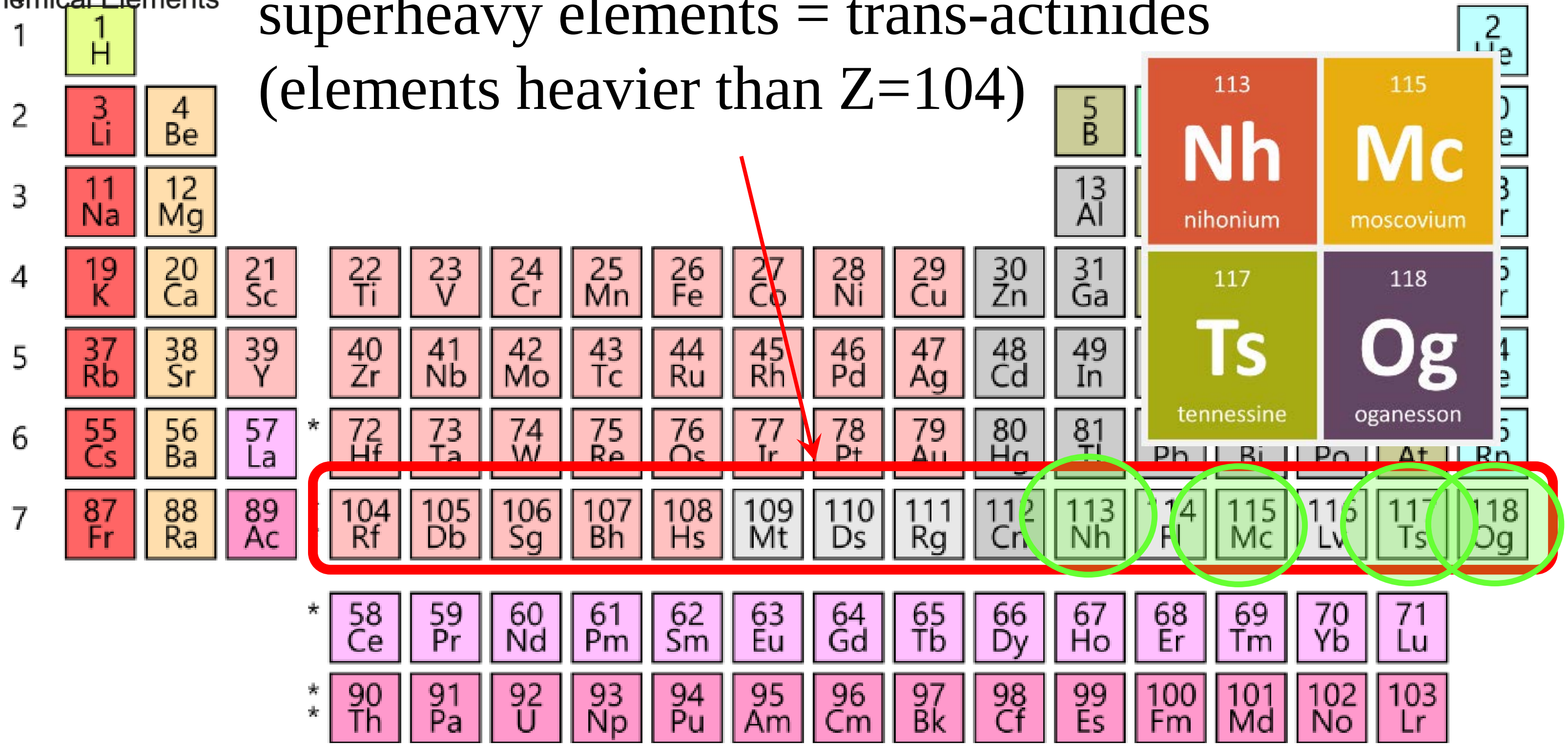
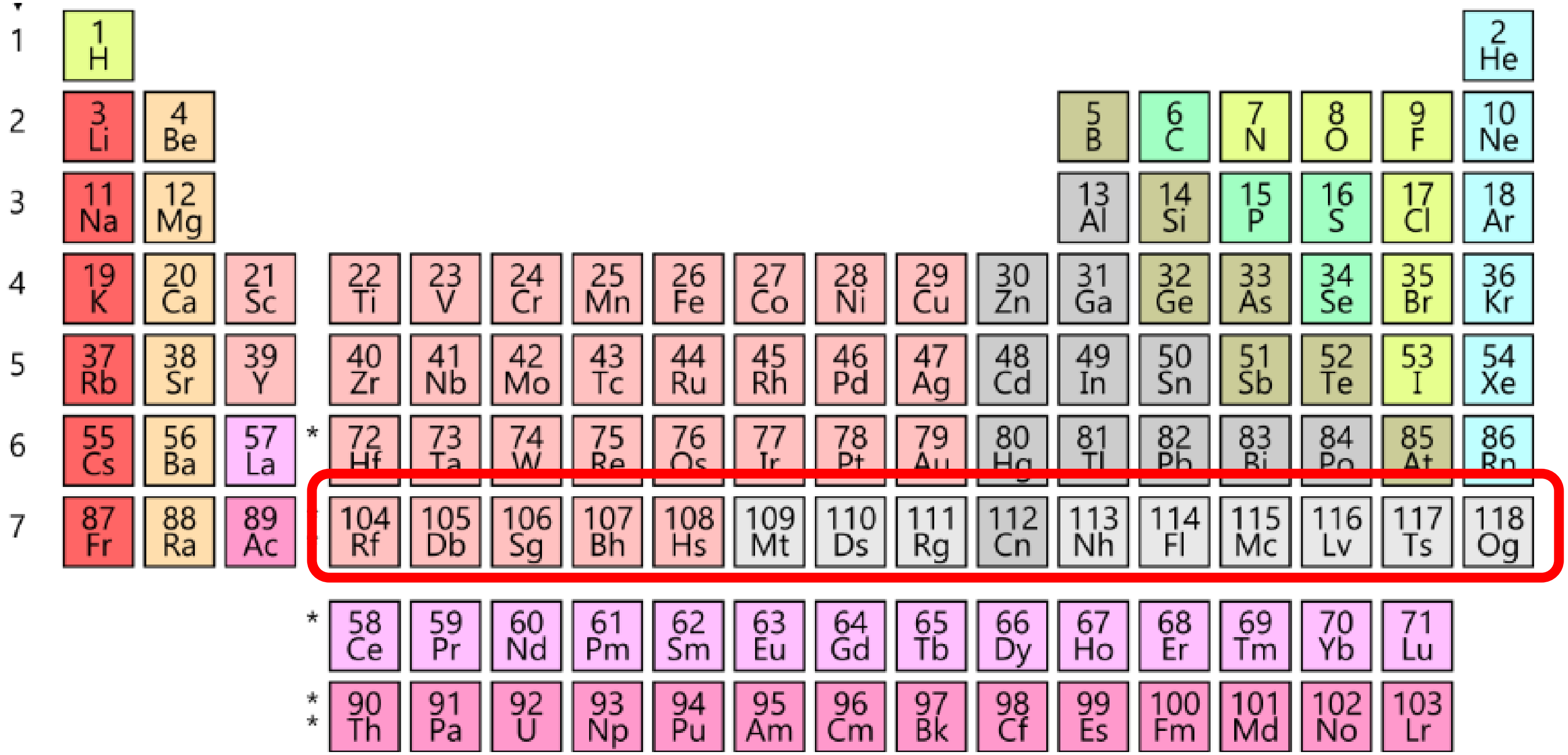
Definition: superheavy elements

superheavy elements = trans-actinides
(elements heavier than Z=104)





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Interests in physics and chemistry of superheavy elements

- what is the heaviest element? → atomic property
- what is the double magicu nucleus next to ^{208}Pb? → nuclear property
- should the periodic table be changed or not? → chemical property
- how do superheavy elements influence the r-process nucleosynthesis?
  → astrophysics

what determines the limit of existence of elements?

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I 53 Iodine
Y 39 Yttrium
Pt 78 Platinum
Ca 20 Calcium
K 19 Potassium

possibilities to be considered:

- ✓ electron orbitals in atom
- ✓ stability of nucleus in atom (← magic number)

what determines the limit of existence of elements?

INTERNATIONAL
YEAR OF THE
PERIODIC TABLE
2019

I	Y	Pt	Ca	K
53	39	78	20	19
Iodine	Yttrium	Platinum	Calcium	Potassium

possibilities to be considered:

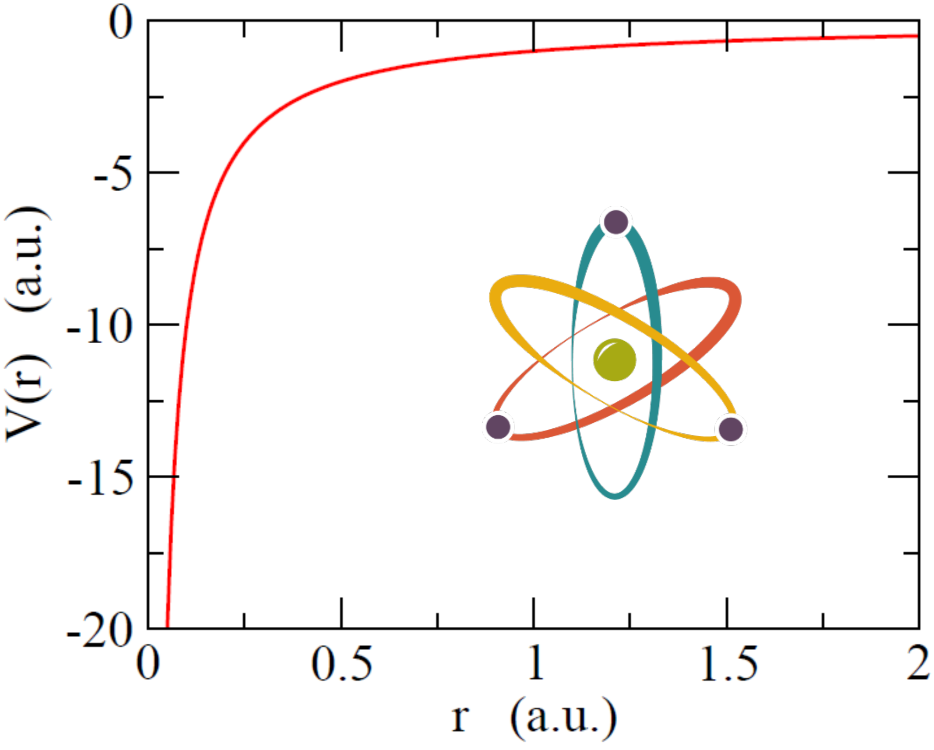
let’s first discuss

- ✓ electron orbitals in atom
- ✓ stability of nucleus in atom (← magic number)

what determines the limit of existence of elements? (i) electron orbits

hydrogen-like atom

$$\boxed{V(r) = -\frac{Ze^2}{r}}$$



1S state

$$\boxed{E_{1S} = -Z^2 \cdot \frac{me^4}{2\hbar^2}}$$

Z →large, E_{1s} →small

$\langle r \rangle \to$ small

what determines the limit of existence of elements? (i) electron orbits

hydrogen-like atom

$$\boxed{V(r) = -\frac{Ze^2}{r}}$$

1S state

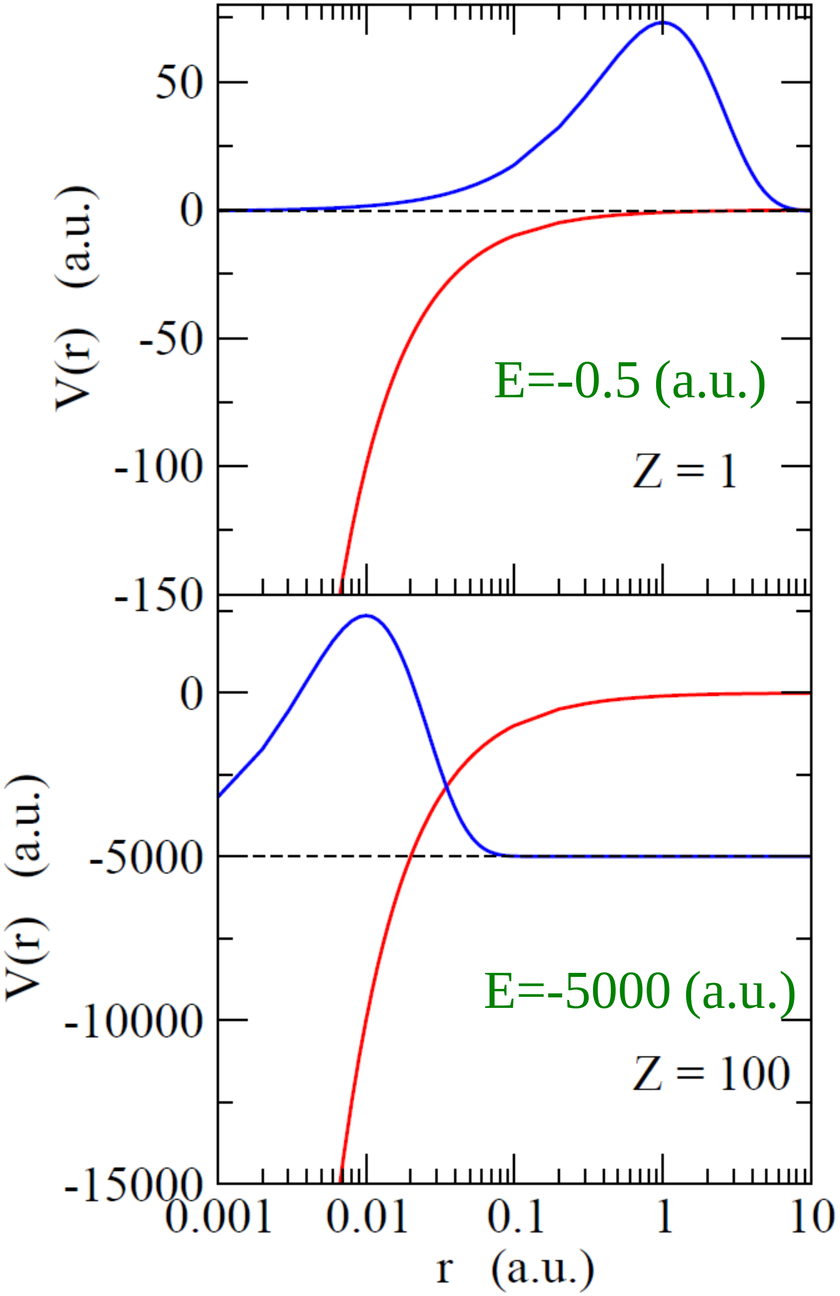
$$\boxed{E_{1S} = -Z^2 \cdot \frac{me^4}{2\hbar^2}}$$

$Z \rightarrow$large, $E_{1s} \rightarrow$small

$\langle r \rangle \rightarrow$ small

$\langle p \rangle \rightarrow$ large (uncertainty)

relativistic effect



what determines the limit of existence of elements? (i) electron orbits

hydrogen-like atom

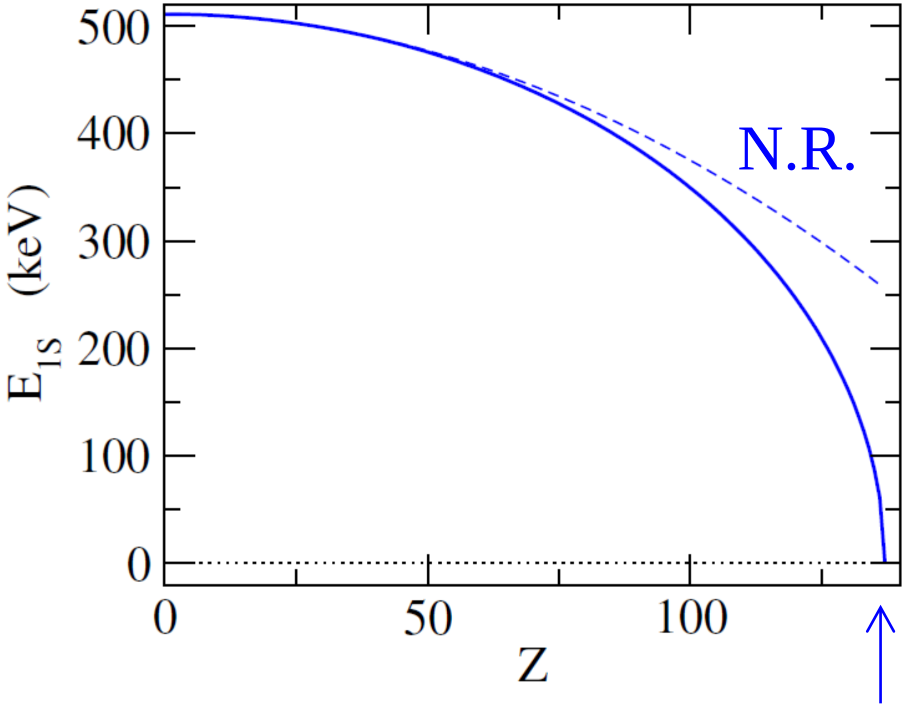
$$\boxed{V(r) = -\frac{Ze^2}{r}}$$

1S state (Dirac equation)

$$\boxed{E_{1S} = mc^2\sqrt{1-(Z\alpha)^2}}$$

$$\alpha = \frac{e^2}{\hbar c} \sim \frac{1}{137}$$

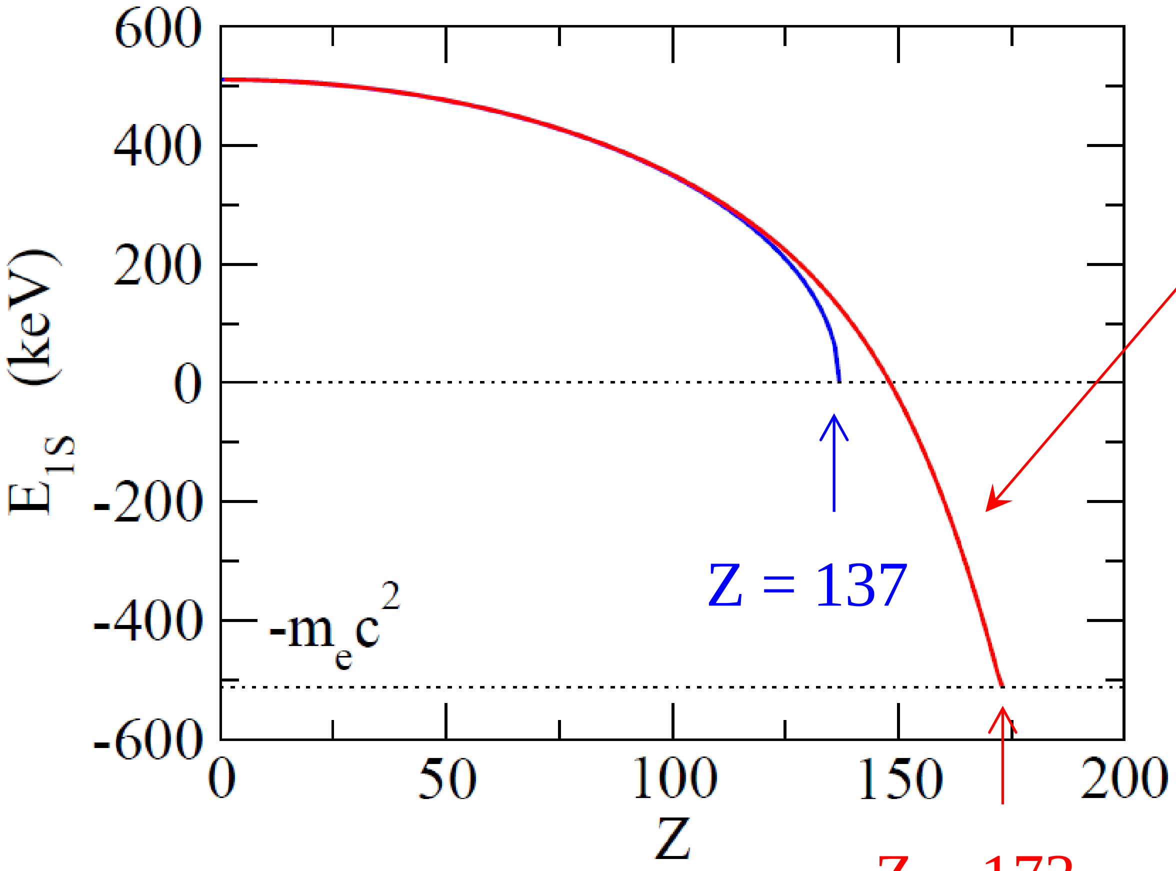
Z > 137 → no solution



Z = 137

what determines the limit of existence of elements? (i) electron orbits

hydrogen-like atom



Z = 137

Z ~ 173

finite size of a nucleus (uniform charge)

$R_N \sim 10^{-4}$ Å
rms $\sim 10^{-3}$ Å
(A=173)

cf. W. Pieper and W. Greiner, Z. Physik 218 (1969) 327

what determines the limit of existence of elements?

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I 53 Iodine
Y 39 Yttrium
Pt 78 Platinum
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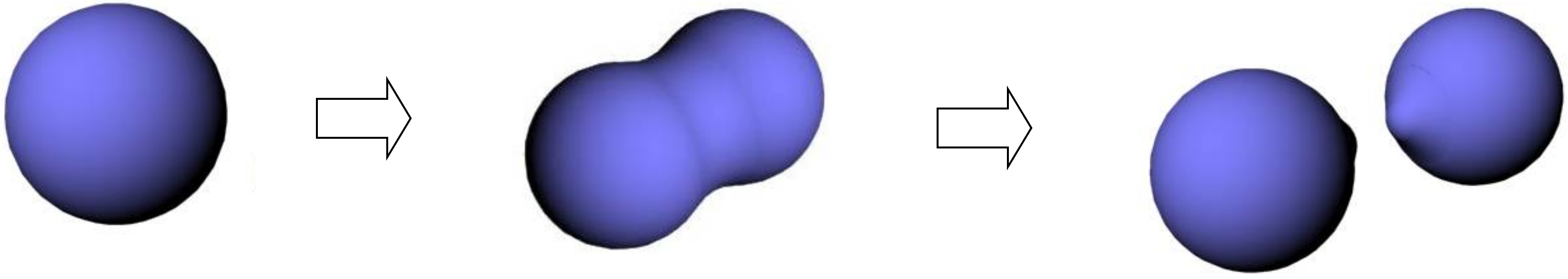
possibilities to be considered:

let’s next discuss

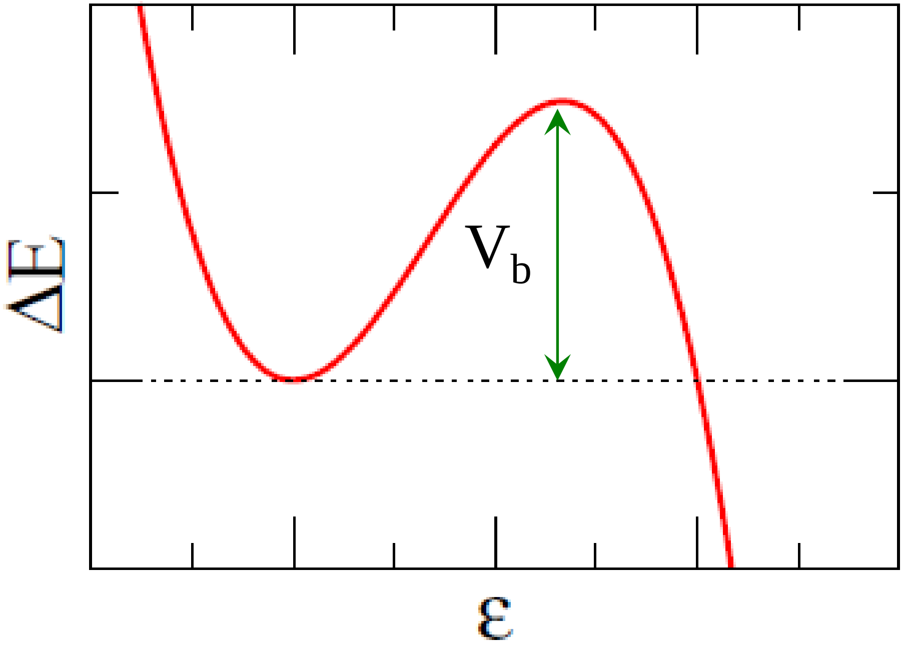
- ✓ electronic orbitals in atom
- ✓ stability of nucleus in atom

what determines the limit of existence of elements? (ii) atomic nucleus

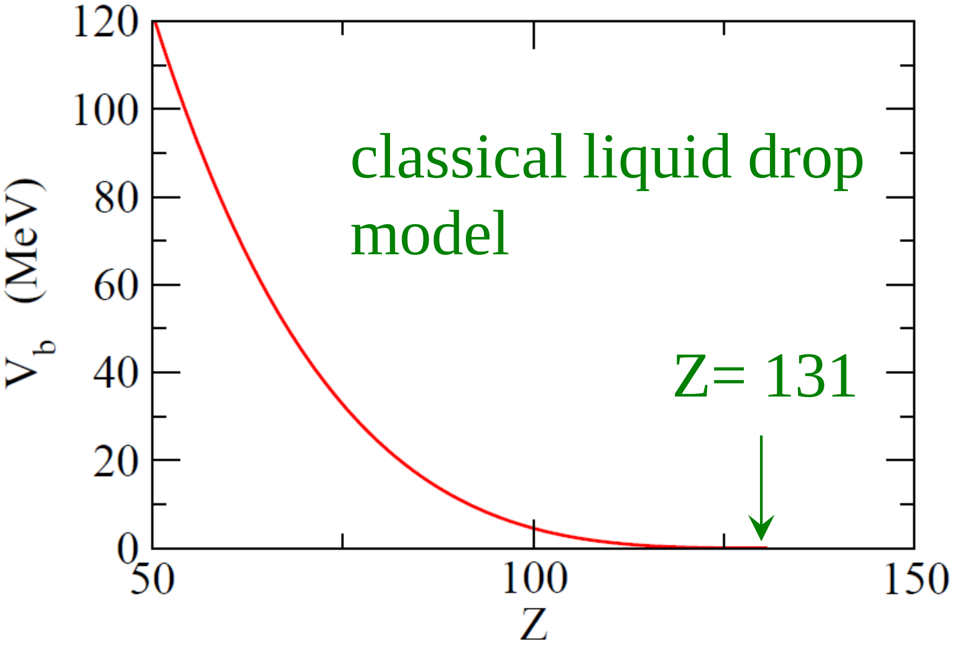
heavy nuclei → unstable against fission



fission barrier

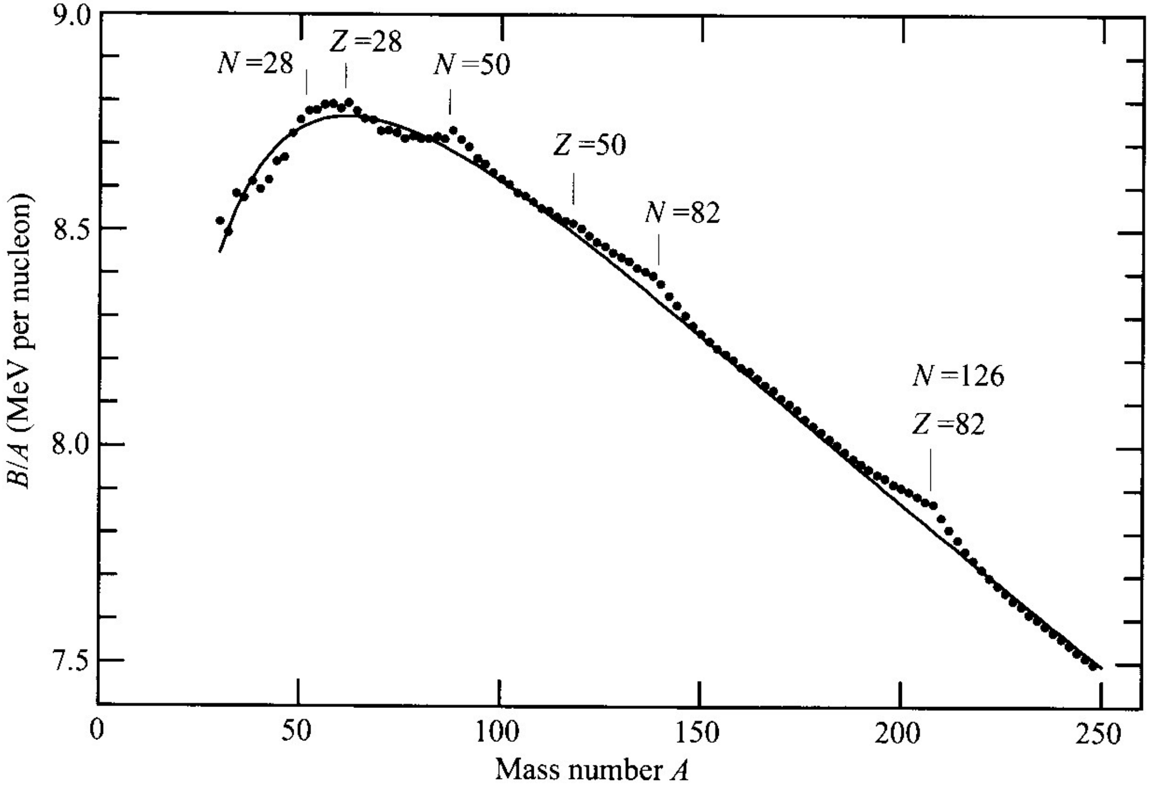


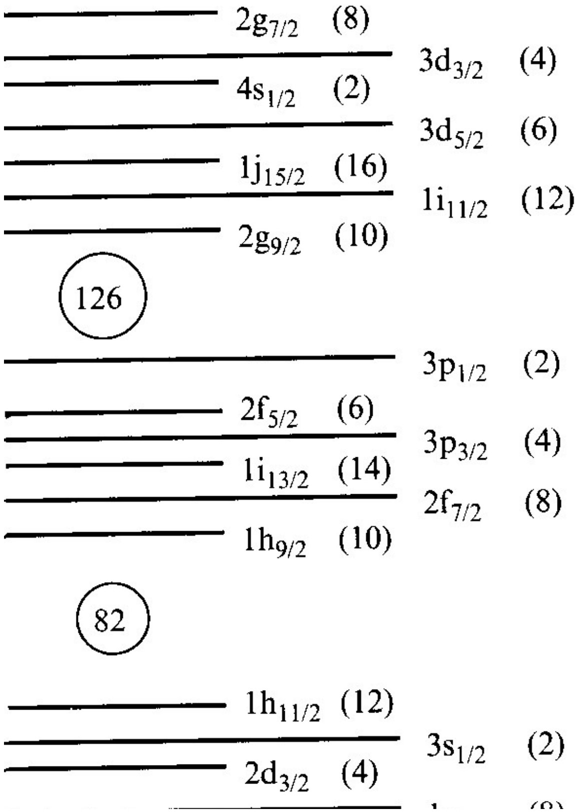
barrier height



shell effect

$$B = B_{LDM} + B_{shell}$$





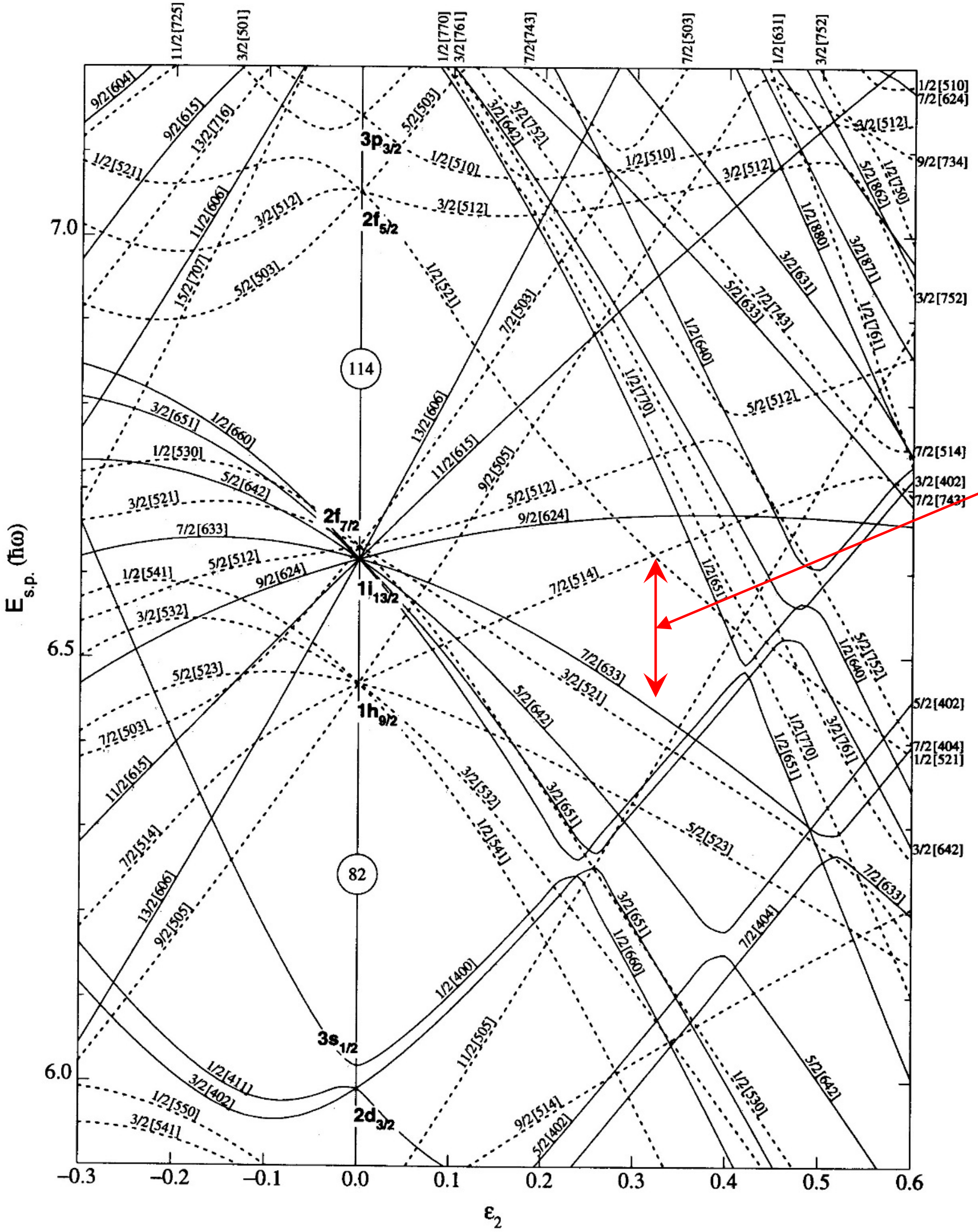
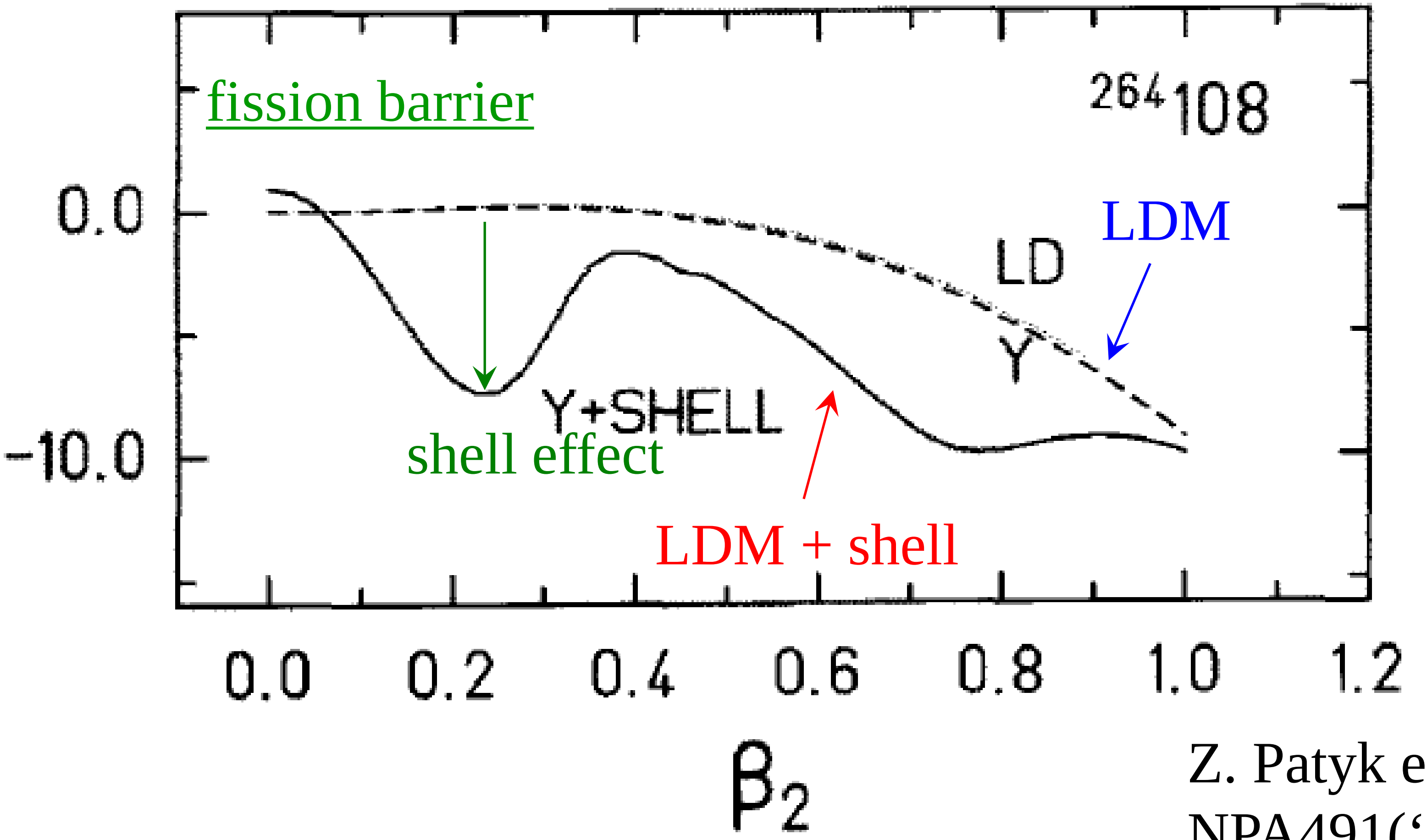


Figure 13. Nilsson diagram for protons, Z ≥ 82 ($\epsilon_4 = \epsilon_2^2/6$).

energy gap if deformed

Nilsson diagram

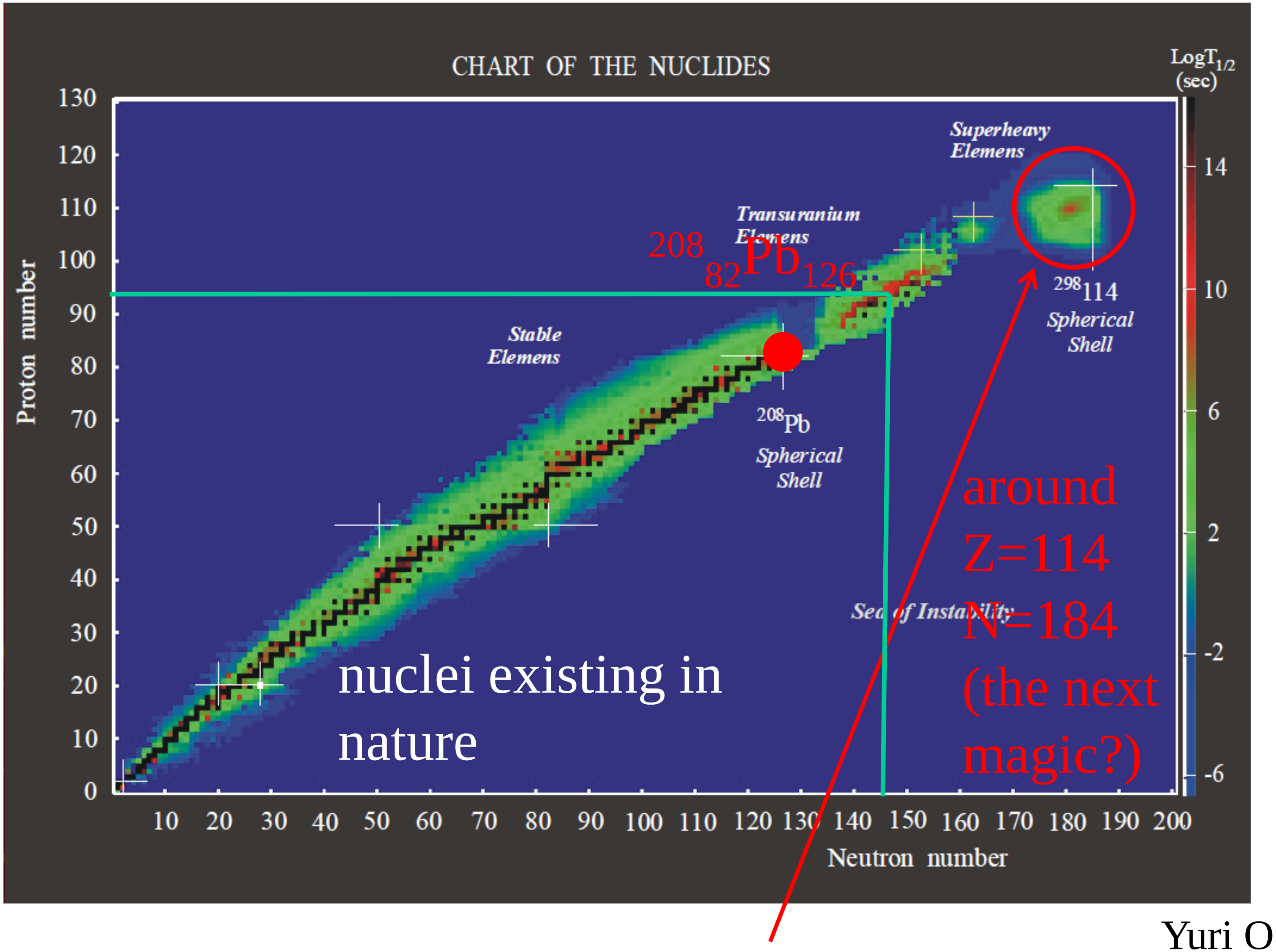
what determines the limit of existence of elements? (ii) atomic nucleus



Z. Patyk et al.,
NPA491('89) 267

QM shell effect (magic numbers) raises B_{fiss} and stabilizes a nucleus

Superheavy elements (the island of stability)



$^{208}_{82}\text{Pb}_{126}$

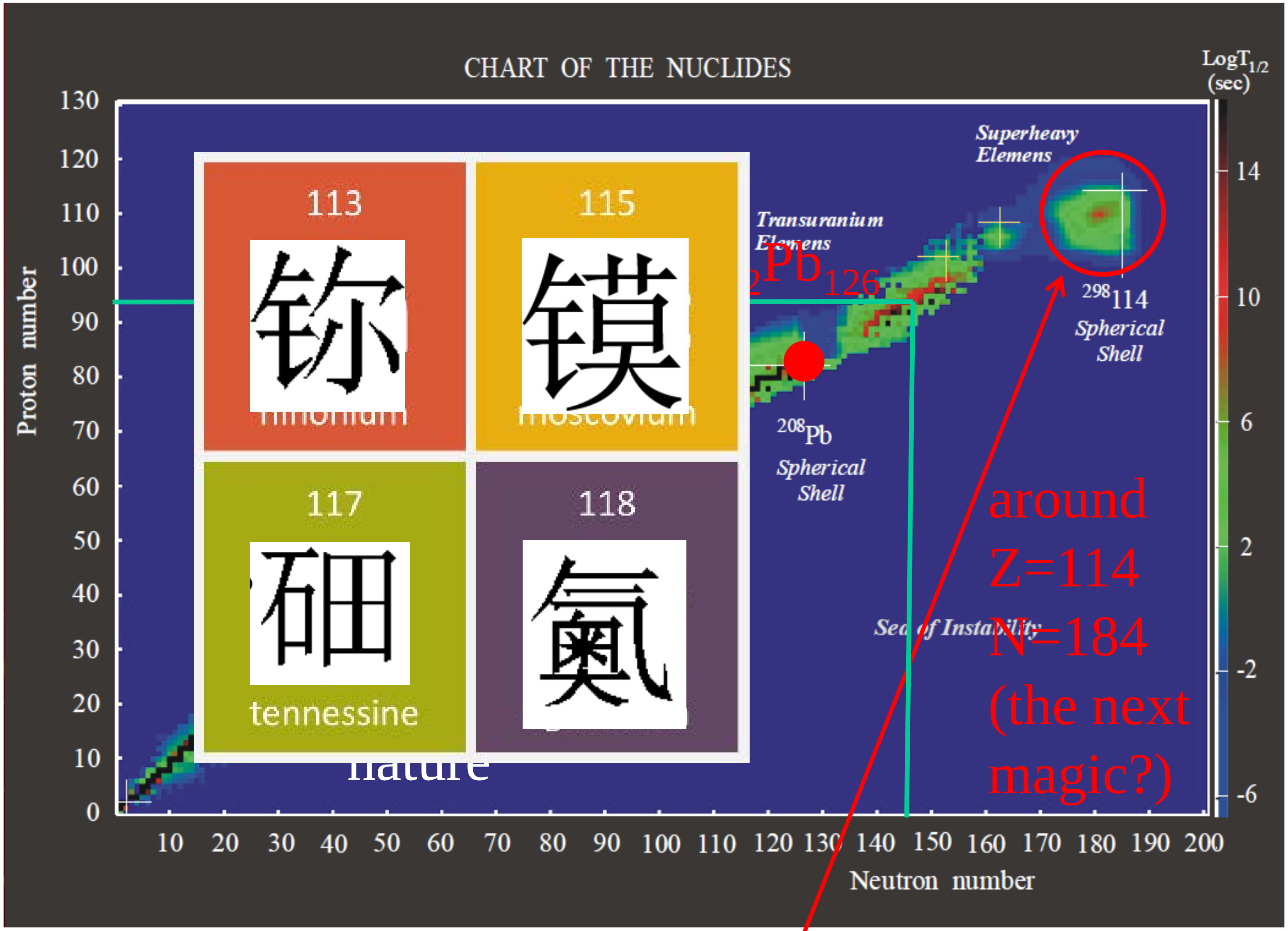
nuclei existing in nature

around Z=114 N=184 (the next magic?)

Yuri Oganessian

long-lived with 10^{3-5} years

Superheavy elements (the island of stability) 超重元素



around Z=114 N=184 (the next magic?)

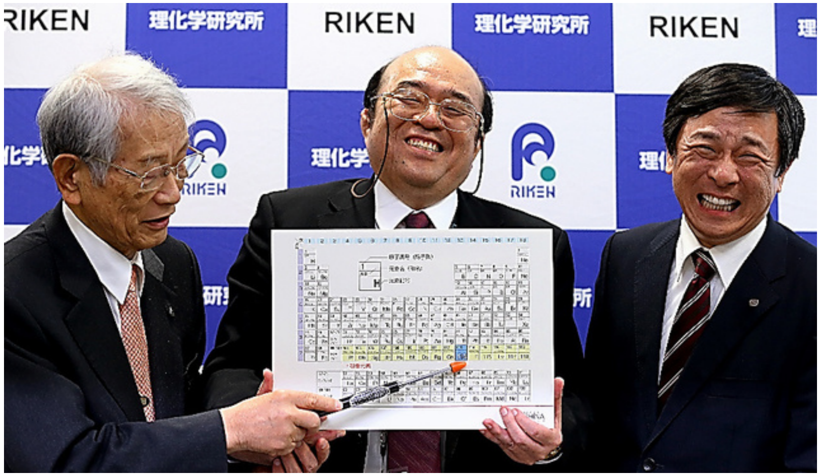
Yuri Oganessian

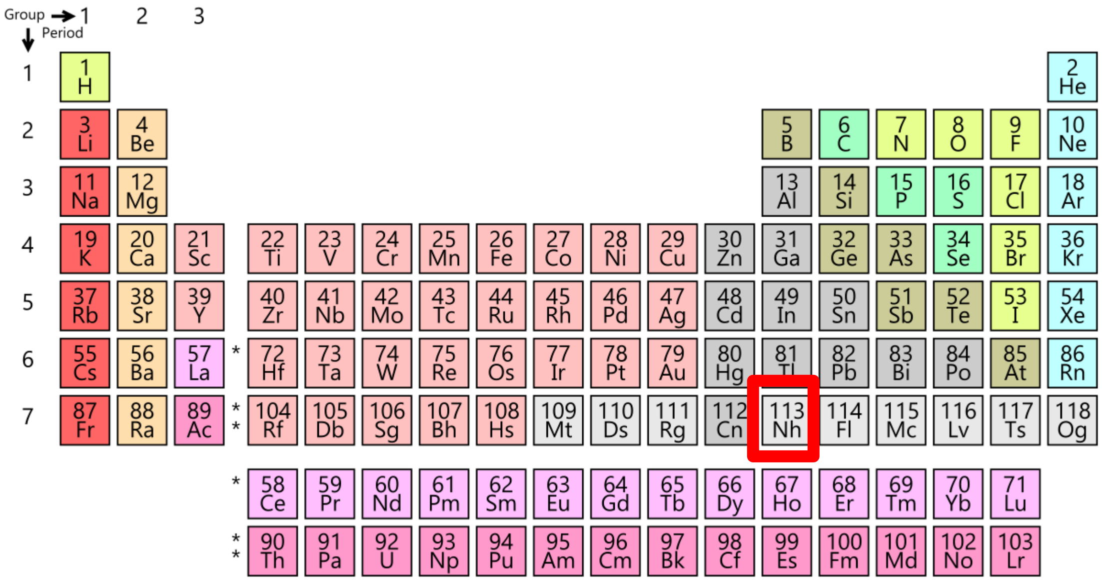
long-lived with $10^{3\text{-}5}$ years

Fusion reactions for SHE

the element 113: Nh

November, 2016





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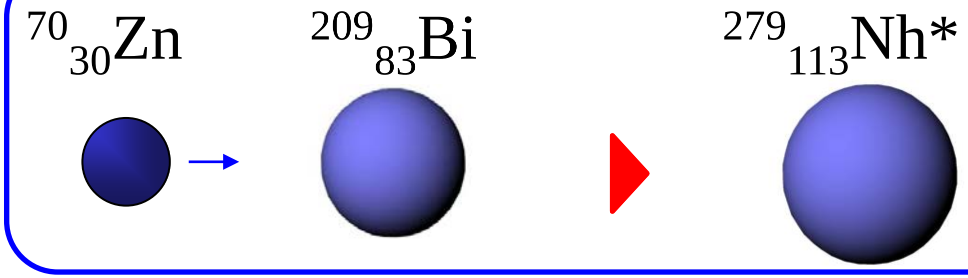
Wikipedia

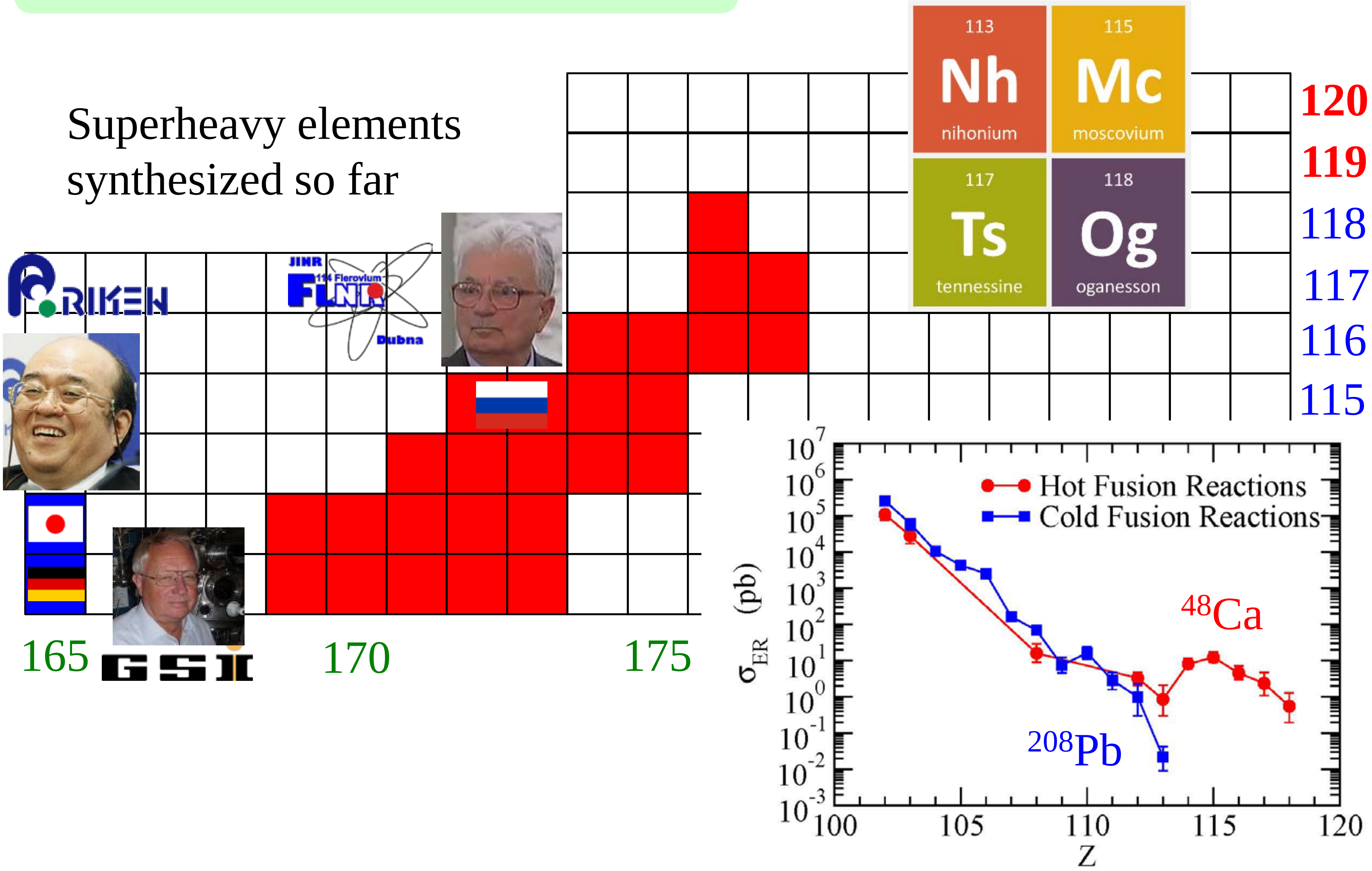


$^{70}_{30}$Zn $^{209}_{83}$Bi $^{279}_{113}$Nh*

Heavy-ion fusion reaction

Fusion for superheavy elements

Superheavy elements synthesized so far



Fusion for superheavy elements

Superheavy elements
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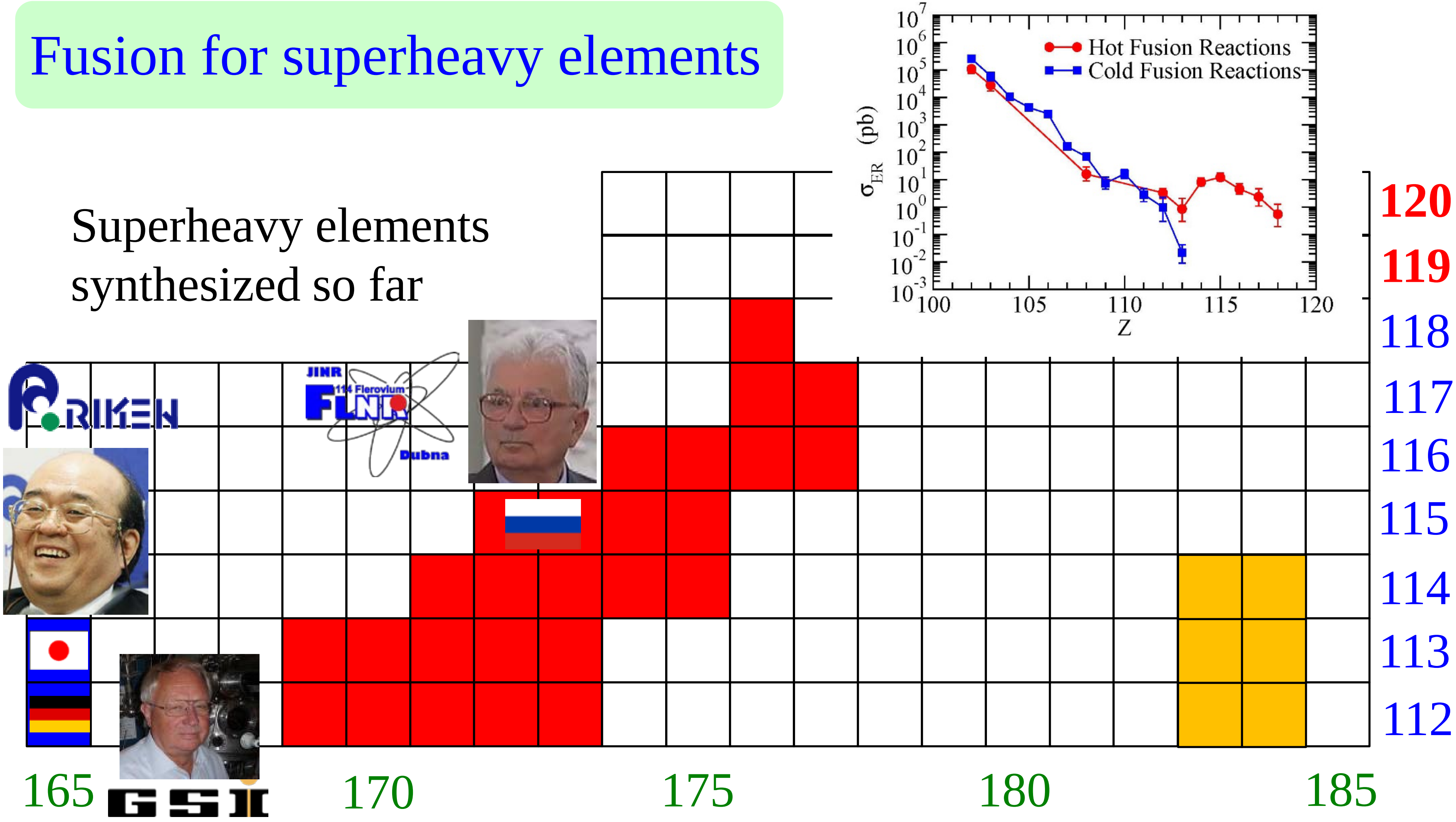
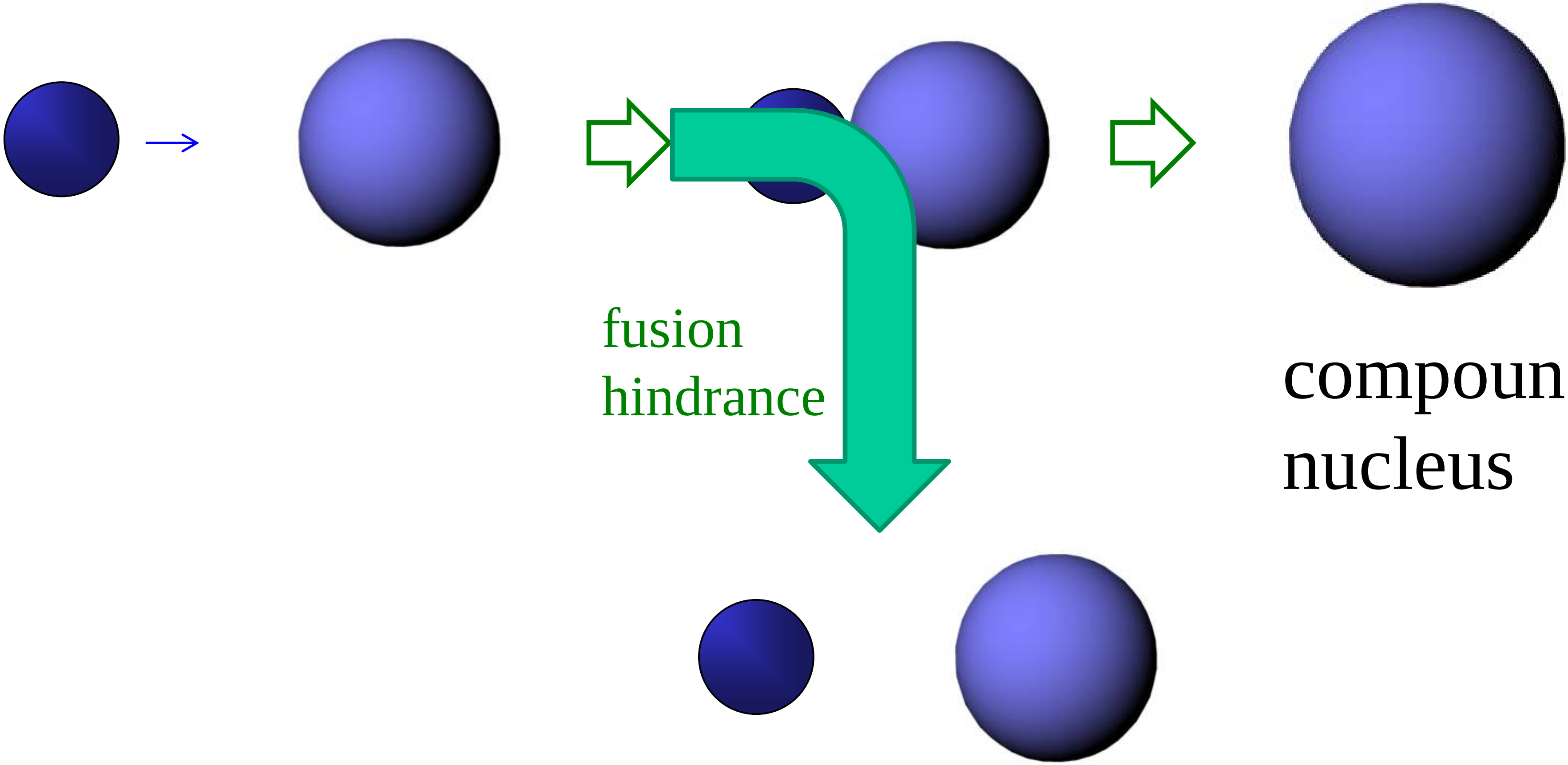


Fusion for SHE: fusion hindrance

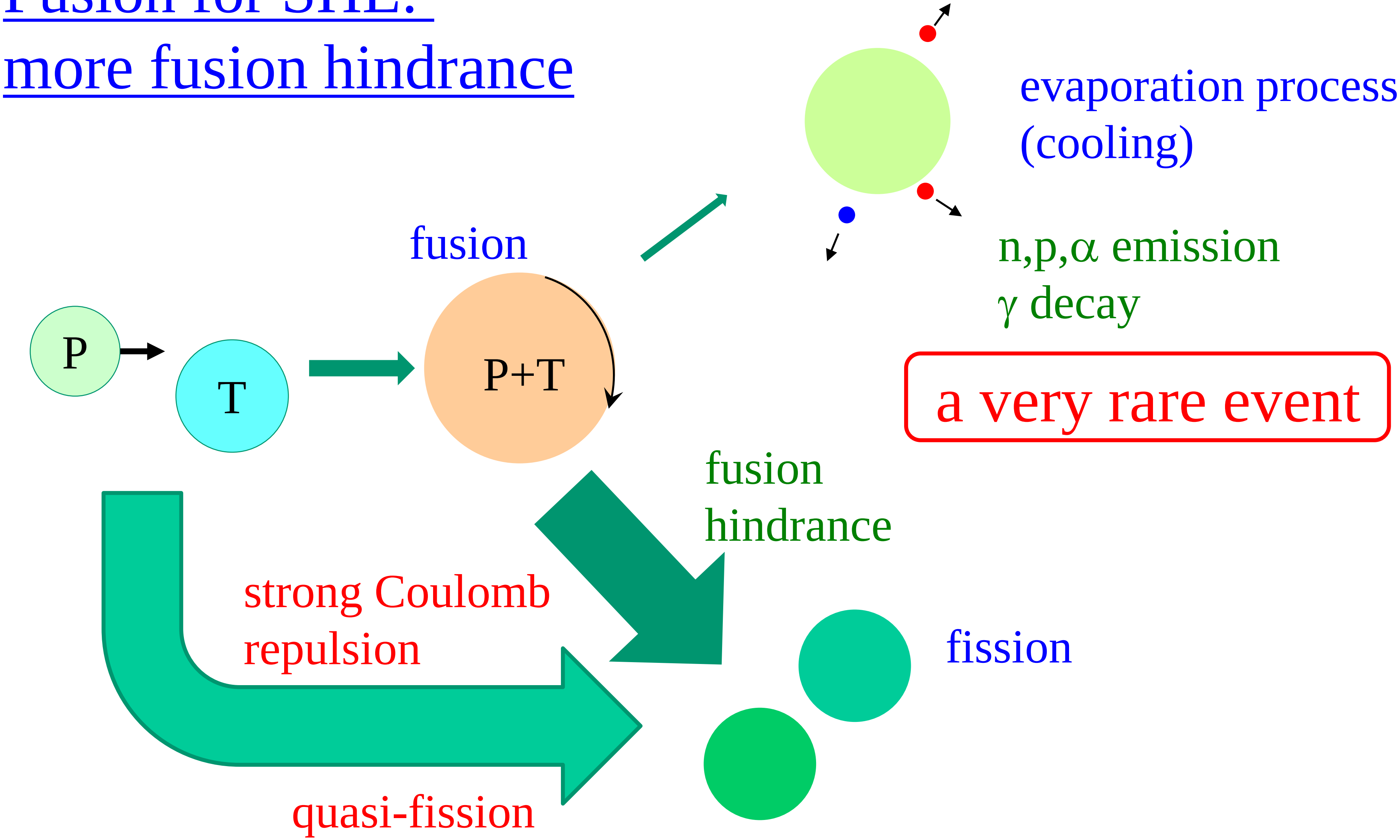


fusion hindrance

compound nucleus

strong Coulomb repulsion
→ re-separation

Fusion for SHE: more fusion hindrance



fusion

evaporation process
(cooling)

n,p,α emission
γ decay

a very rare event

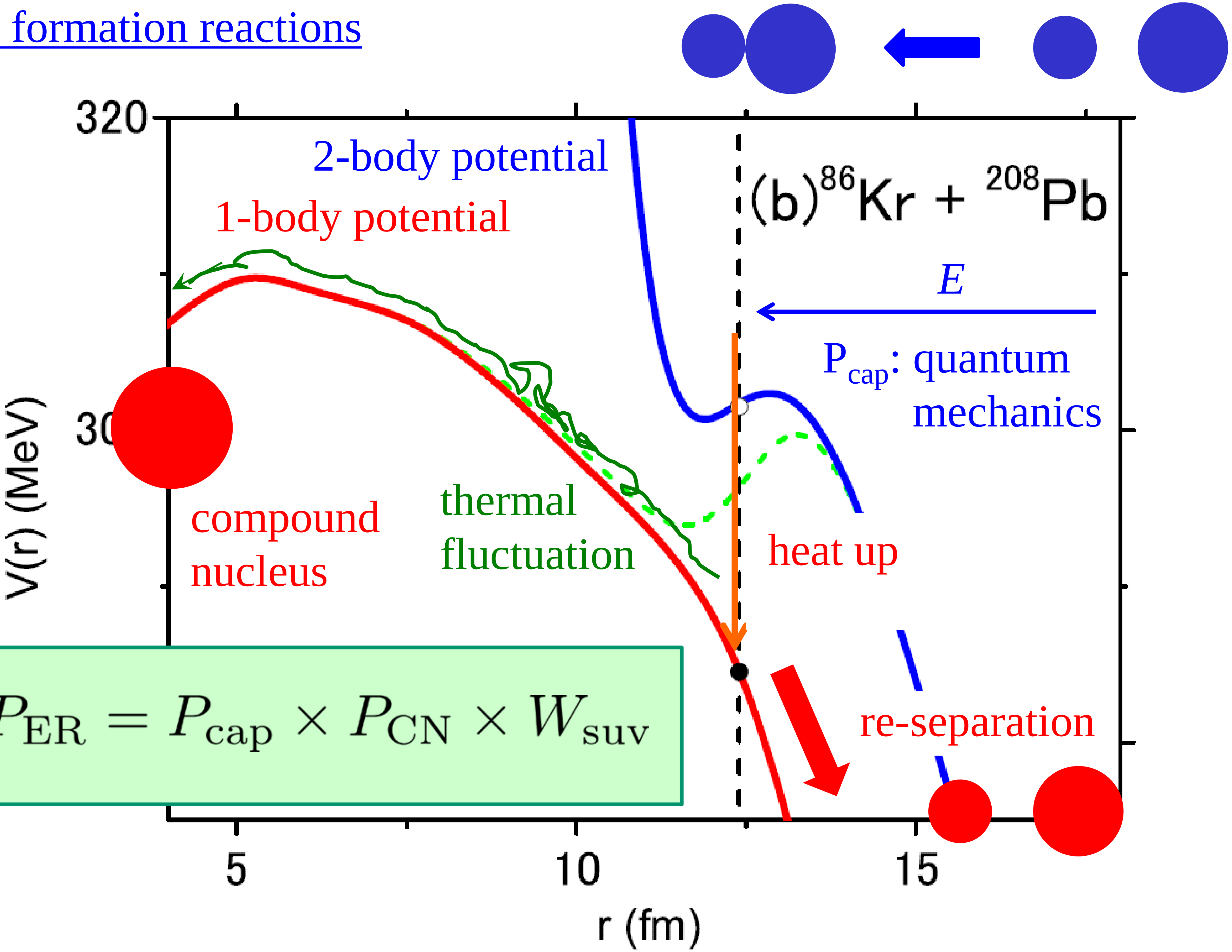
fusion
hindrance

strong Coulomb
repulsion

fission

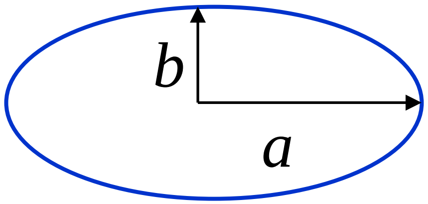
quasi-fission

SHE formation reactions



$$P_{\mathrm{ER}} = P_{\mathrm{cap}} \times P_{\mathrm{CN}} \times W_{\mathrm{suv}}$$

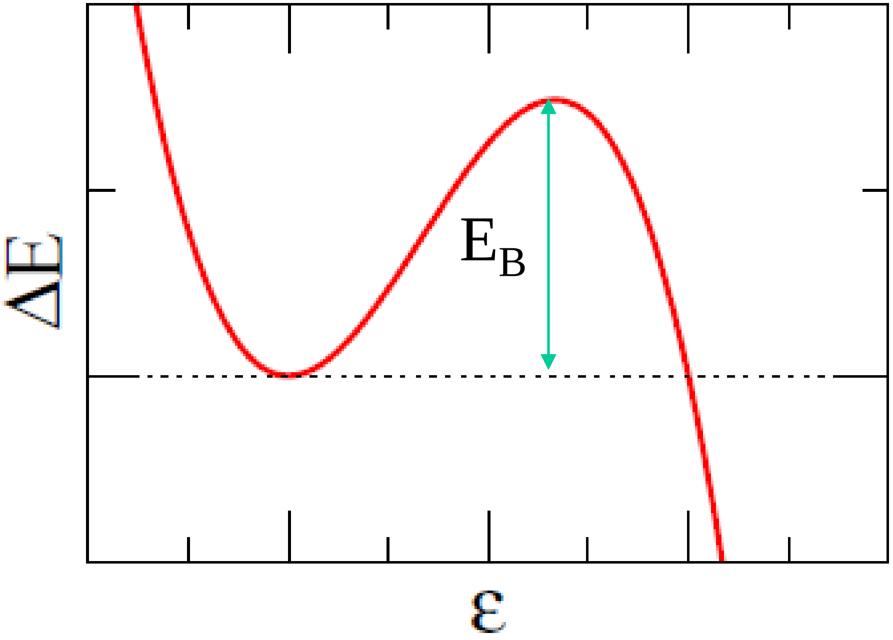
(note) fission barrier in the liquid drop model



$$\begin{aligned} a &= R\cdot(1+\epsilon) \\ b &= R\cdot(1+\epsilon)^{-1/2} \end{aligned}$$

$$ab^2 = R^3 = \text{constant}$$

$$\begin{aligned} \Delta E &= \Delta E_{\text{surf}} + \Delta E_{\text{coul}} \\ &= E_S^{(0)}\left\{\frac{2}{5}(1-x)\epsilon^2 - \frac{4}{105}(1+2x)\epsilon^3 + \cdots\right\} \end{aligned}$$

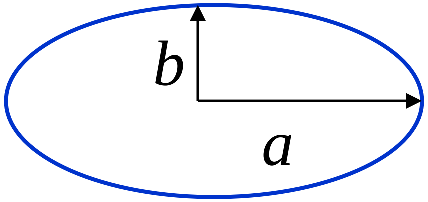


$$E_S^{(0)} = +a_S A^{2/3}$$

$$x \equiv \frac{E_C^{(0)}}{2E_S^{(0)}} = \frac{a_C}{2a_S}\cdot\frac{Z^2}{A} \sim \frac{1}{53.3}\cdot\frac{Z^2}{A}$$

$$E_C^{(0)} = a_C Z(Z-1)/A^{1/3}$$

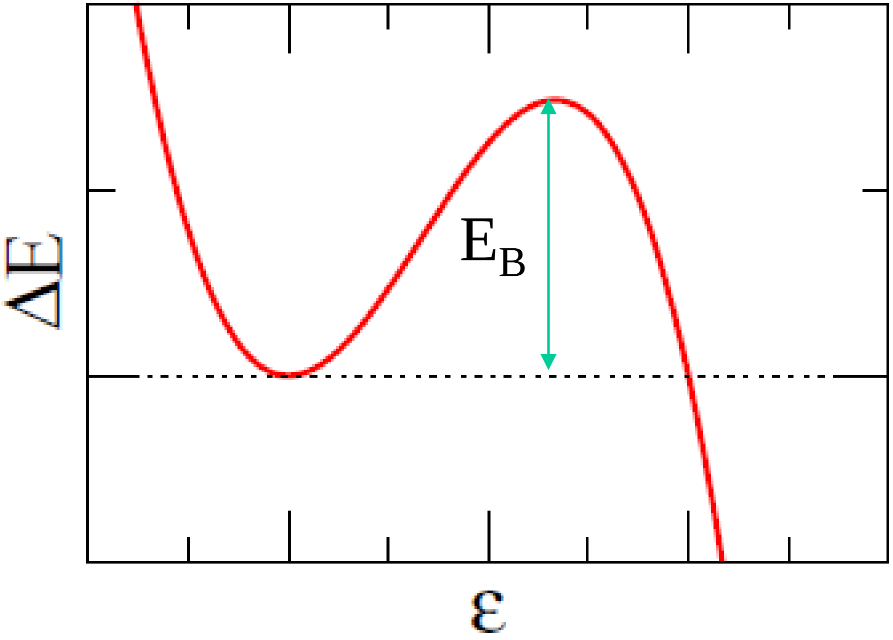
(note) fission barrier in the liquid drop model



$$a = R \cdot (1+\epsilon)$$
$$b = R \cdot (1+\epsilon)^{-1/2}$$

$$ab^2 = R^3 = \text{constant}$$

$$\begin{aligned} \Delta E &= \Delta E_{\mathrm{surf}} + \Delta E_{\mathrm{coul}} \\ &= E_S^{(0)} \left\{ \frac{2}{5}(1-x)\epsilon^2 - \frac{4}{105}(1+2x)\epsilon^3 + \cdots \right\} \end{aligned}$$

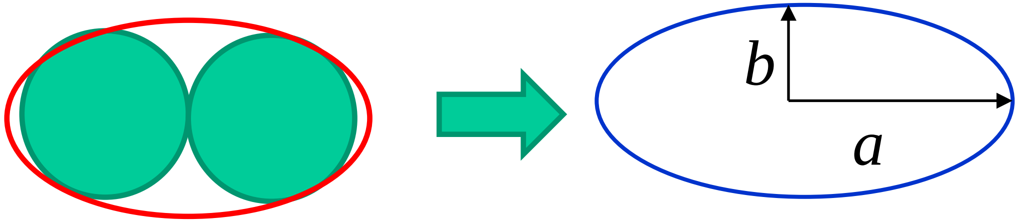


fission barrier:

$$\epsilon_B = \frac{21(1-x)}{3(1+2x)}$$

$$E_B = \frac{98}{15} \cdot \frac{(1-x)^3}{(1+2x)^2} \cdot E_S^{(0)}$$

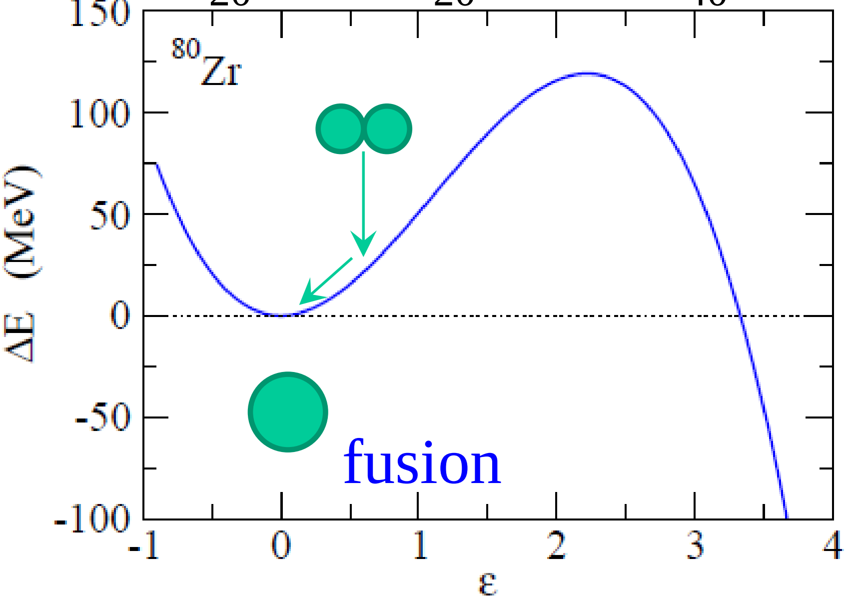
if two identical nuclei contact:



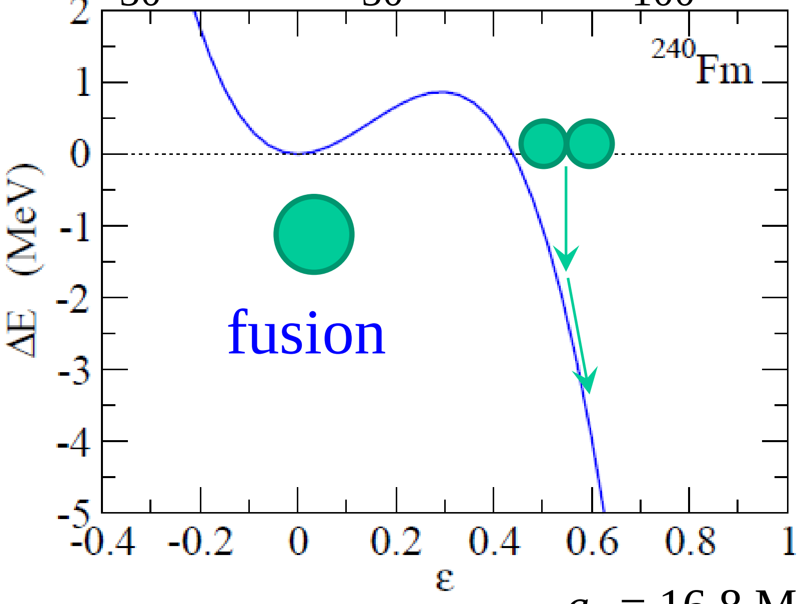
$$a = R_0 \cdot (1 + \epsilon)$$
$$b = R_0 \cdot (1 + \epsilon)^{-1/2}$$

$$\frac{a}{b} \sim \frac{2R}{R} = 2 \to \epsilon \sim 0.587$$

${}^{40}_{20}\mathrm{Ca} + {}^{40}_{20}\mathrm{Ca} \longrightarrow {}^{80}_{40}\mathrm{Zr}$



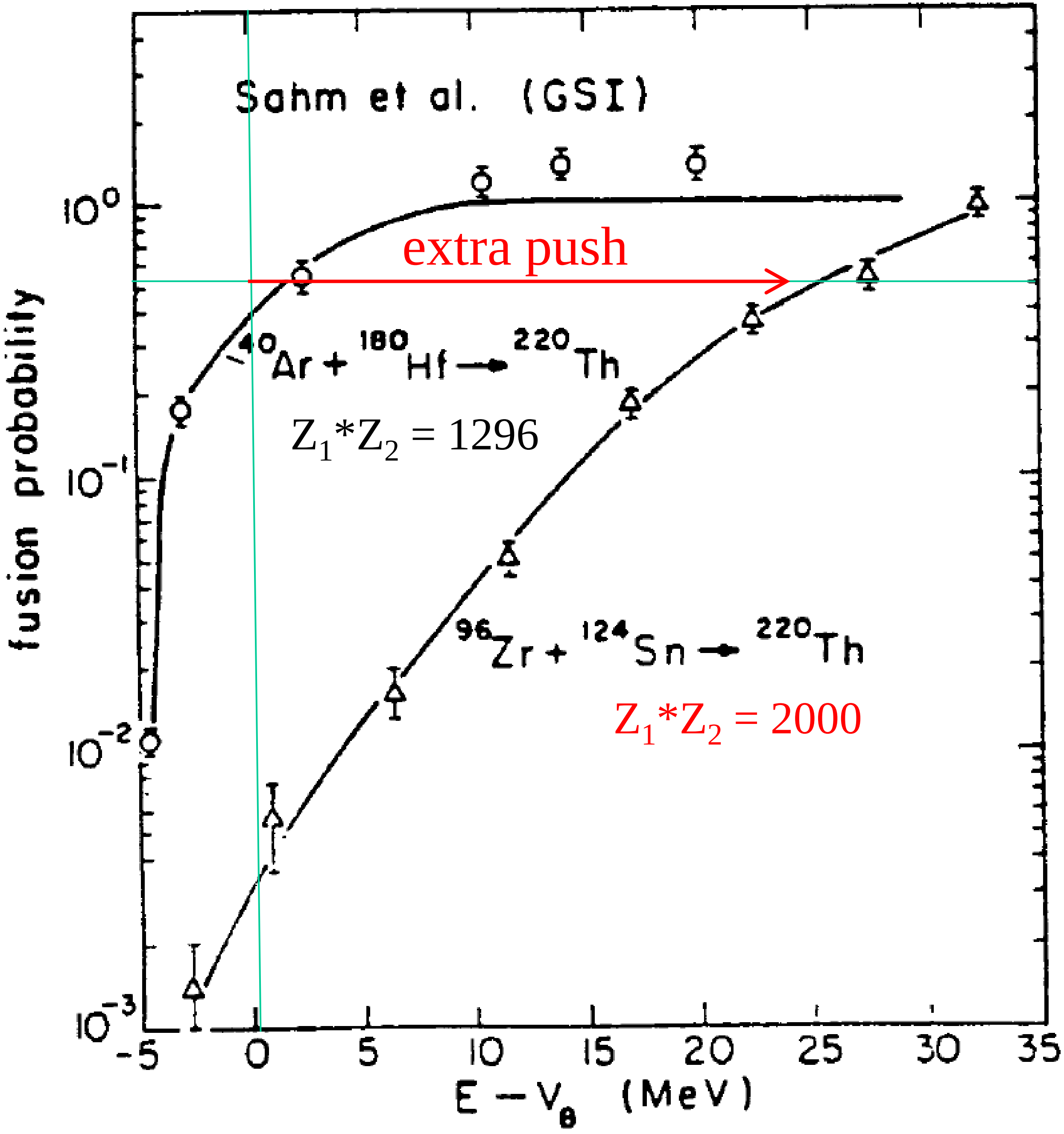
${}^{120}_{50}\mathrm{Sn} + {}^{120}_{50}\mathrm{Sn} \longrightarrow {}^{240}_{100}\mathrm{Fm}$



a_S = 16.8 MeV

a_C = 0.72 MeV

threshold: $Z_1 * Z_2$ = 1600 ~ 1800

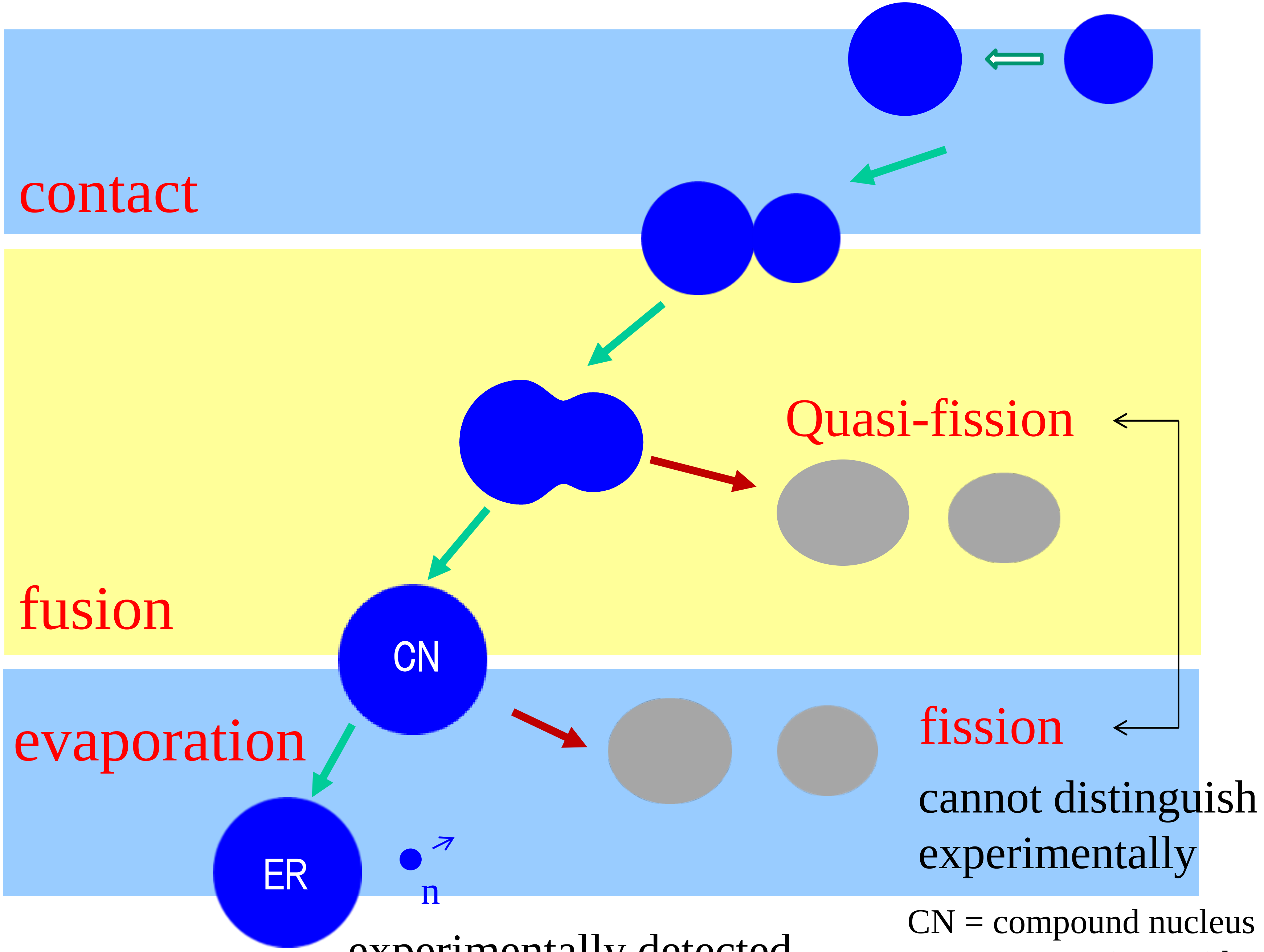


extra push

$Z_1 * Z_2 = 1296$

$Z_1 * Z_2 = 2000$

C.-C. Sahm et al.,
Z. Phys. A319(‘84)113



contact

fusion

evaporation

Quasi-fission

fission

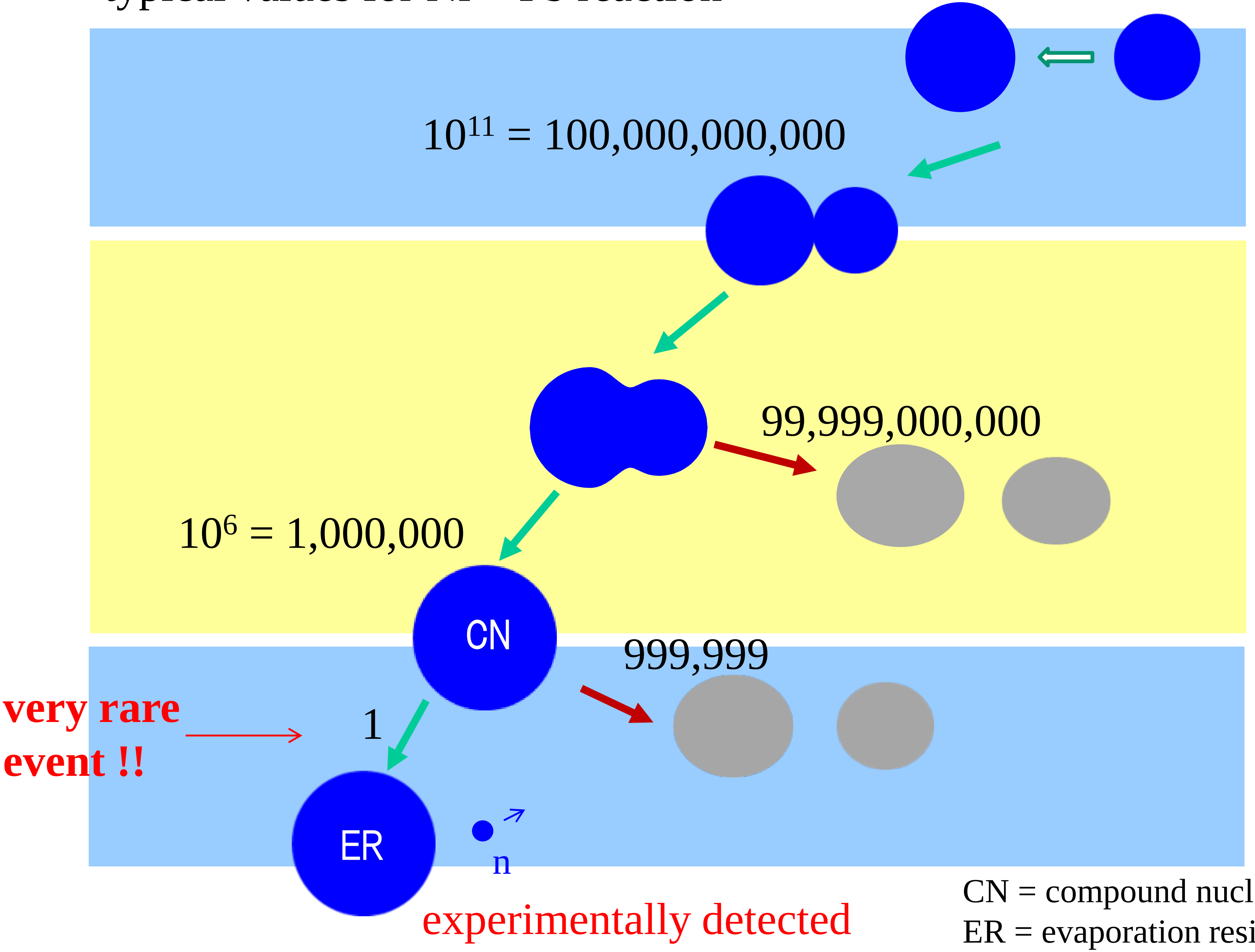
cannot distinguish experimentally

experimentally detected

CN = compound nucleus

ER = evaporation residue

typical values for Ni + Pb reaction



10^{11} = 100,000,000,000

99,999,000,000

10^{6} = 1,000,000

CN

999,999

very rare event !!

1

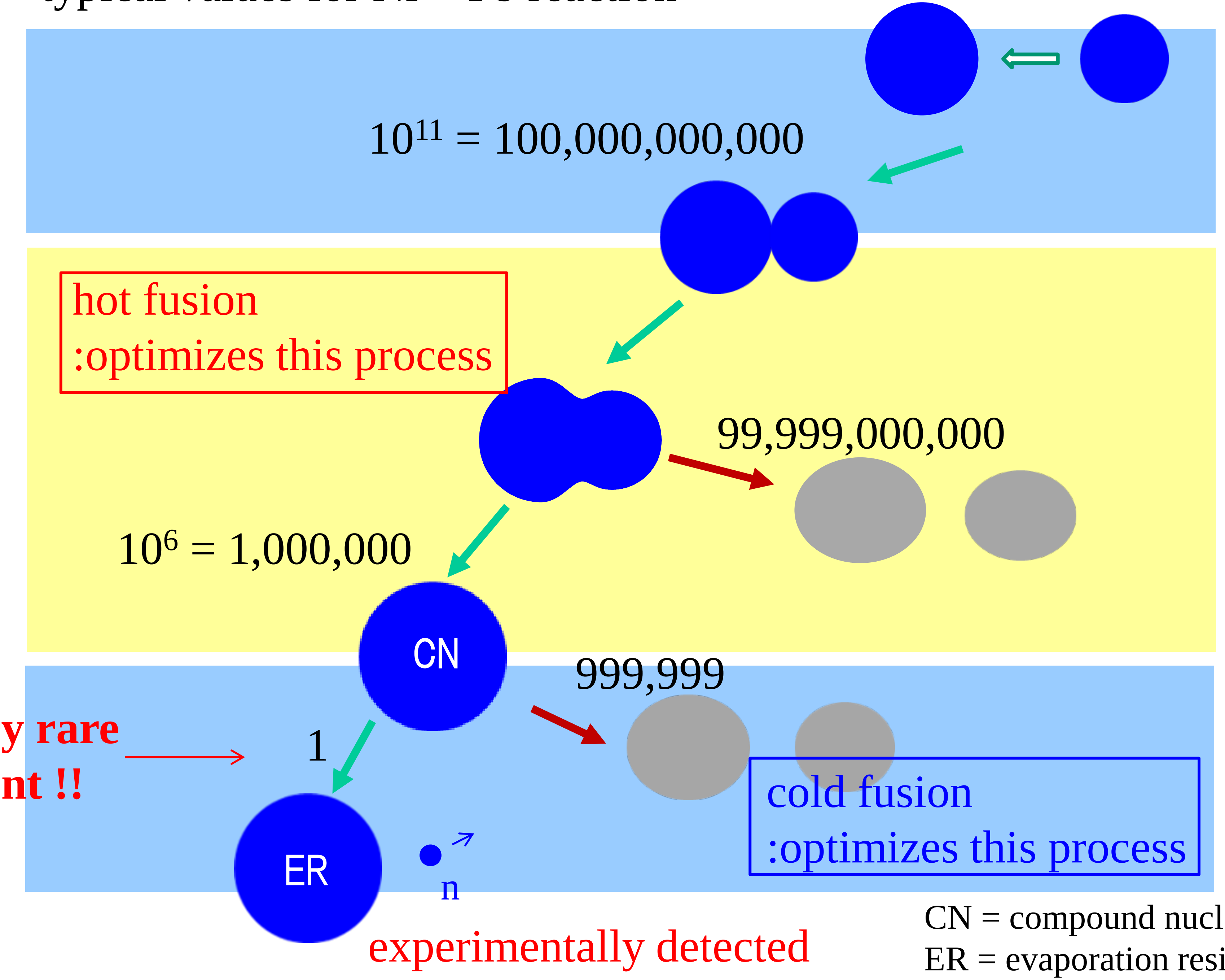
ER

n

experimentally detected

CN = compound nucleus
ER = evaporation residue

typical values for Ni + Pb reaction



10^{11} = 100,000,000,000

hot fusion
:optimizes this process

99,999,000,000

10^{6} = 1,000,000

999,999

very rare event !!

1

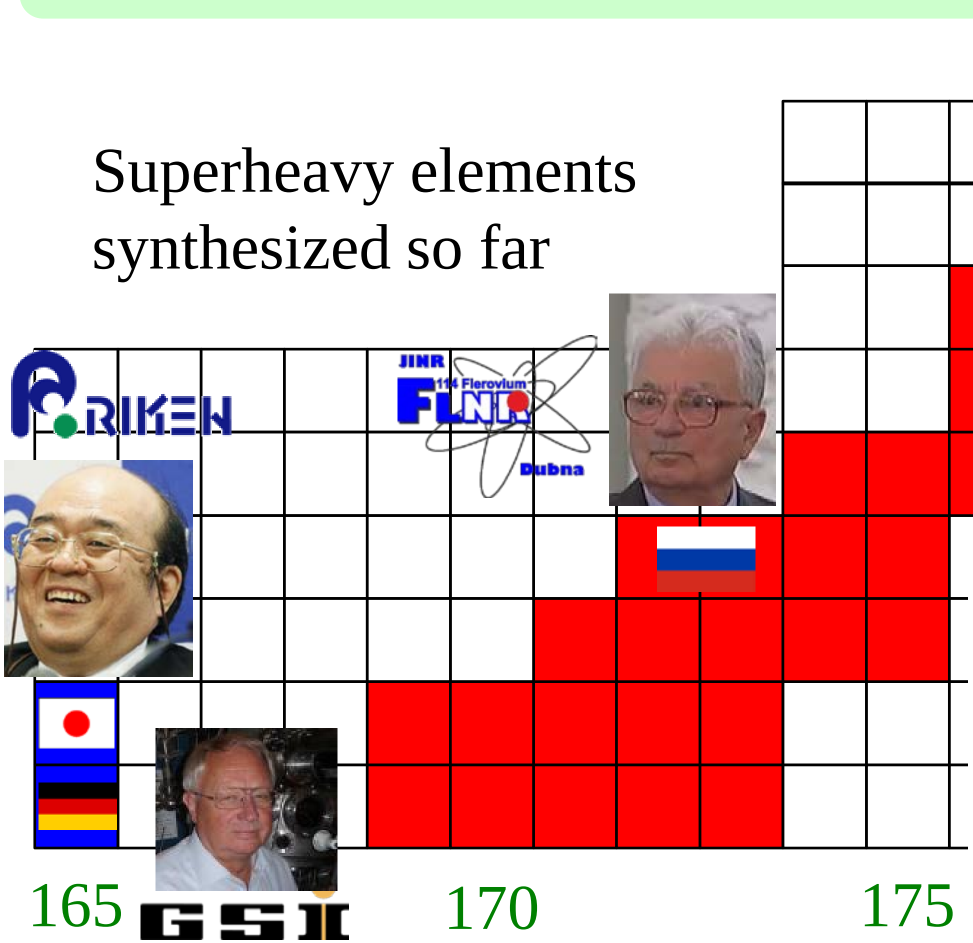
cold fusion
:optimizes this process

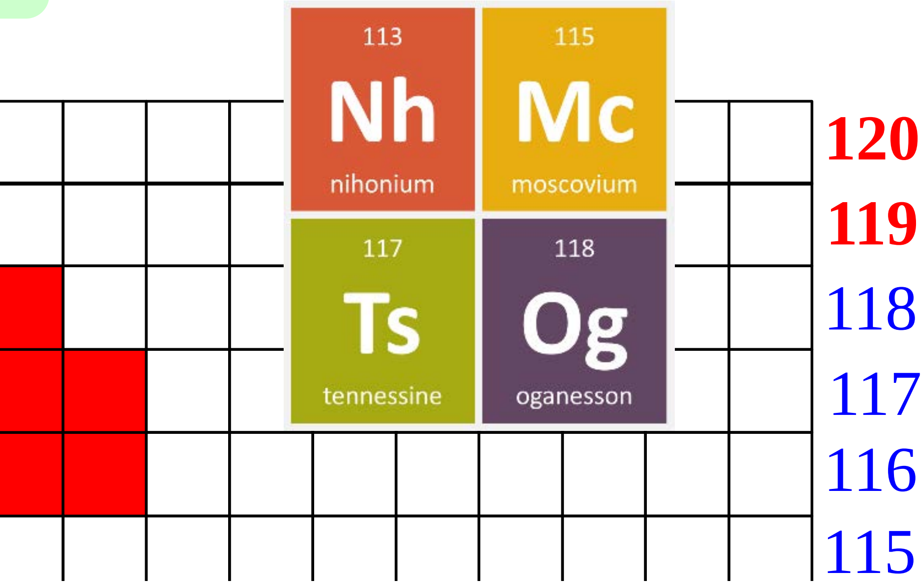
experimentally detected

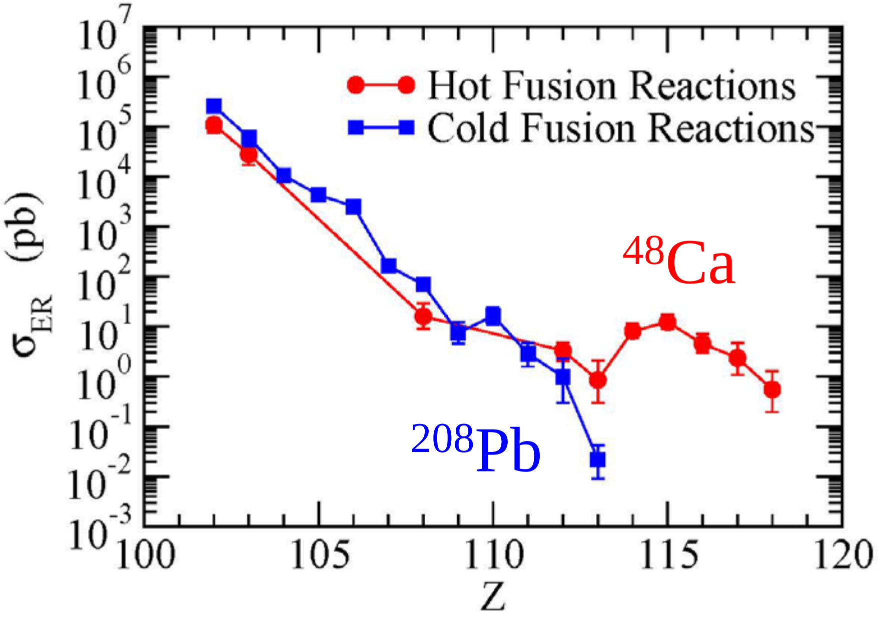
CN = compound nucleus
ER = evaporation residue

Fusion for superheavy elements

Superheavy elements synthesized so far







Theoretical challenges

formation of SHE: very rare

→ a large theoretical uncertainty

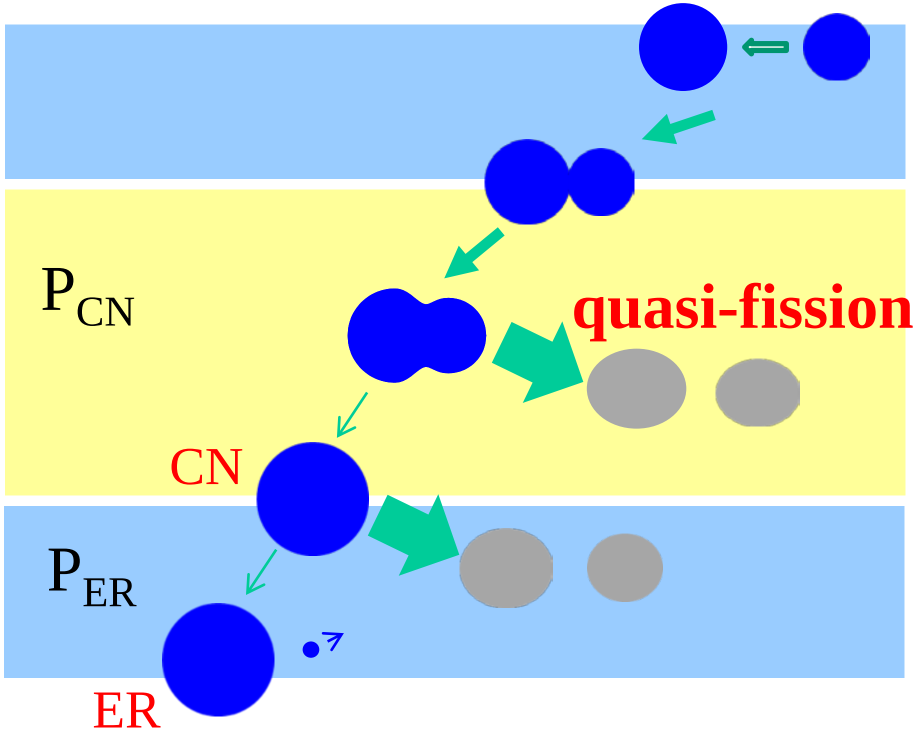
$$P_{\rm ER} = P_{\rm cap} \cdot P_{\rm CN} \cdot W_{\rm suv}$$

✓no exp. data for $P_{\rm CN}$
✓exp. data: $P_{\rm ER}$ only

CN＝複合核、ER=蒸発残留核

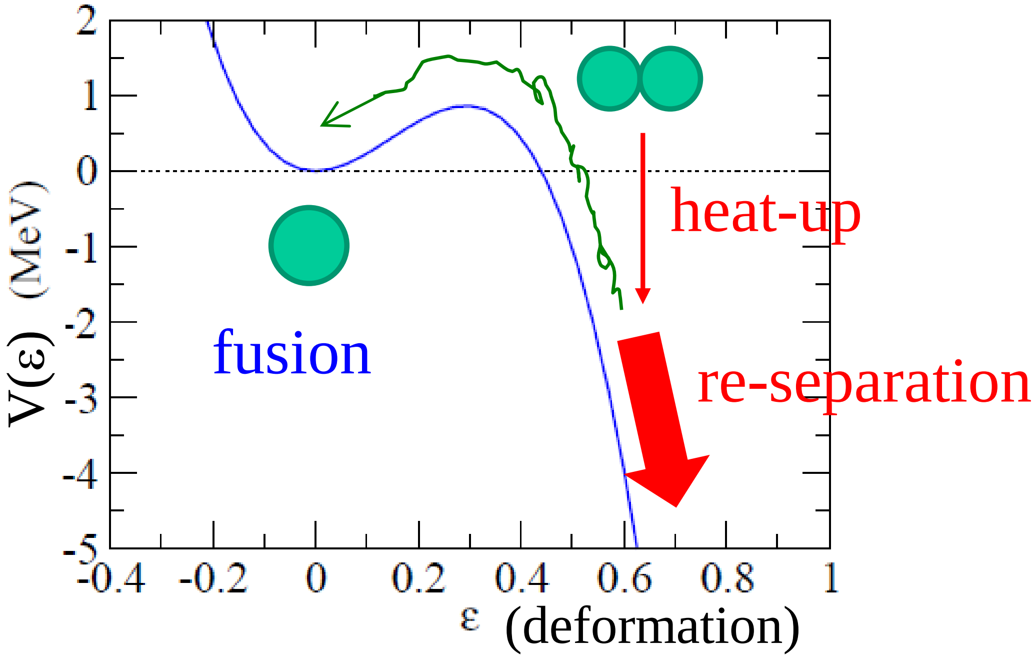
theoretical challenges:
to reduce the uncertainties and
make reliable predictions

fusion hindrance



➡ Physics of open quantum systems
量子開放系

Langevin approach



thermal fluctuation

⟶ Langevin method
(Brownian method)

classical Langevin equation

$$m\frac{d^2q}{dt^2} = -\frac{dV(q)}{dq} \underline{- \gamma\frac{dq}{dt}} \; \underline{+ R(t)}$$

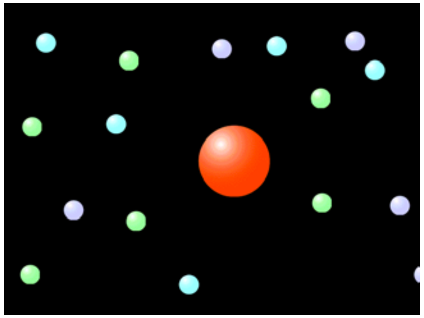
friction random interaction → $\langle R(t) \rangle = 0$

classical: $\boxed{\langle R(t)R(t') \rangle = 2D\,\delta(t-t')}$

$D = \gamma T$ (Einstein relation)

(white noise; no memory)

Brownian motion



interaction of a Brownian
particle with atoms

classical Langevin equation

$$m\frac{d^2q}{dt^2} = -\frac{dV(q)}{dq} \underline{-\gamma\frac{dq}{dt}} + \underline{R(t)}$$

friction random interaction → $\langle R(t)\rangle = 0$

classical: $\boxed{\langle R(t)R(t')\rangle = 2D\,\delta(t-t')}$

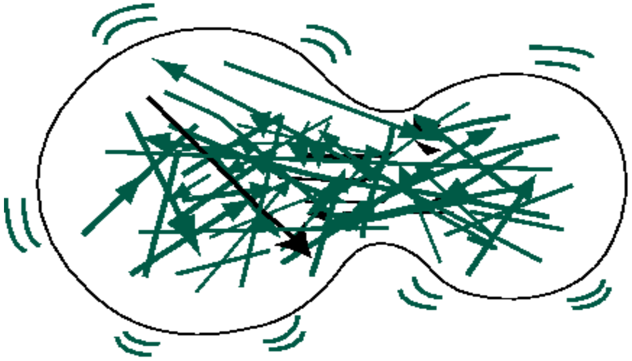
$D = \gamma T$ (Einstein relation)

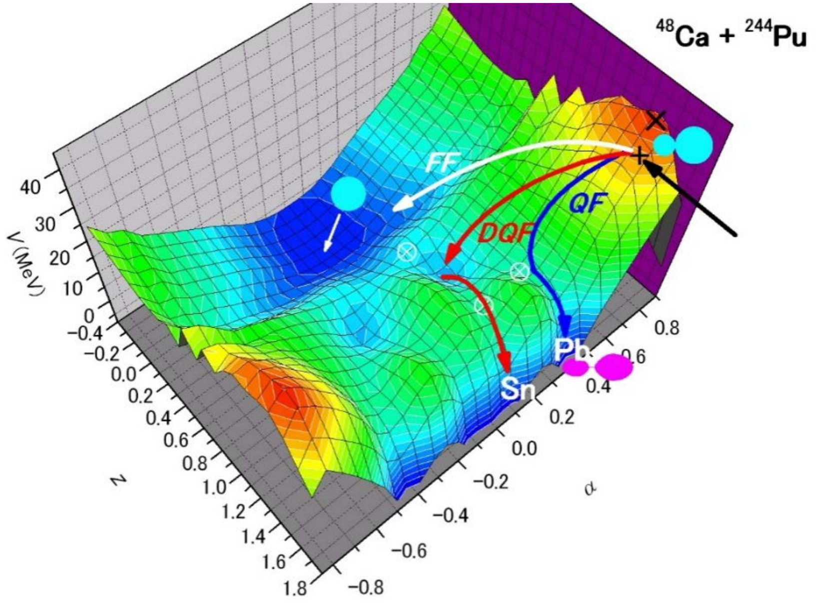
(white noise; no memory)

nuclear reactions:

q = the relative distance etc.

"atoms" = nucleonic d.o.f





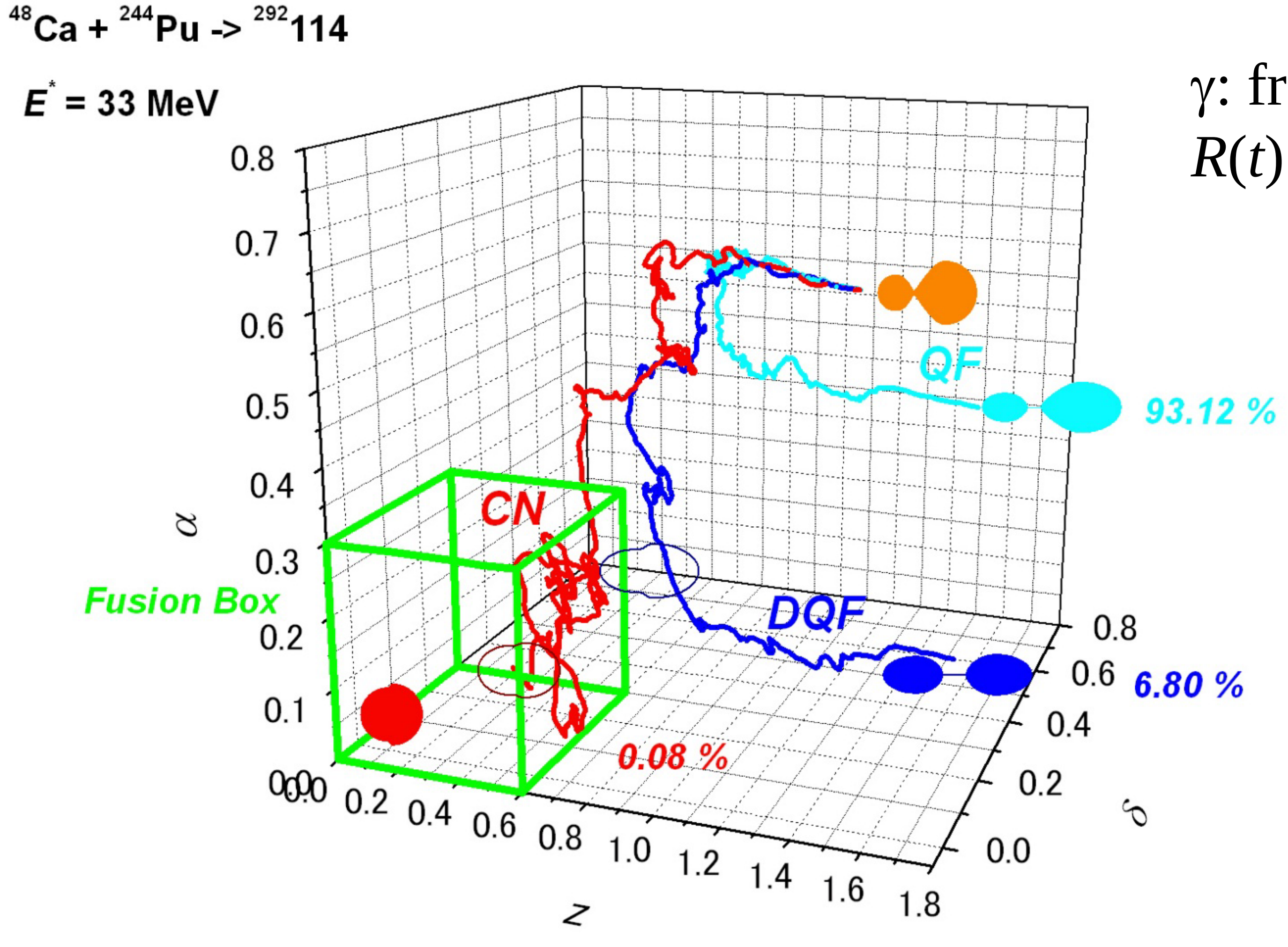
Theory: Lagenvin approach

multi-dimensional extension of:

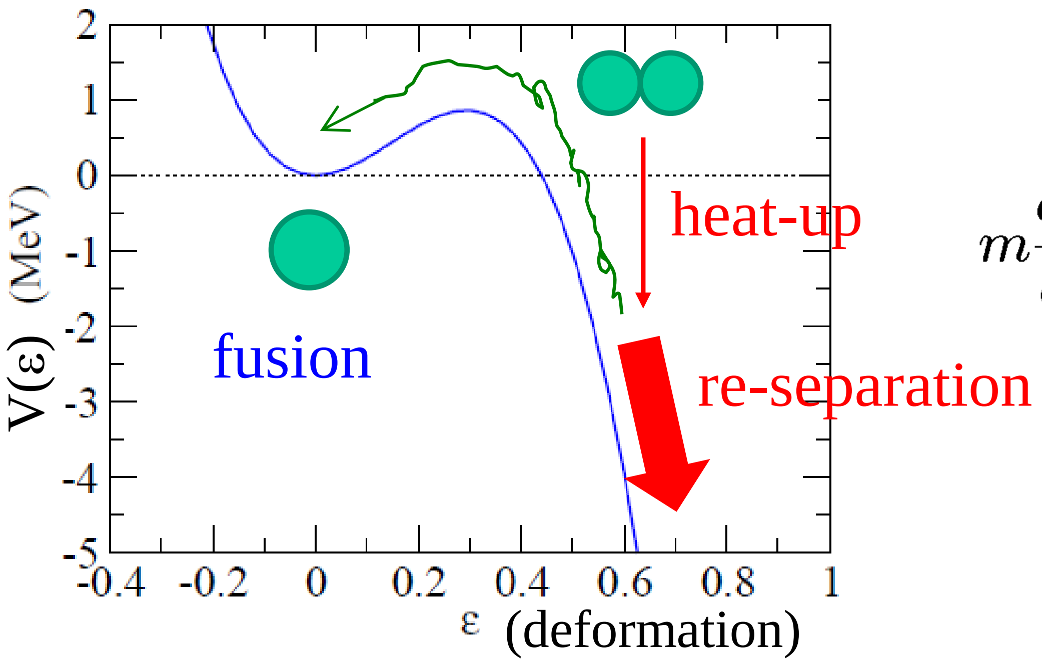
$$m\frac{d^2q}{dt^2} = -\frac{dV(q)}{dq} - \gamma\frac{dq}{dt} + R(t)$$

γ: friction coefficient

$R(t)$: random force



Langevin approach



$$m\frac{d^2q}{dt^2} = -\frac{dV(q)}{dq} - \gamma\frac{dq}{dt} + R(t)$$

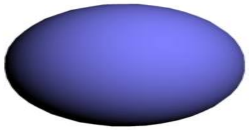
Theoretical issues

- ✓how to thermaize? mechanisms?
- ✓is thermal equilibrium OK?
- ✓Is Markovian approximation OK?
- ✓quantum effects?
- ✓quantal-to-classical transitions (decoherence)?

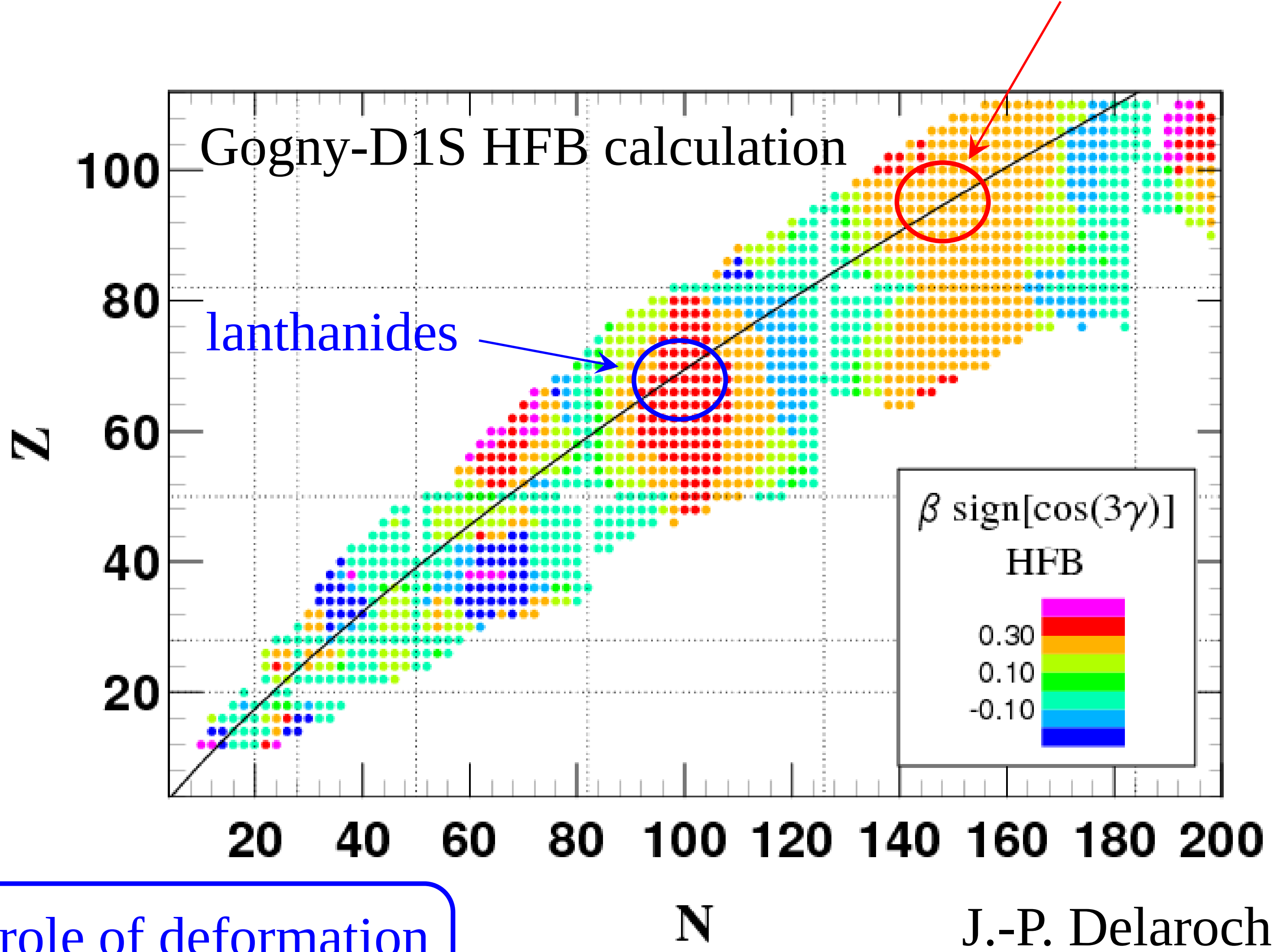
⇨ microscopic models?

⇨ open quantum systems

hot fusion: Nuclear Deformation



hot fusion: ^{48}Ca + deformed target



actinides

lanthanides

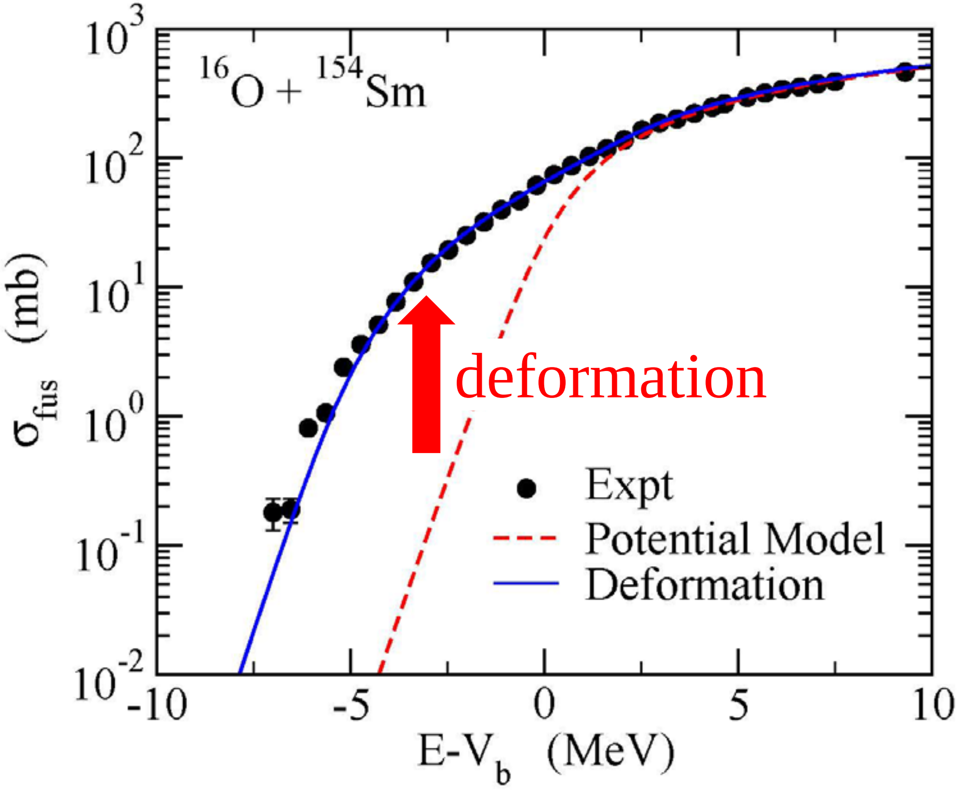
J.-P. Delaroche et al.,
PRC81 ('10) 014303

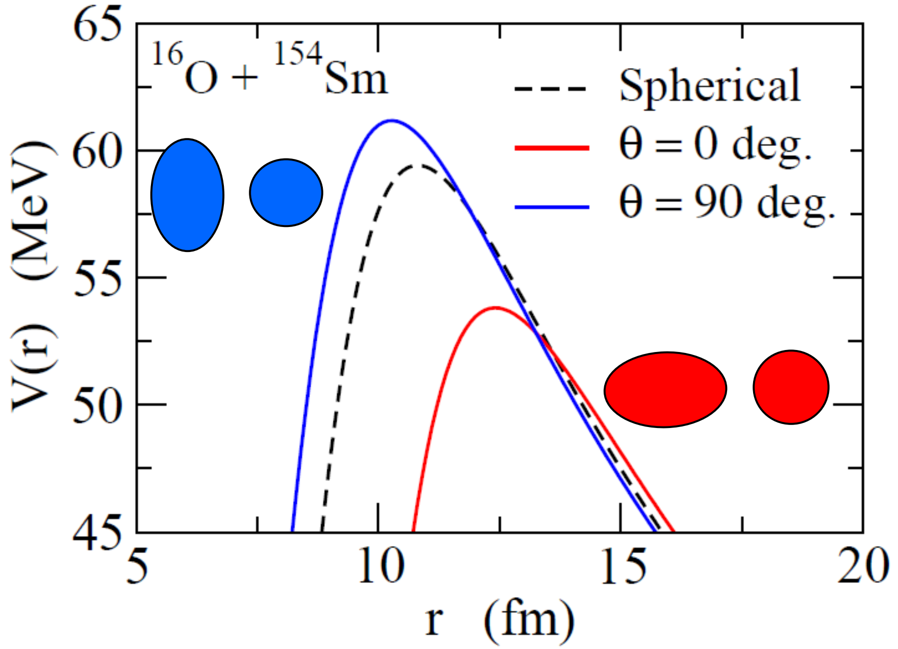
the role of deformation
in heavy-ion reactions?

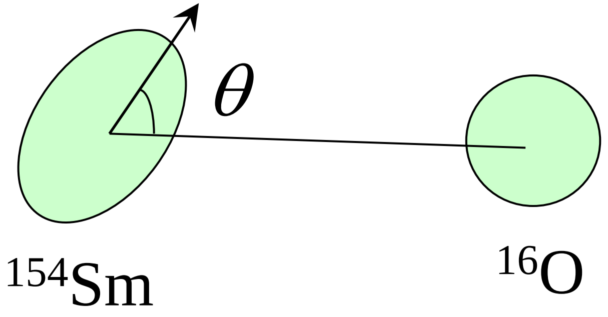
Nuclear deformation and barrier distribution

Nuclear deformation → a large sub-barrier enhancement of fusion cross sections

^{16}O+^{154}Sm

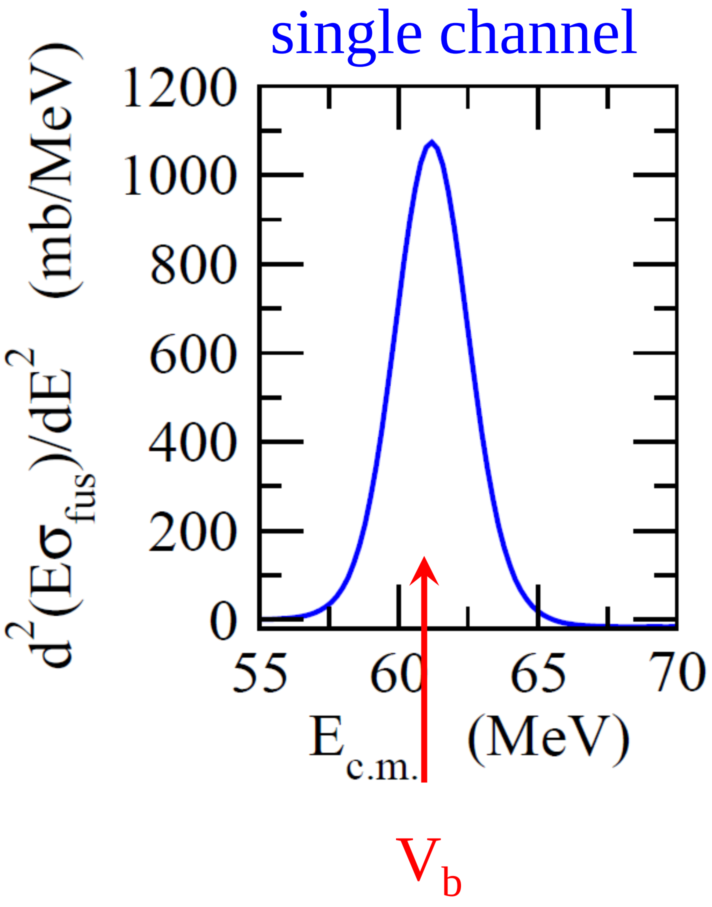






Fusion barrier distribution [Rowley, Satchler, Stelson, PLB254('91)]

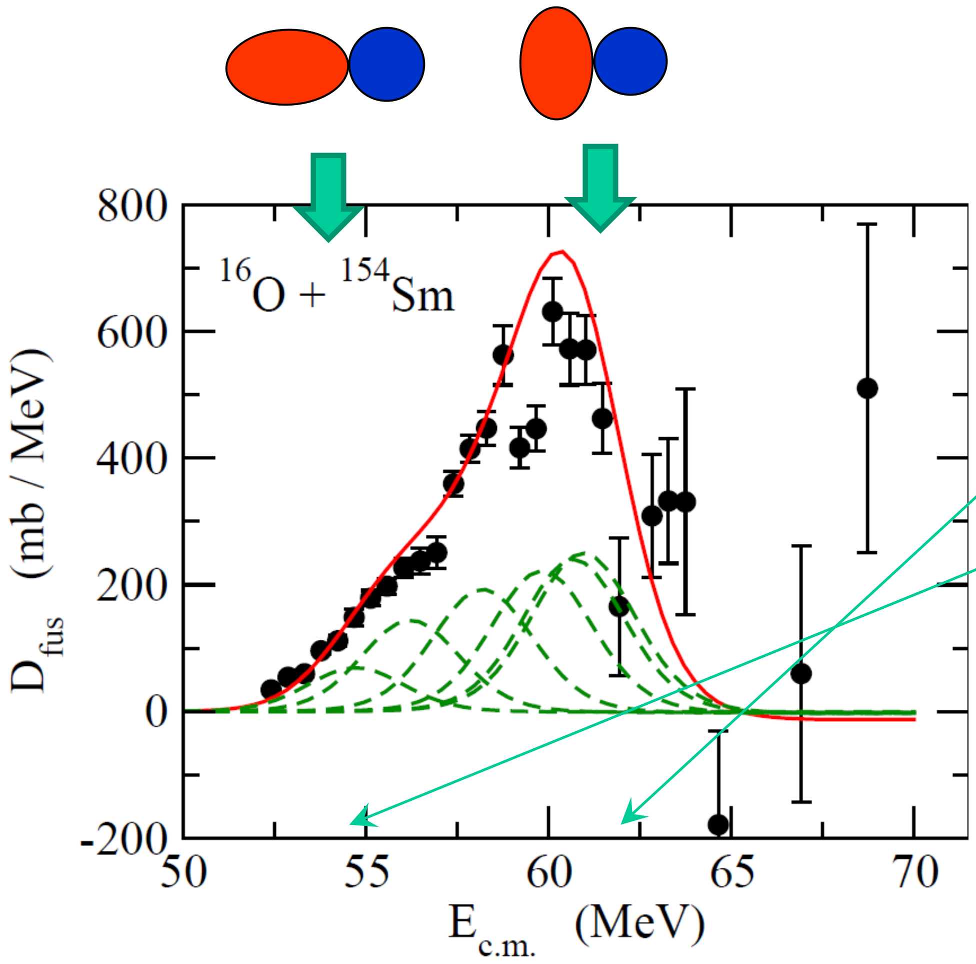
$$\boxed{D_{\text{fus}}(E) = \frac{d^2(E\sigma_{\text{fus}})}{dE^2}} \propto \frac{dP_{l=0}}{dE}$$

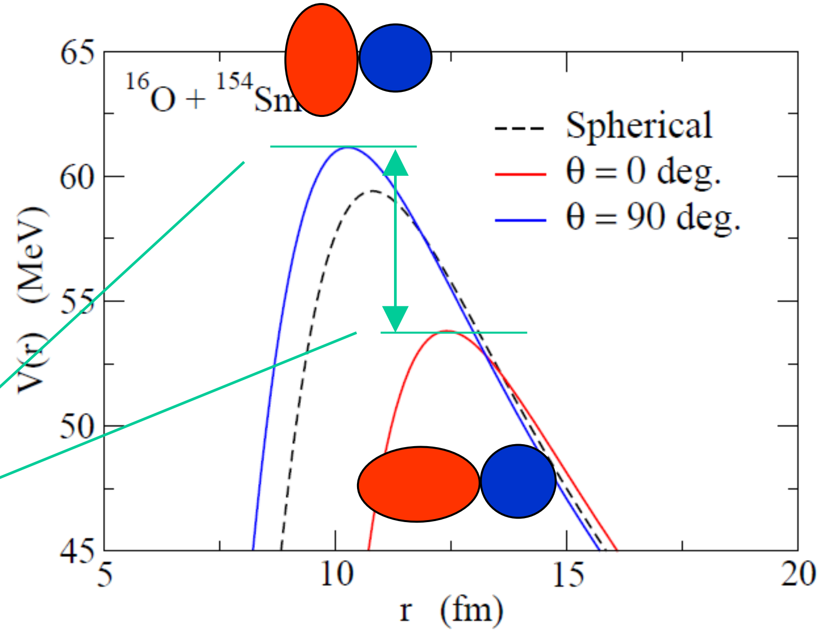


K.H., N. Takigawa, PTP128 ('12) 1061

✓ Fusion barrier distribution (Rowley, Satchler, Stelson, PLB254('91))

$$D_{\text{fus}}(E) = \frac{d^2(E\sigma_{\text{fus}})}{dE^2}$$



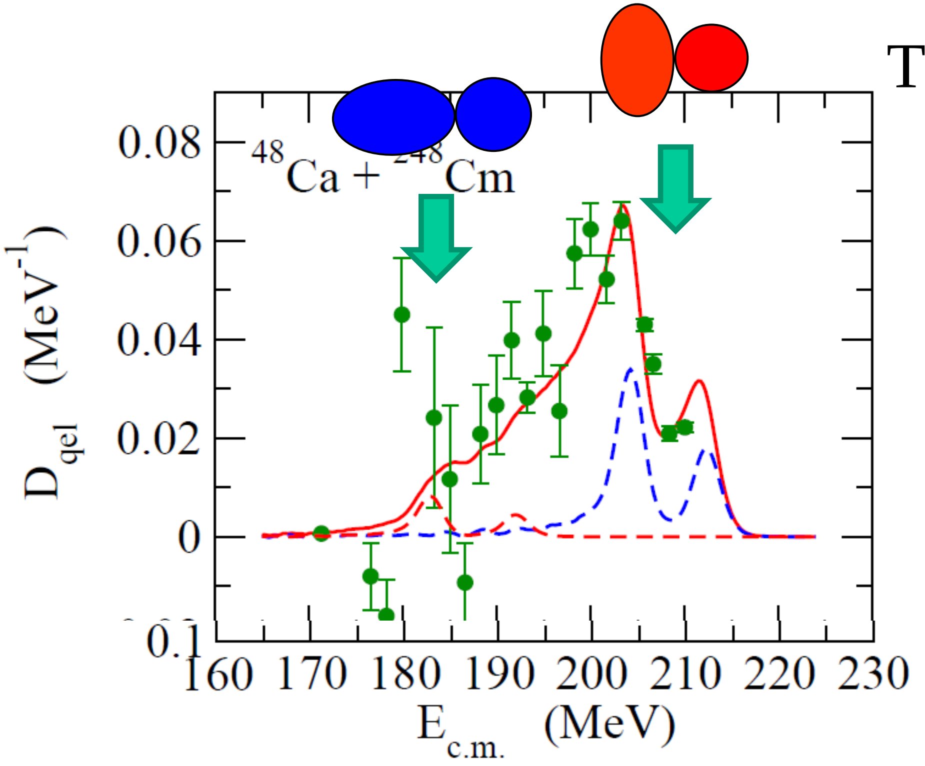


Data: J.R. Leigh et al.,
PRC52 ('95) 3151

can be used to identify
the side/tip collisions

Application to hot fusion reactions

$^{48}\text{Ca} + {}^{248}\text{Cm} \rightarrow {}^{296}_{116}\text{Lv}^*$

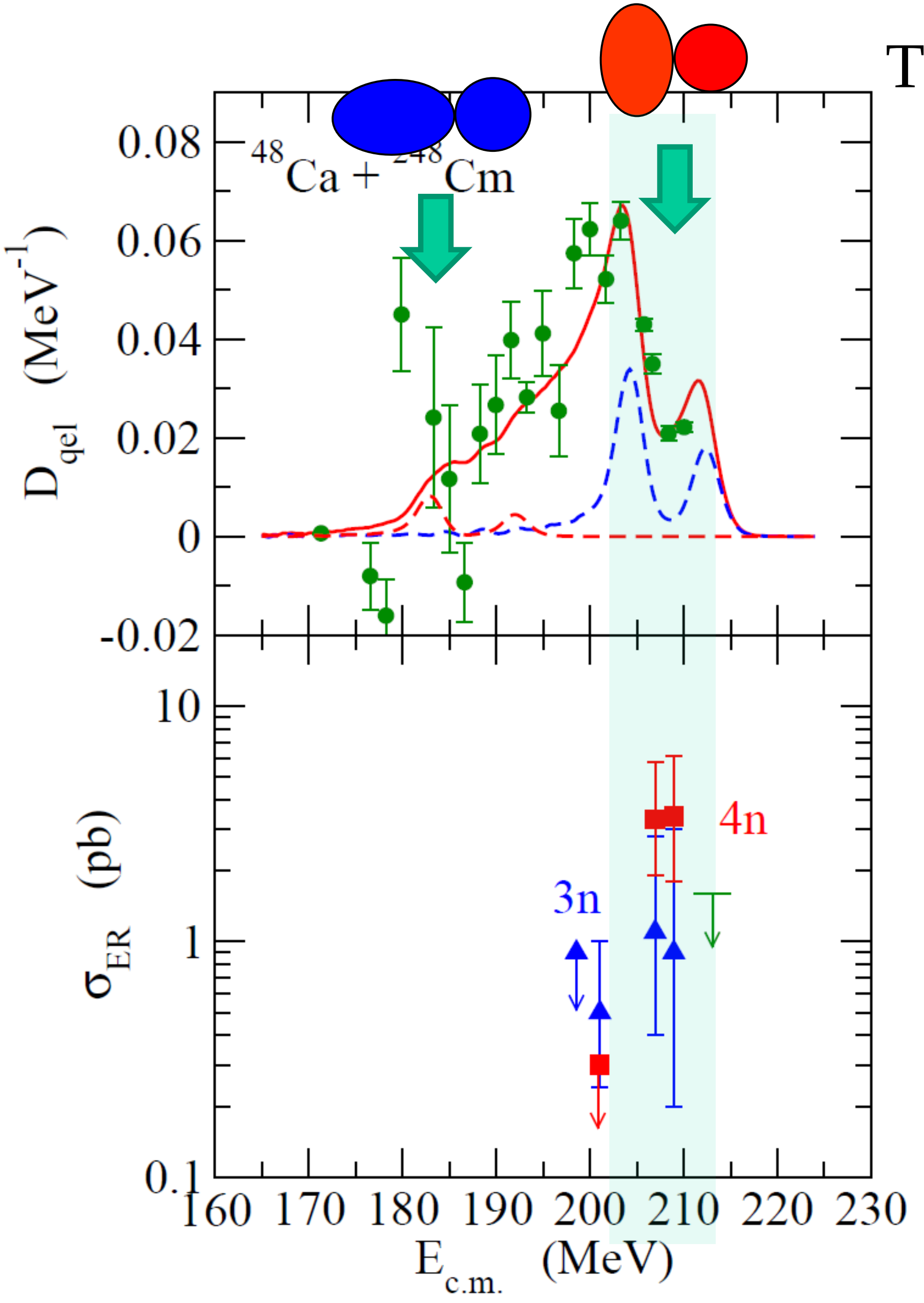


T. Tanaka,..., K.H., et al.,
JPSJ 87 ('18) 014201
PRL124 ('20) 052502

capture barrier distribution

Application to hot fusion reactions

$^{48}\text{Ca} + {}^{248}\text{Cm} \rightarrow {}^{296}_{116}\text{Lv}^*$

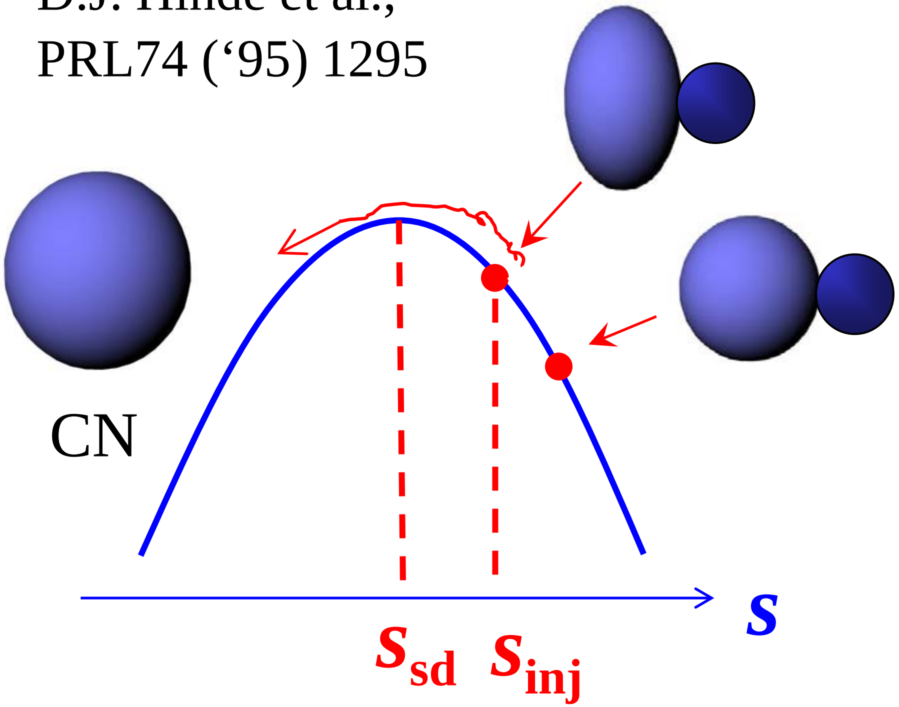


T. Tanaka,..., K.H., et al.,
JPSJ 87 ('18) 014201
PRL124 ('20) 052502

capture barrier distribution

cf. notion of compactness:

D.J. Hinde et al.,
PRL74 ('95) 1295



Application to hot fusion reactions

$^{48}\mathrm{Ca} + {}^{248}\mathrm{Cm} \longrightarrow {}^{296}_{116}\mathrm{Lv}^{*}$

T. Tanaka,..., K.H., et al.,
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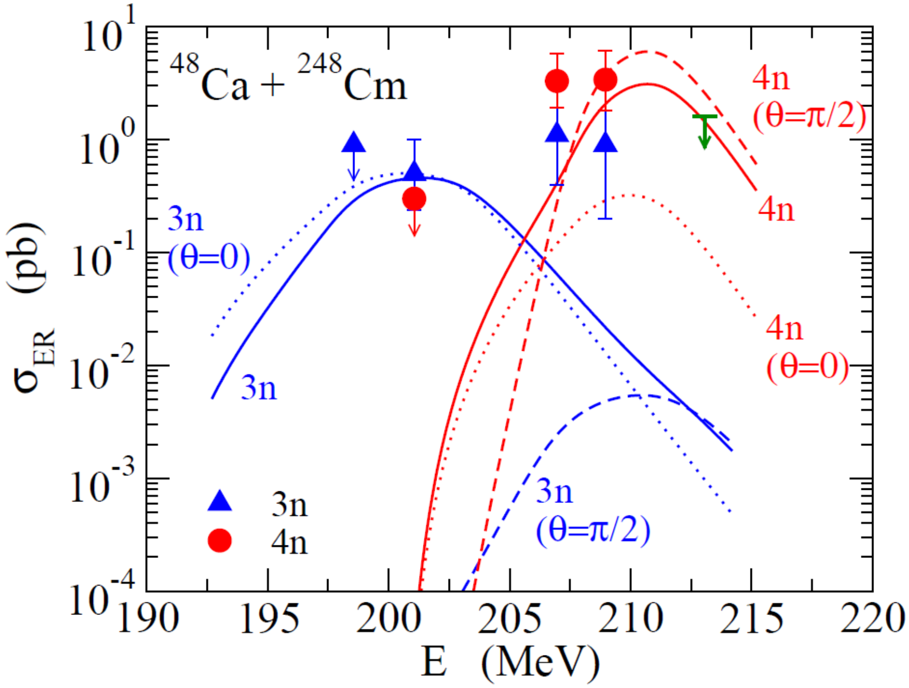
PRL124 ('20) 052502

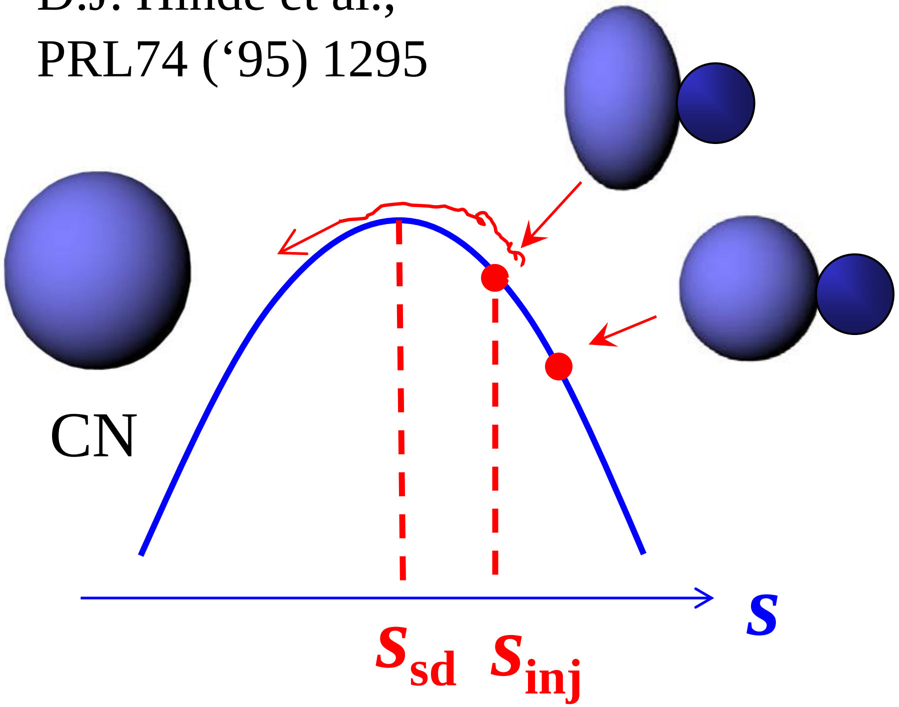


K. Hagino, PRC98 ('18) 014607

capture barrier distribution

cf. notion of compactness:

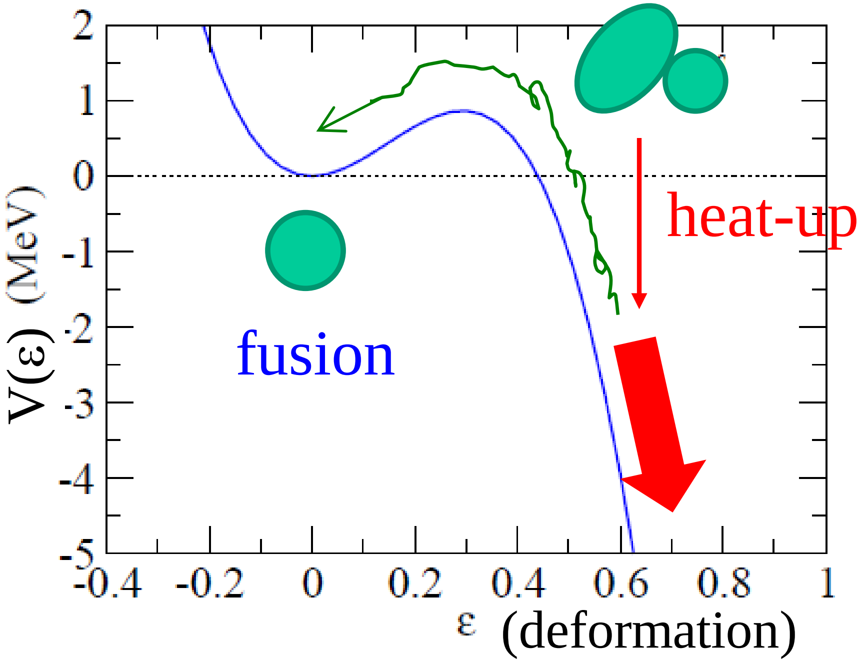
D.J. Hinde et al.,
PRL74 ('95) 1295

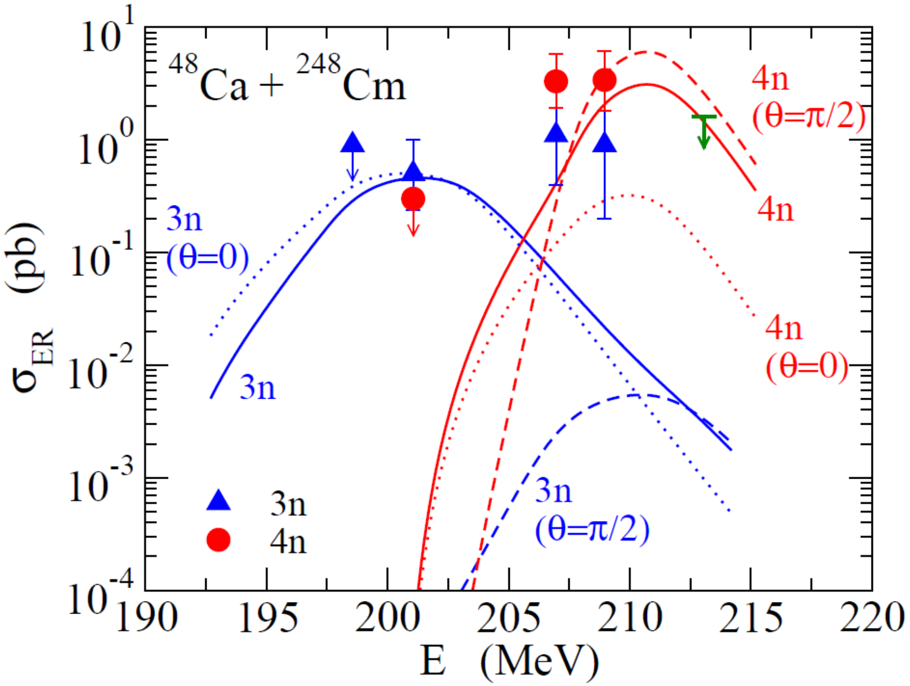


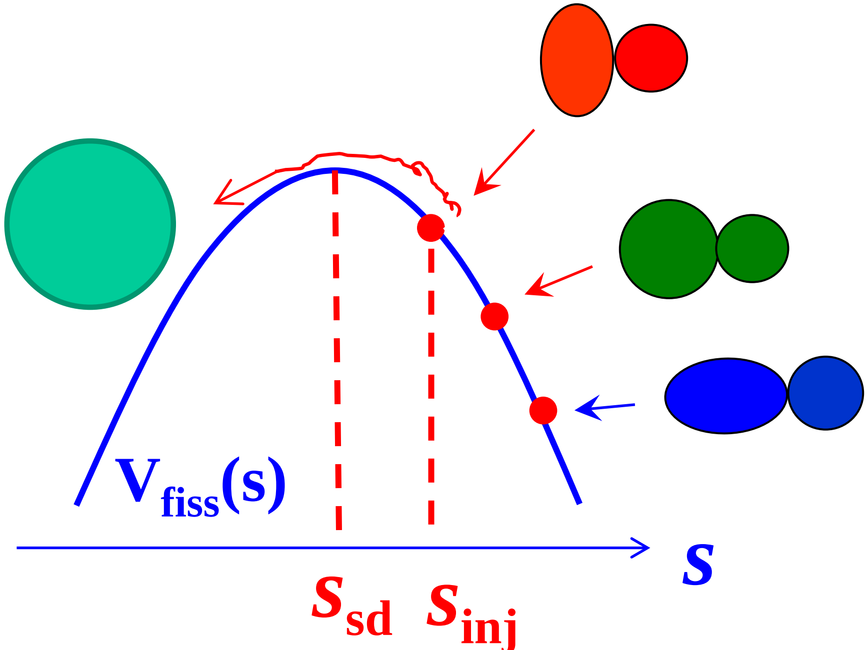
the 2nd stage of fusion reaction

hot fusion:
^{48}Ca + deformed target

effect of deformation

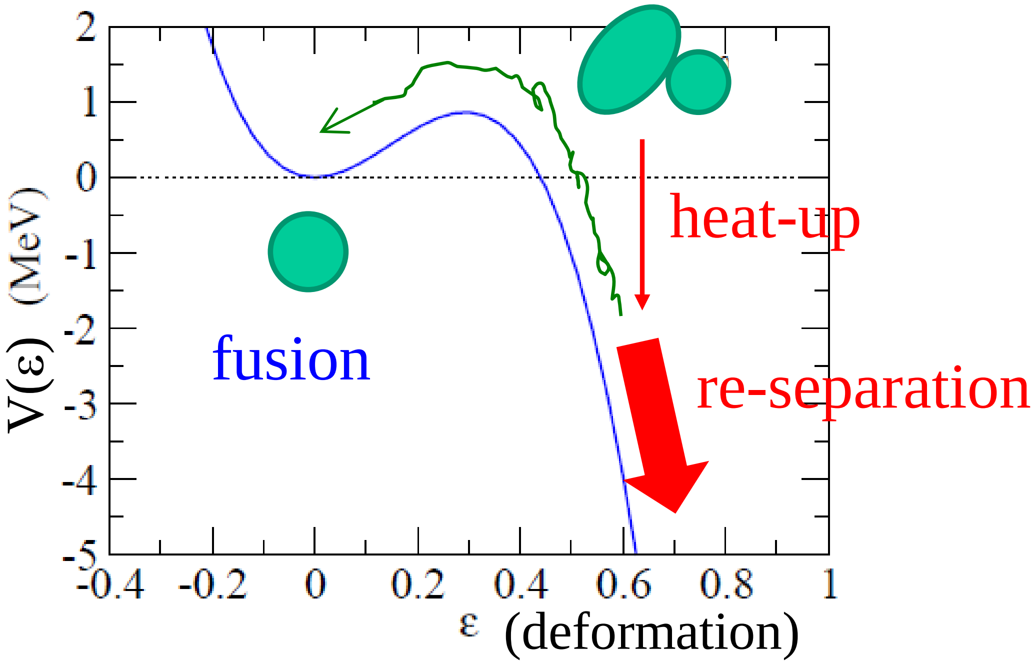


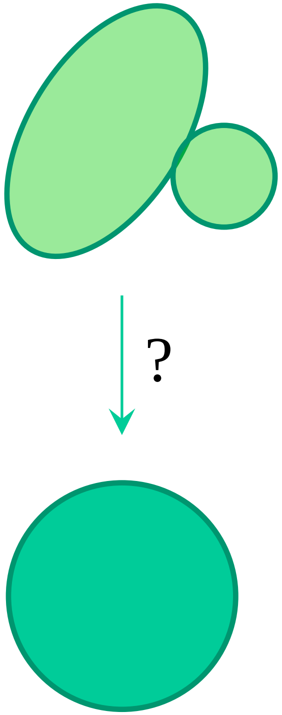




K. Hagino, PRC98 (‘18) 014607

open problems



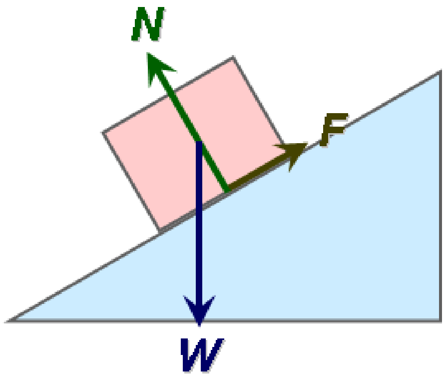


- how is the shape evolved to a compound nucleus?
- Deformation: a quantum effect
  how does the deformation disappear during heat-up?

quantum friction/open quantum systems

M. Tokieda and K.H., Ann. of Phys. 412 (‘20) 168005.
Front. in Phys. 8 (‘20) 8.

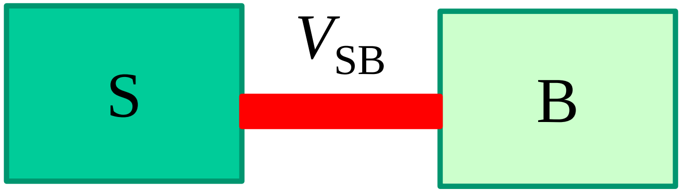
quantum friction



heat generation when a rigid body stops

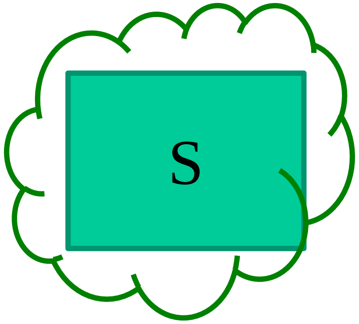
the energy conversion from the rigid body to intrinsic d.o.f. (atoms)

in quantum mechanics :



system

internal d.o.f.



“quasi” particle

solve the whole H without introducing the quasi-particle

M. Tokieda and K.H. (2020)

quantum Langevin?

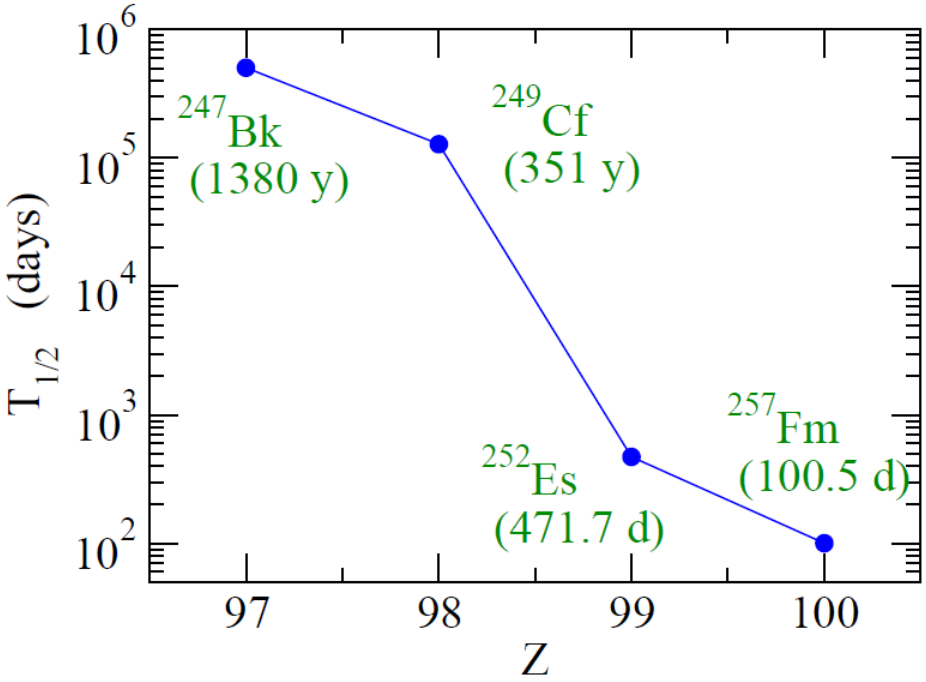
Hot fusion towards Z=119 and 120 nuclei

hot fusion reactions with ^{48}Ca:

$^{48}_{20}\mathrm{Ca} + {}_{99}\mathrm{Es} \rightarrow 119$

$^{48}_{20}\mathrm{Ca} + {}_{100}\mathrm{Fm} \rightarrow 120$

short lived → not available with sufficient amounts



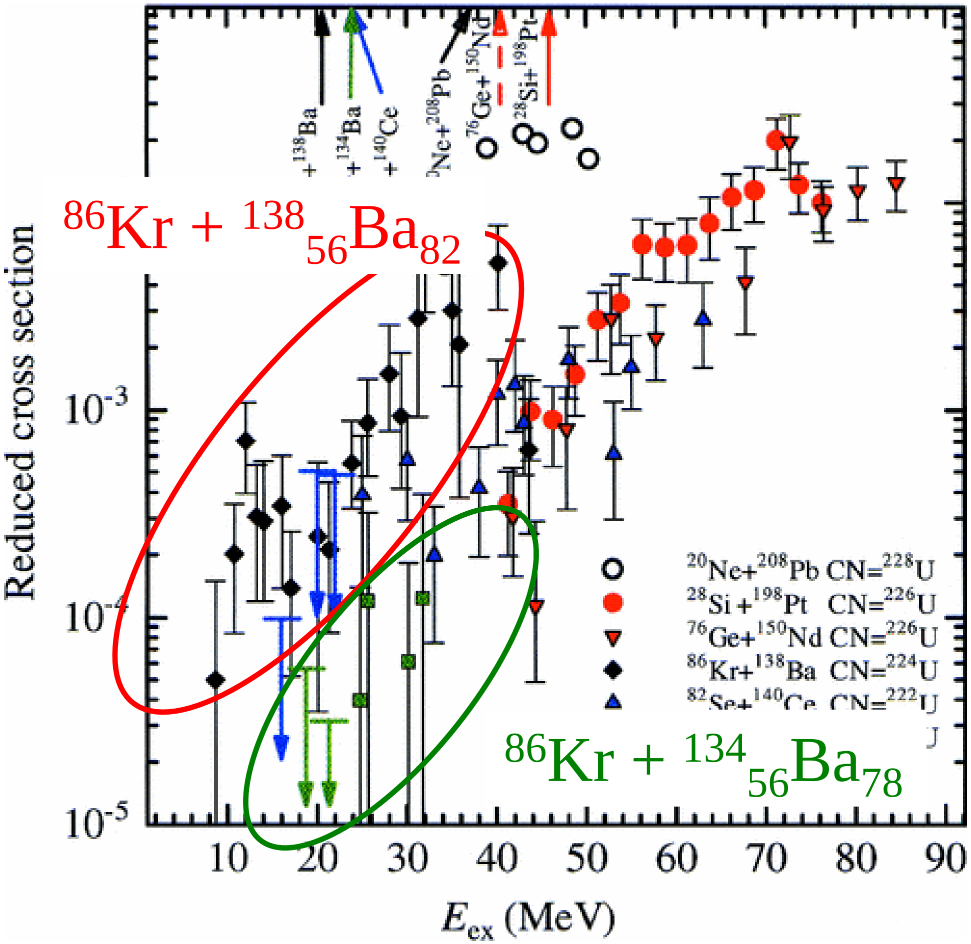
$^{48}\mathrm{Ca} \rightarrow {}^{50}_{22}\mathrm{Ti},\ {}^{51}_{23}\mathrm{V},\ {}^{54}_{24}\mathrm{Cr}$ projectiles

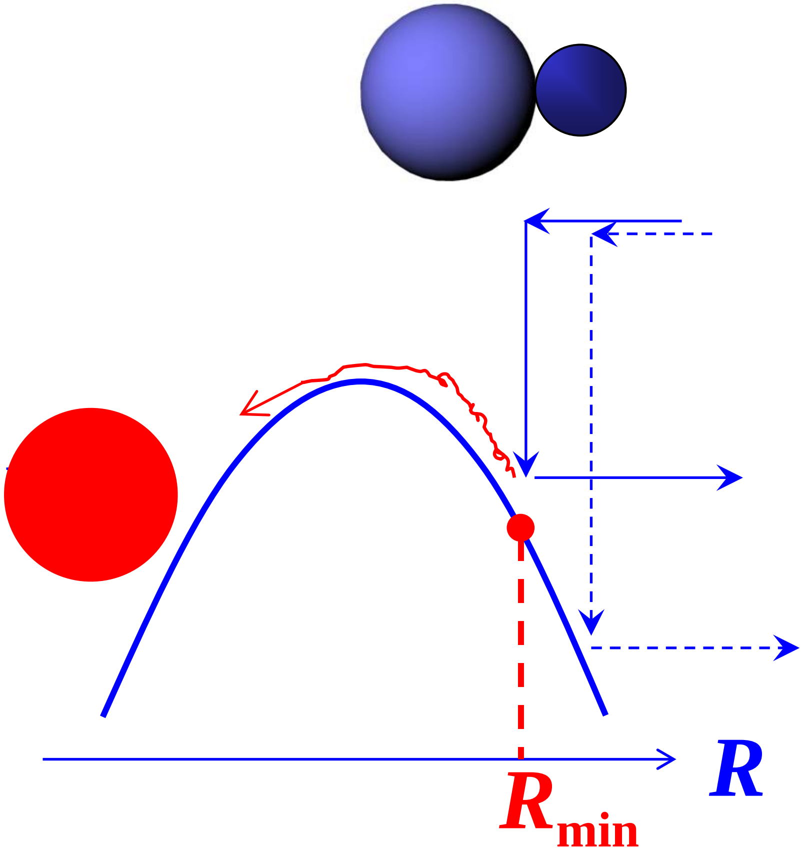
closed shell → open shells

how much will cross sections be affected?

Role of magicity

can proceed deeper
with less friction





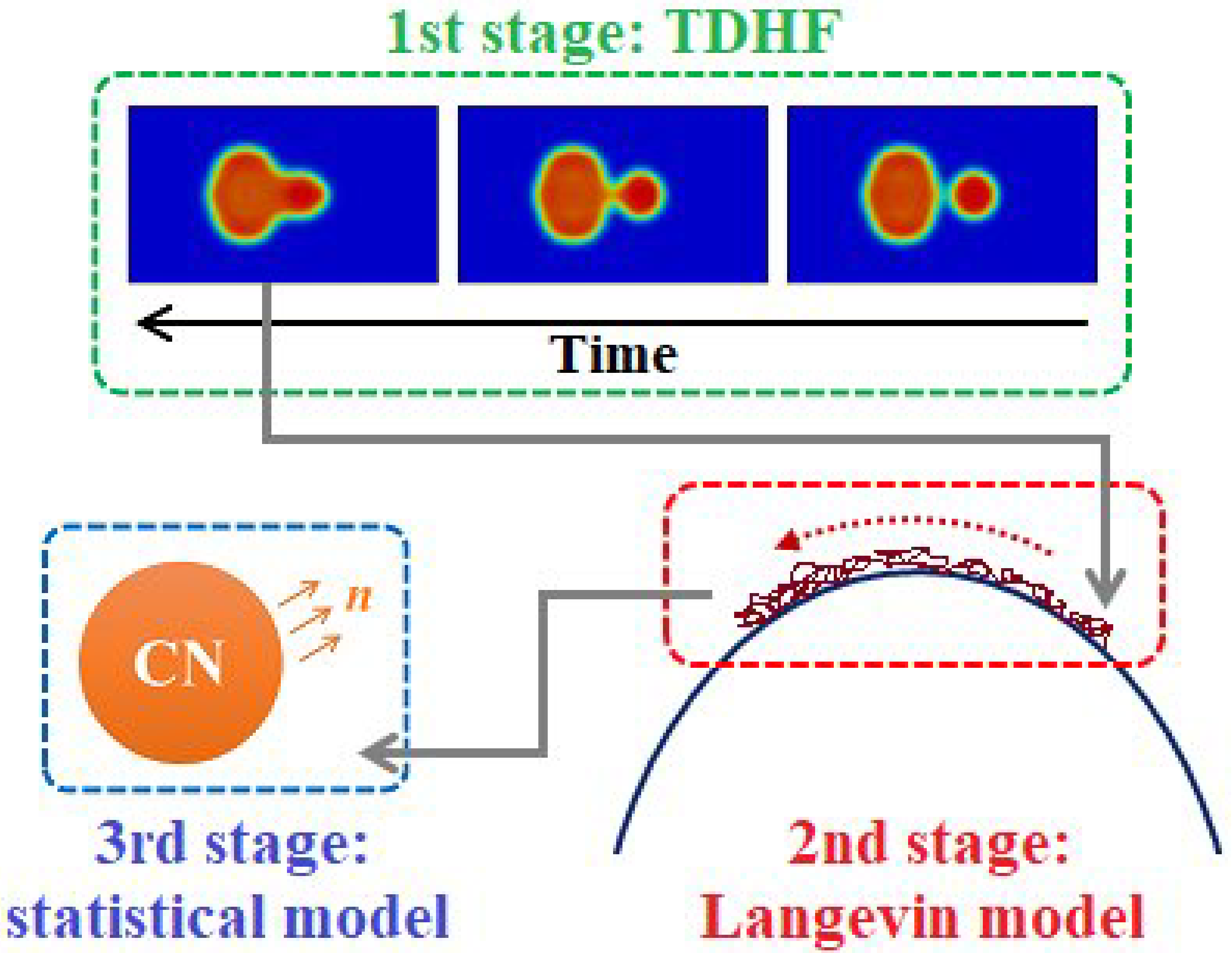
K. Satou, H. Ikezoe et al.,
PRC73 ('06) 034609

cf. P. Moller et al.,
Z. Phys. A359 ('97) 251.

similar effect for ^{48}Ca?

New hybrid model: TDHF + Langevin approach

K. Sekizawa and K.H., PRC99 (2019) 051602(R)



1st stage: TDHF

2nd stage:
Langevin model

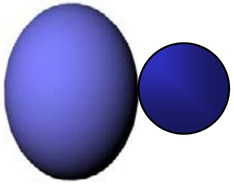
3rd stage:
statistical model

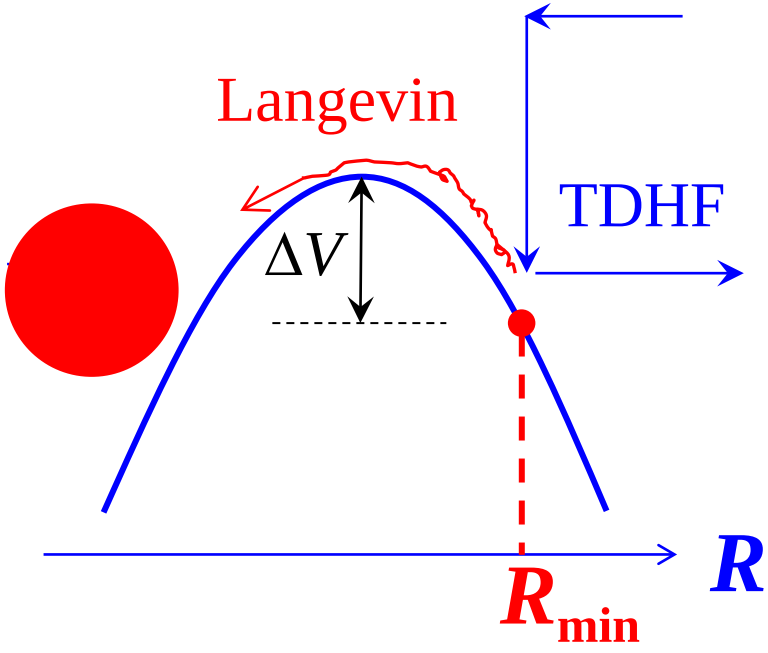
Furthermore : TDHF + Langevin approach and quantum friction

TDHF + Langevin approach :

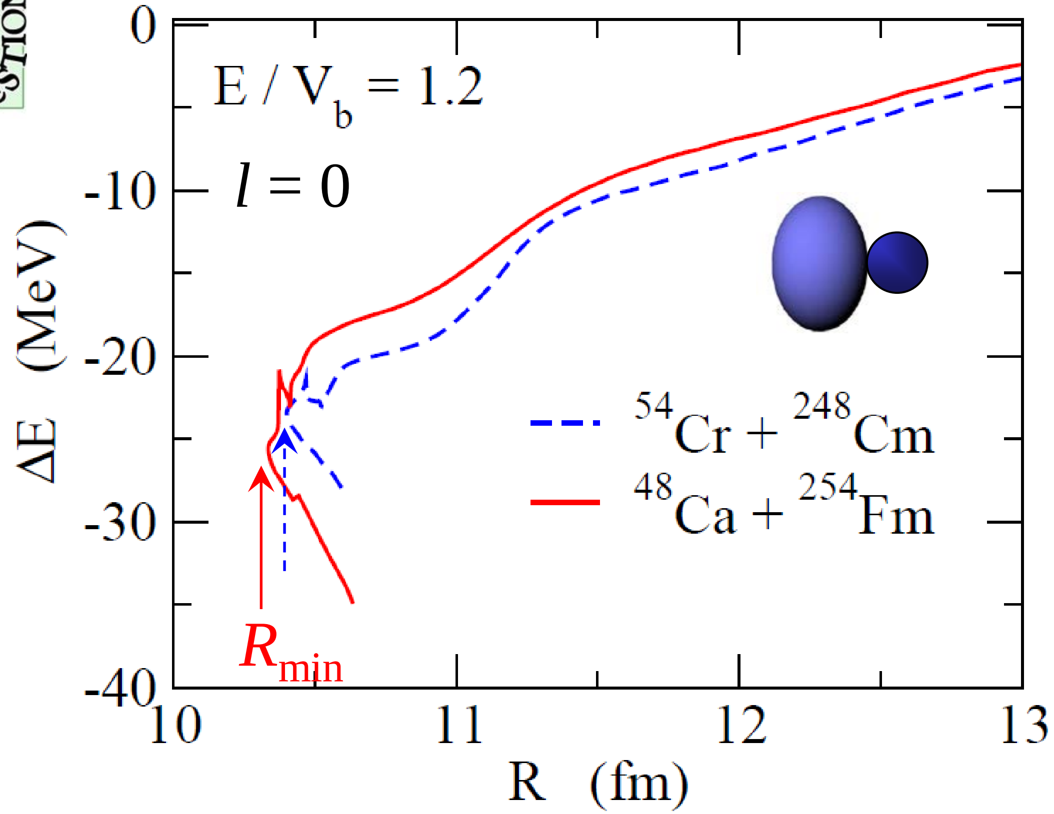
K. Sekizawa and K. H.,
PRC99 (2019) 051602(R)

side
collision





$^{54}Cr + {}^{248}Cm \rightarrow {}^{302}120$
$^{48}Ca + {}^{254}Fm \rightarrow {}^{302}120$

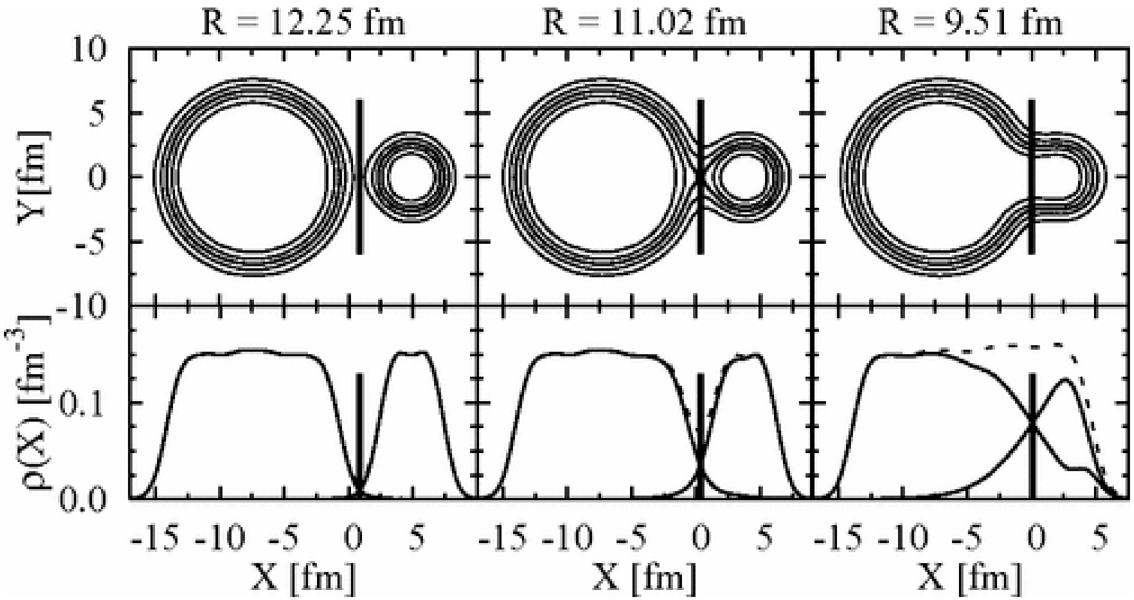


→ Langevin caluclation

Mapping TDHF onto a classical equation of motion

K. Washiyama and D. Lacroix, PRC78 (‘08) 024610

TDHF simulations

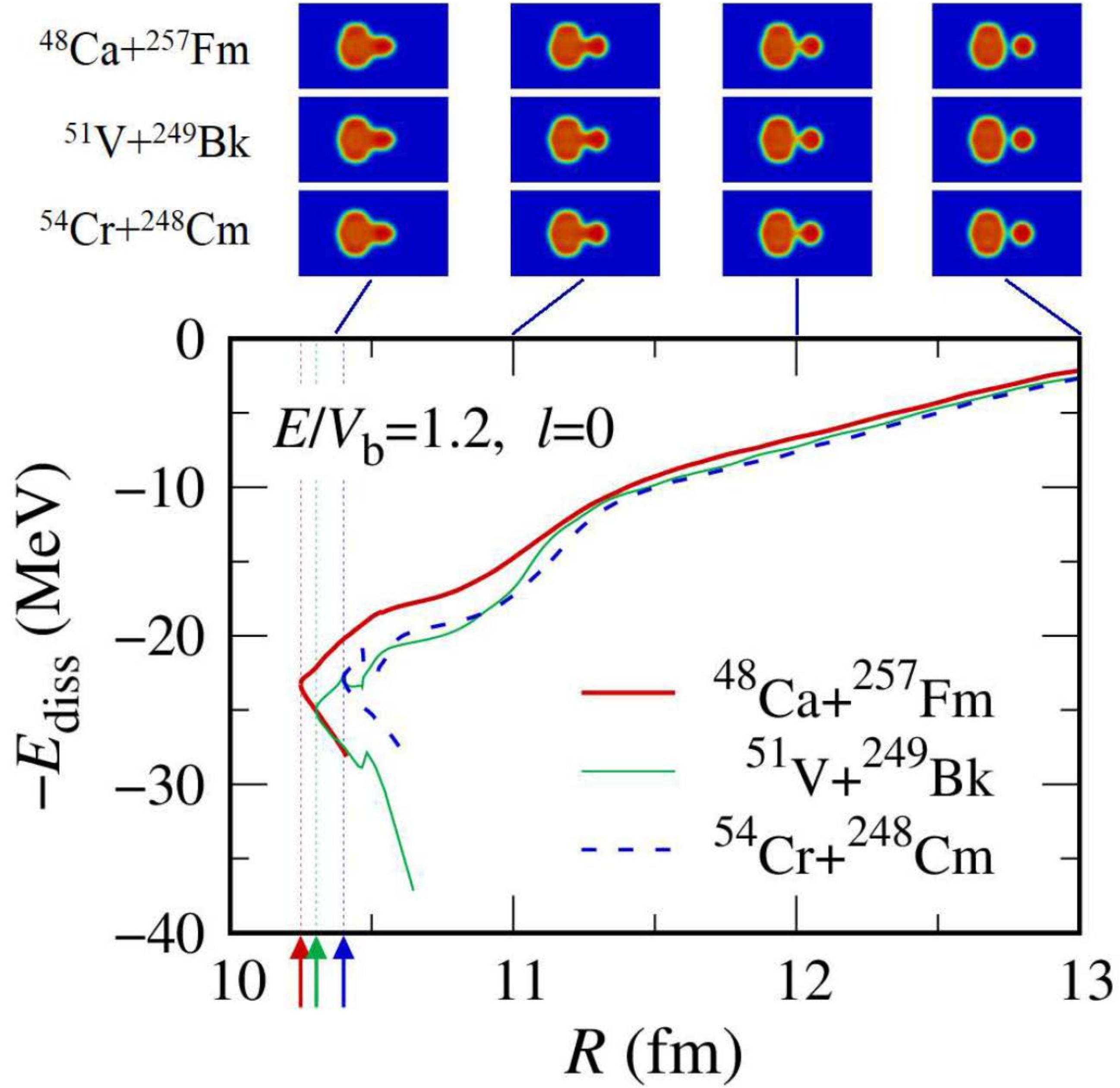


$\longrightarrow$ $R(t)$, $P(t)$

$$\boxed{\dot{P} = -\frac{dV}{dR} - \frac{d}{dR}\left(\frac{P^2}{2\mu}\right) - \gamma \dot{R}}$$

$\longrightarrow$ $V(R)$, $\gamma(R)$

$$\longrightarrow \quad \boxed{\Delta E(t) = -E_{\text{diss}}(t) = \frac{P(t)^2}{2\mu(R(t))} + V(R(t)) - E_{\text{ini}}}$$



K. Sekizawa and K.H., PRC99 (2019) 051602(R)

New model for fusion for SHE: TDHF + Langevin approach

K. Sekizawa and K.H., PRC99 (2019) 051602(R)

SUGGESTION

how special is ^{48}Ca ?

System	CN	E^* (MeV)	$R_{\rm min}$ (fm)	$P_{\rm CN}$ $(\times 10^4)$	$W_{\rm sur}$ $(\times 10^9)$	$P_{\rm CN}\,W_{\rm sur}$ $(\times 10^{13})$
^{48}Ca + ^{254}Fm	^{302}120	29.0	12.93	1.72	176	302
^{54}Cr + ^{248}Cm	^{302}120	33.2	13.09	1.89	1.31	2.47
^{51}V + ^{249}Bk	^{300}120	37.0	12.94	3.95	0.117	0.461
^{48}Ca + ^{257}Fm	^{305}120	30.5	12.94	2.49	0.729	1.82

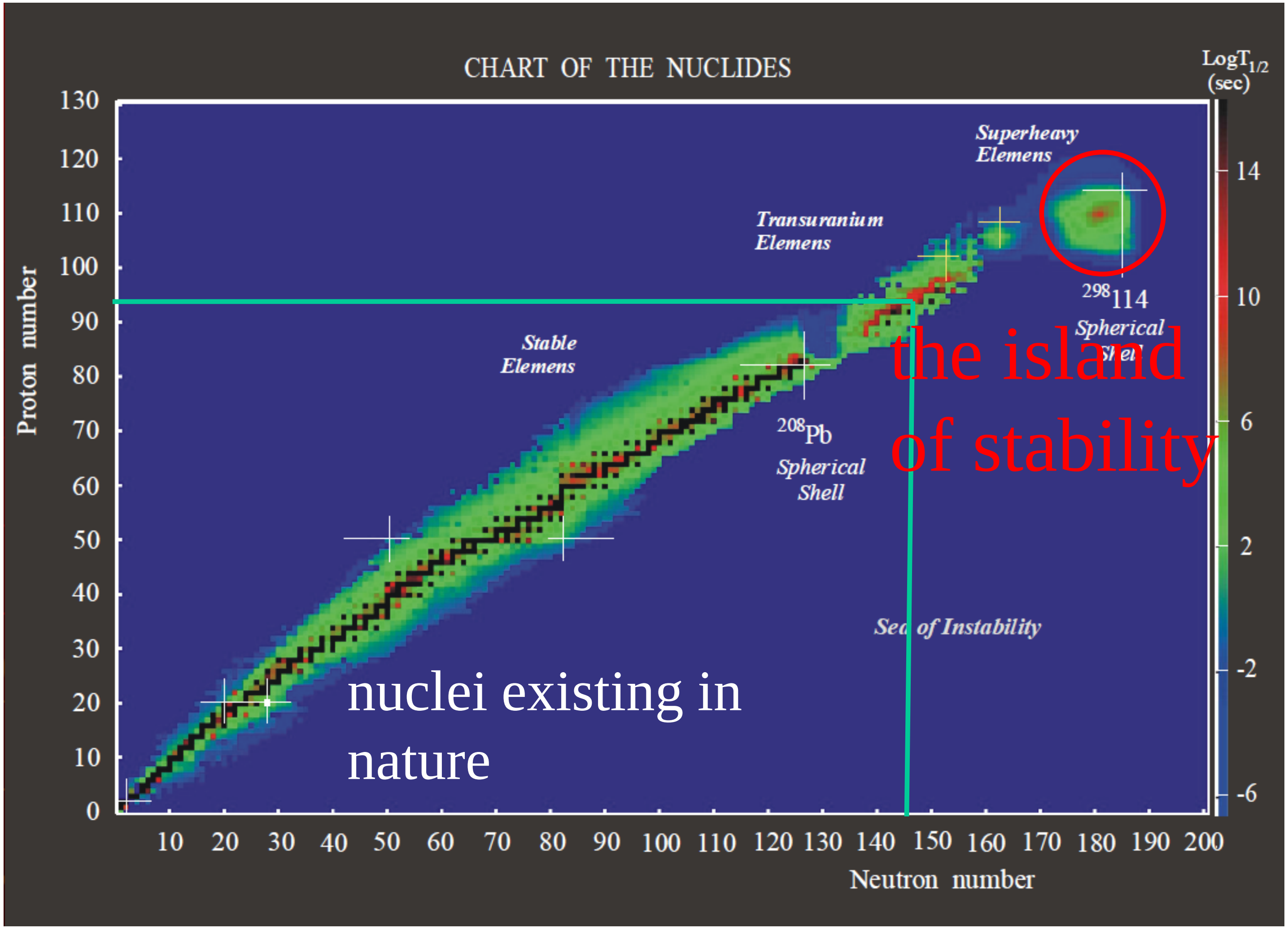
$$P_{\rm ER} = P_{\rm cap} \cdot P_{\rm CN} \cdot W_{\rm suv}$$

similar $P_{\rm CN}$

✓ no special role of ^{48}Ca in the entrance channel

✓ non-^{48}Ca proj.: about 2 order of magnitude smaller due mainly to $W_{\rm sur}$

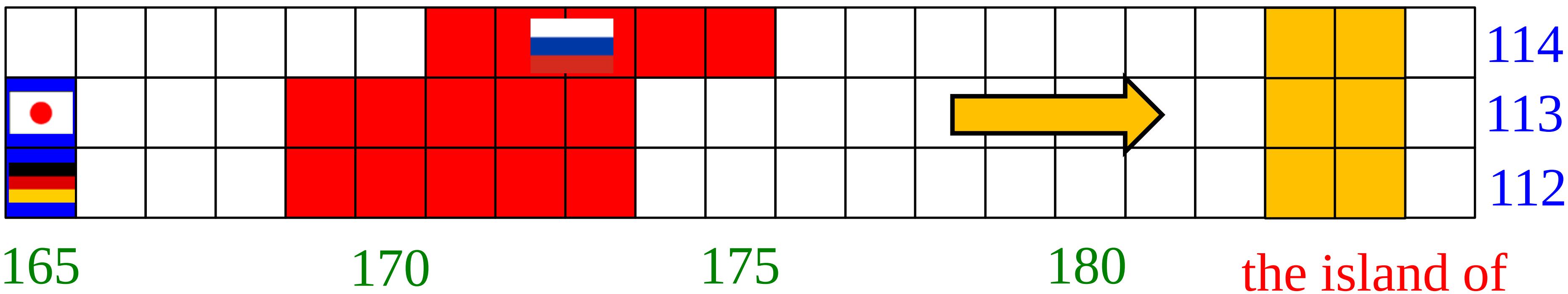
Another important issue: physics of neutron-rich nuclei



Yuri Oganessian

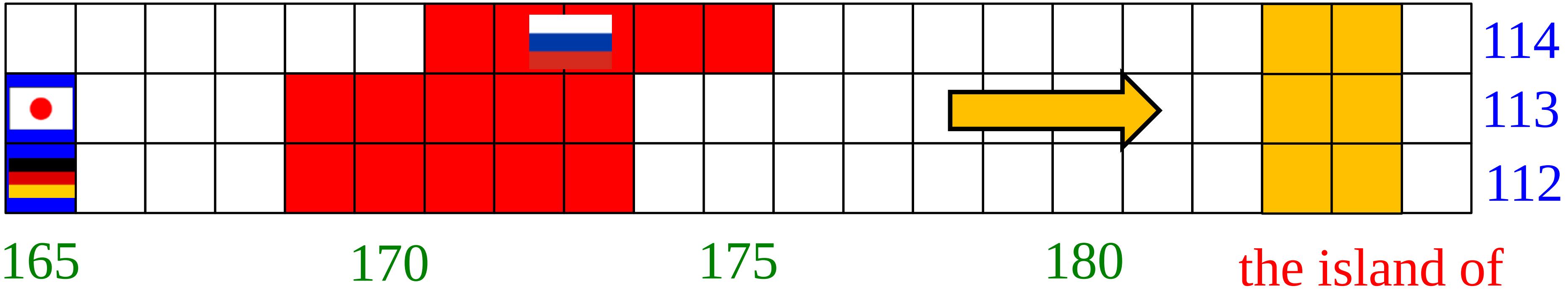
how to reach the island of stability?

Fusion of unstable nuclei



the island of stability (?)

Fusion of unstable nuclei



the island of stability (?)

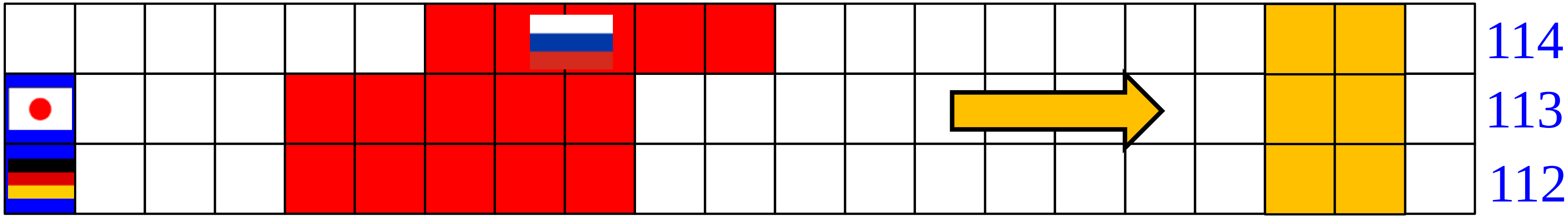
neutron-rich beams: indispensable

- ➢ how to deal with low beam intensity?
- ➢ reaction dynamics of neutron-rich beams?
  - ✓ capture: role of breakup and (multi-neutron) transfer?
  - ✓ diffusion: neutron emission during a shape evolution?
  - ✓ survival: validity of the statistical model?

structure of exotic nuclei

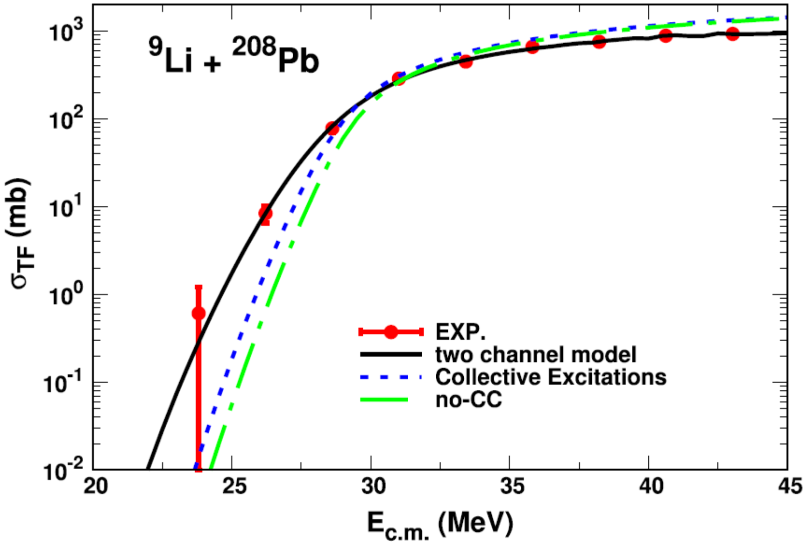
more studies are required

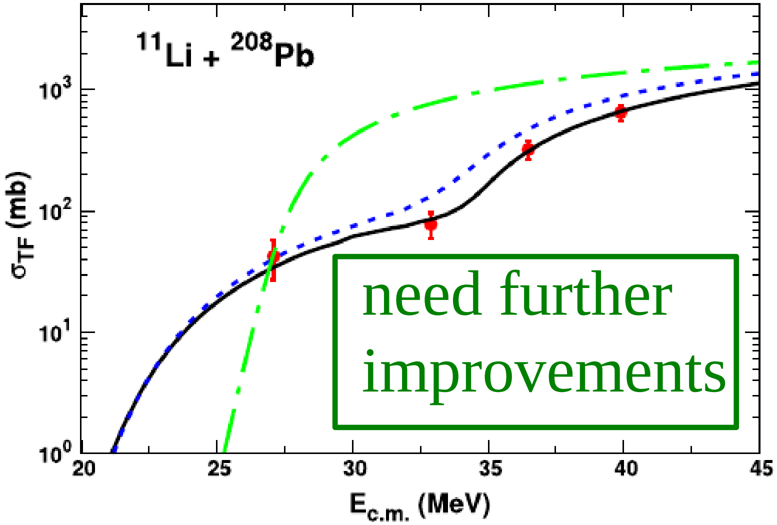
Fusion of unstable nuclei



neutron-rich beams: indispensable
→reaction dynamics?

K.-S. Choi, K. Hagino et al.,
Phys. Lett. B780 ('18) 455



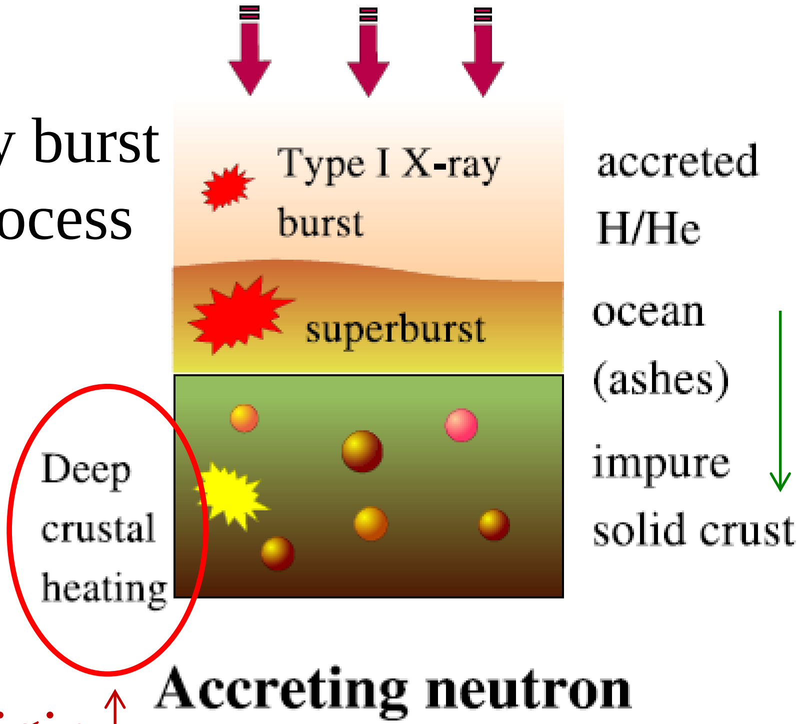


need further improvements

simultaneous explanation for ^{9}Li+^{208}Pb and ^{11}Li+^{208}Pb with:
^{11}Li+^{208}Pb ⟵⟶ ^{9}Li+^{210}Pb ⟵⟶ ^{7}Li+^{212}Pb transfer couplings

fusion of neutron-rich nuclei in accreting（質量降着）neutron stars

X-ray burst
rp-process



electron capture

$(A,Z) + e^- \rightarrow (A,Z-1) + \nu_e$

towards neutron-rich nuclei

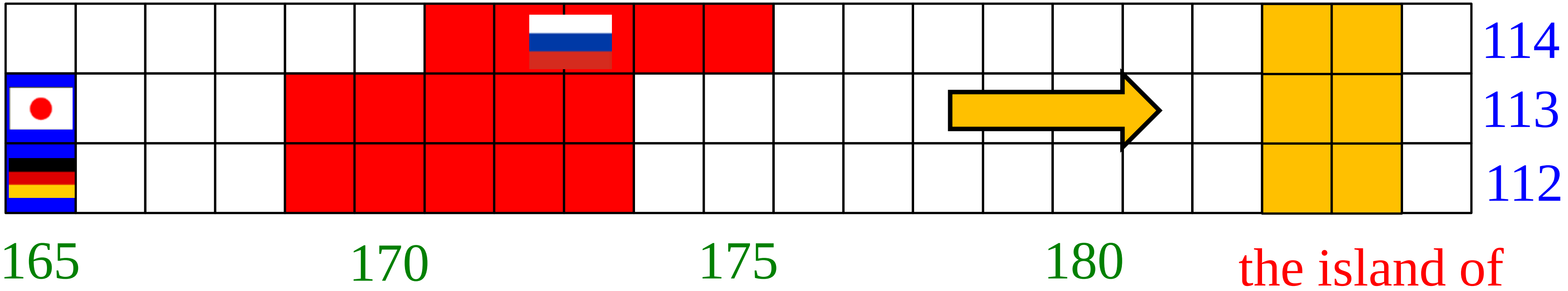
origin ↑

fusion of neutron-rich nuclei
when Z becomes small enough

$^{24}O + ^{24}O$, $^{28}Ne + ^{28}Ne$ etc.

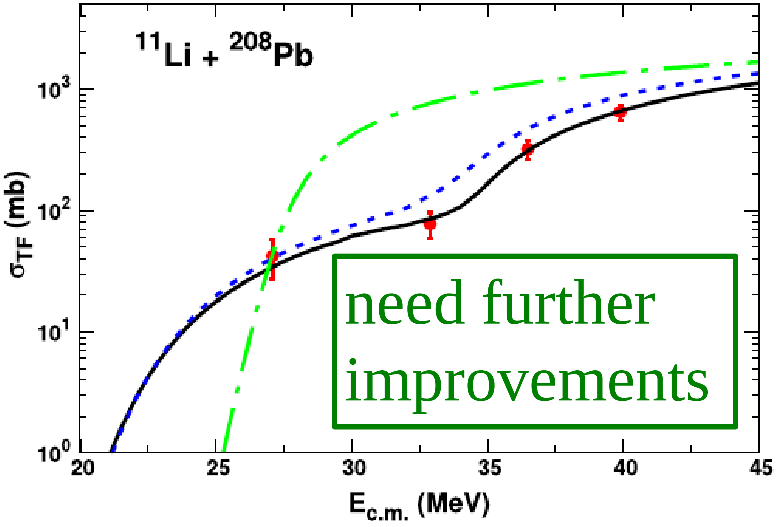
N. Chamel and P. Haensel,
Living Rev. Relativity, 11 (‘08) 10.

Fusion of unstable nuclei



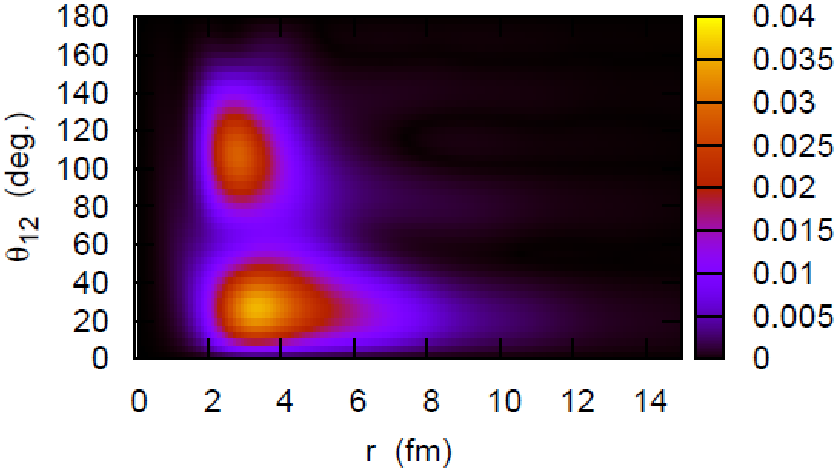
the island of stability

neutron-rich beams: indispensable→reaction dynamics?



need further improvements

K.-S. Choi, K. Hagino et al., Phys. Lett. B780 (’18) 455

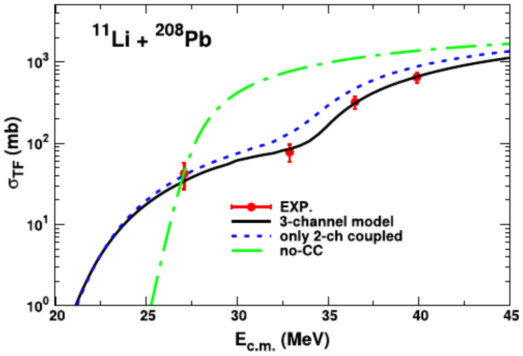


K.H. and H. Sagawa, PRC72(‘05)044321

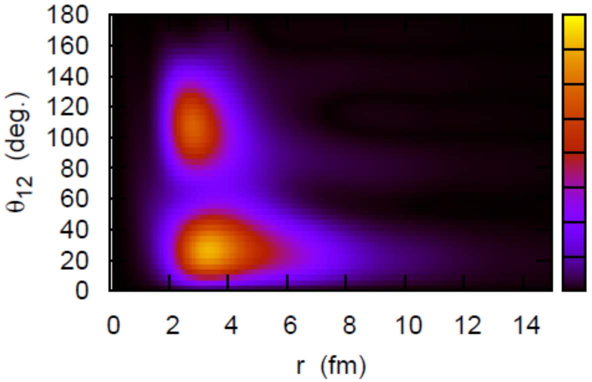
good understandings of the structure of neutron-rich nuclei is also important

Physics of SHE

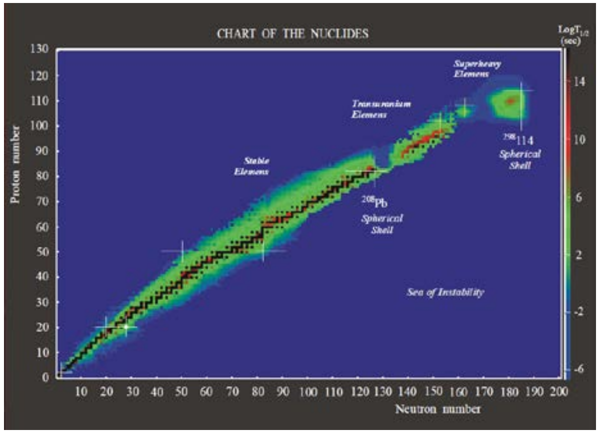
Reactions of n-rich nucl.



Structure of n-rich nucl.



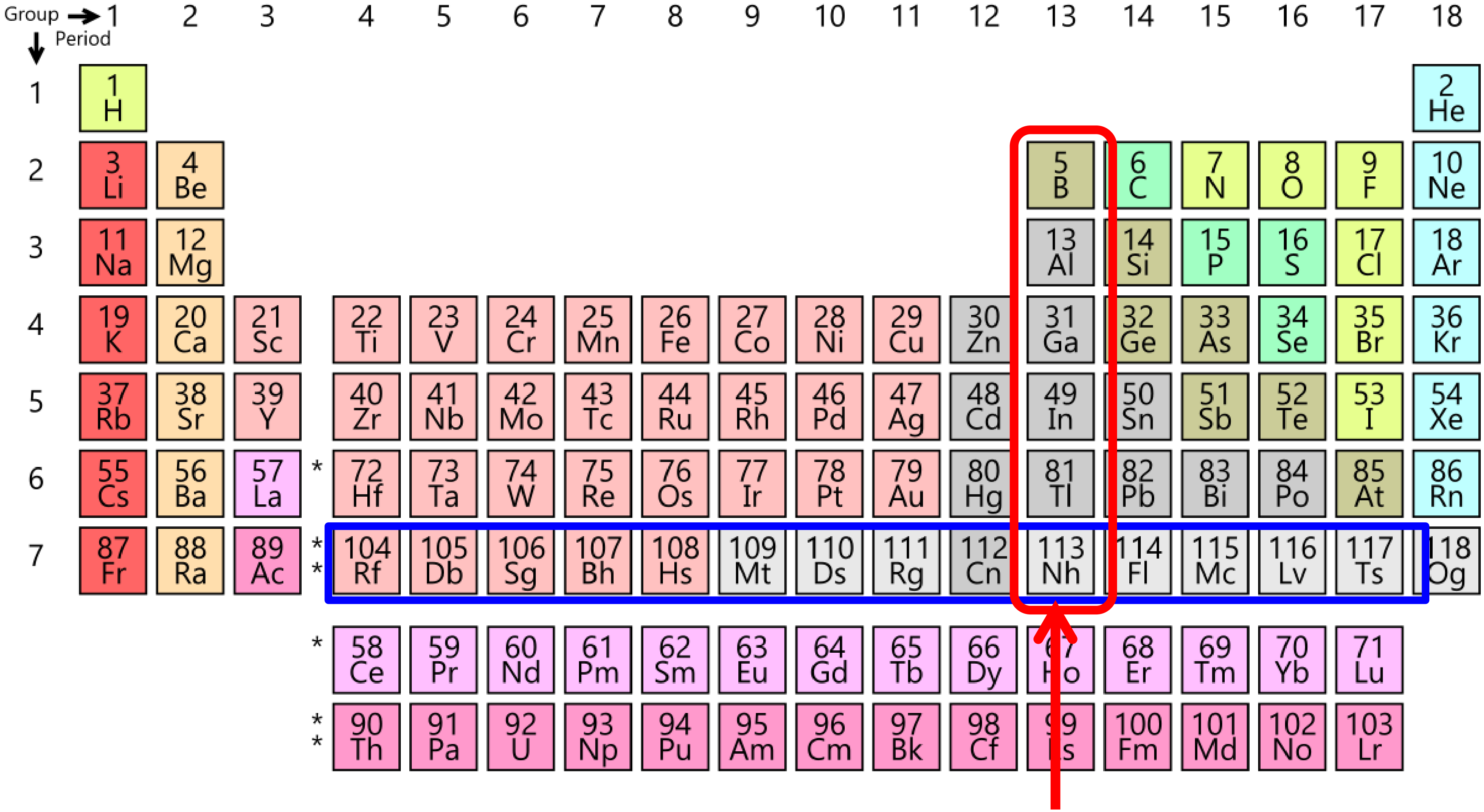
- SHE
- the island of stability



open quantum systems (OQS)

SHE + neutron-rich nuclei + OQS → new direction

Chemistry of superheavy elements



Group → Period ↓	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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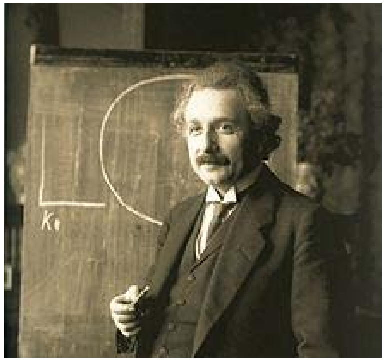
5	37 Rb	38 Sr	39 Y		40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
				*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
				**	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

- Are they here in the periodic table?
- Does Nh show the same chemical properties as B, Al, Ga, In, and Tl?

relativistic effect : important for large Z

$$E = mc^2$$

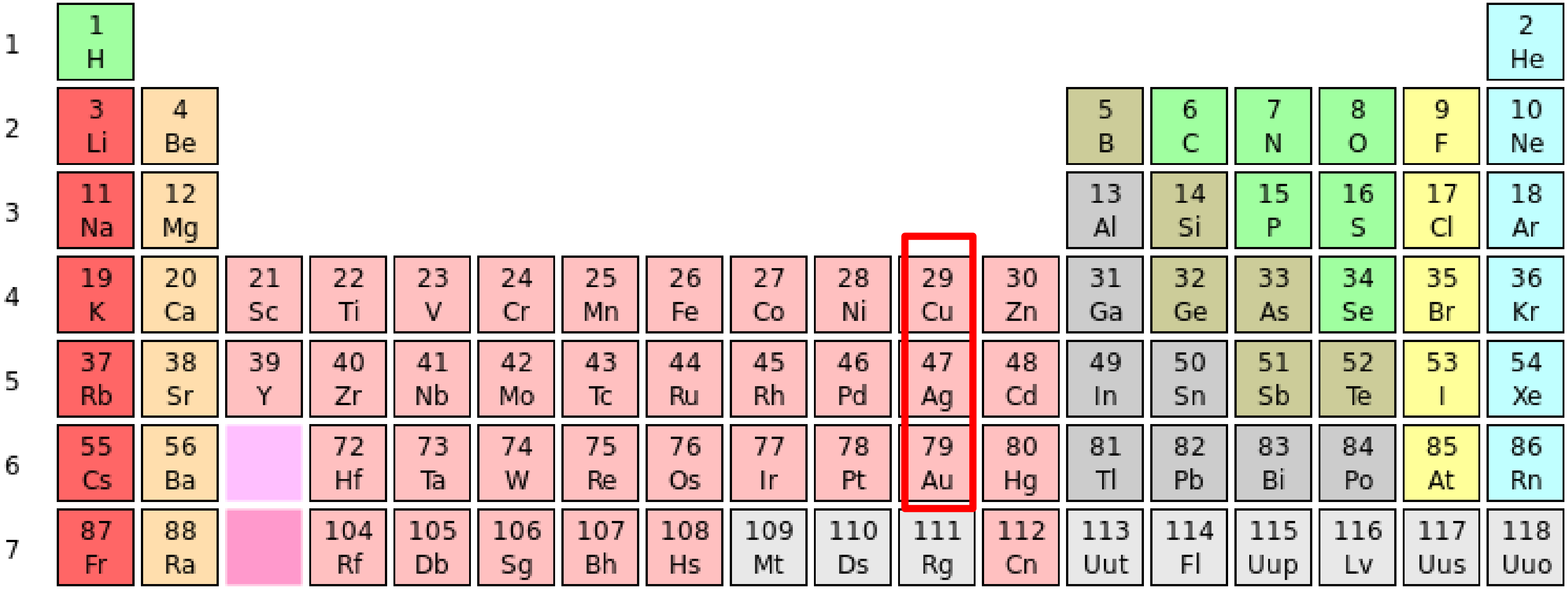


Solution of the Dirac equation (relativistic quantum mechanics) for a hydrogen-like atom:

$$E_{1S} = mc^2\sqrt{1-(Z\alpha)^2} \sim mc^2\left(1 - \frac{(Z\alpha)^2}{2} \underbrace{- \frac{(Z\alpha)^4}{8} + \cdots}\right)$$

relativistic effect

Famous example of relativistic effects: the color of gold



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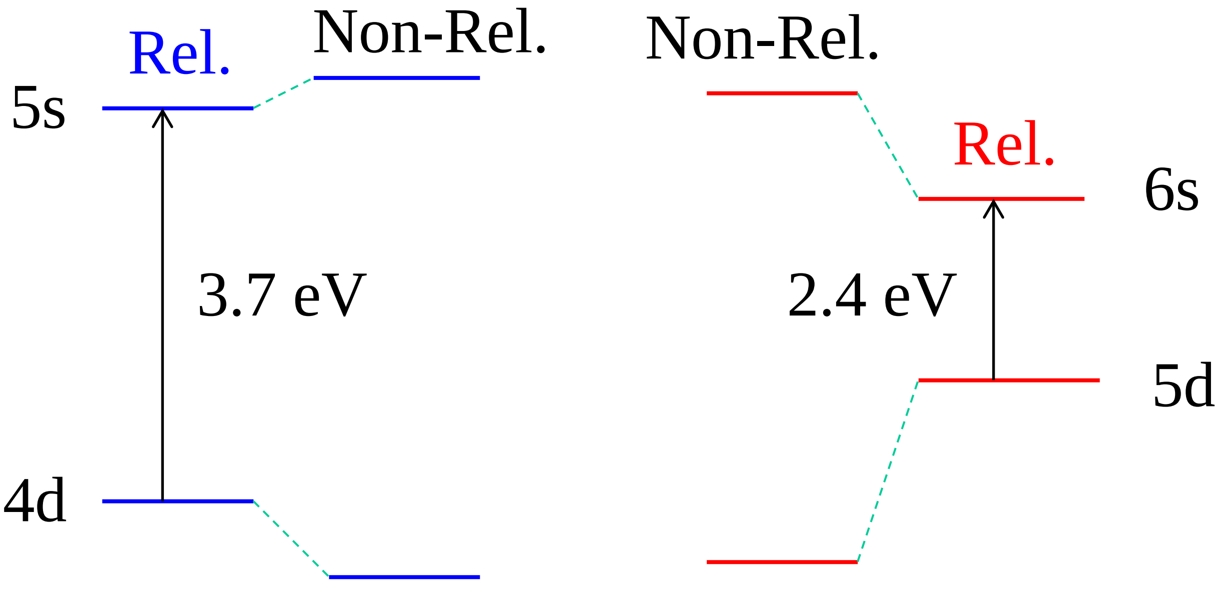
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo

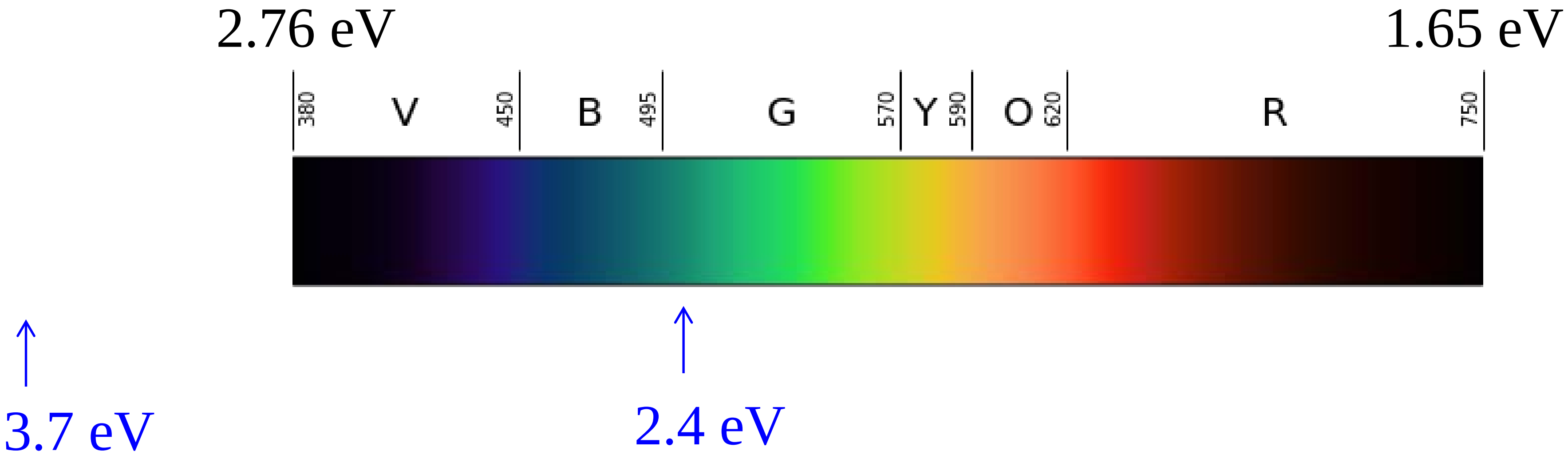
Gold looked like silver if there was no relativistic effects!

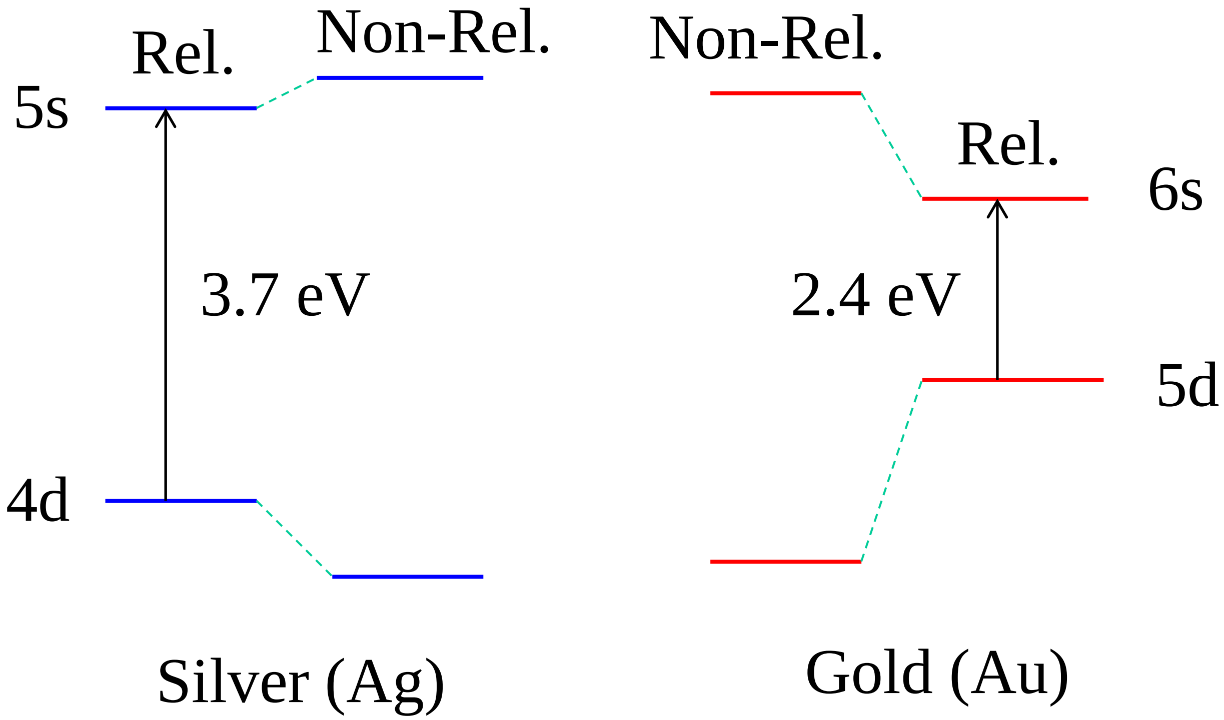


Silver (Ag)

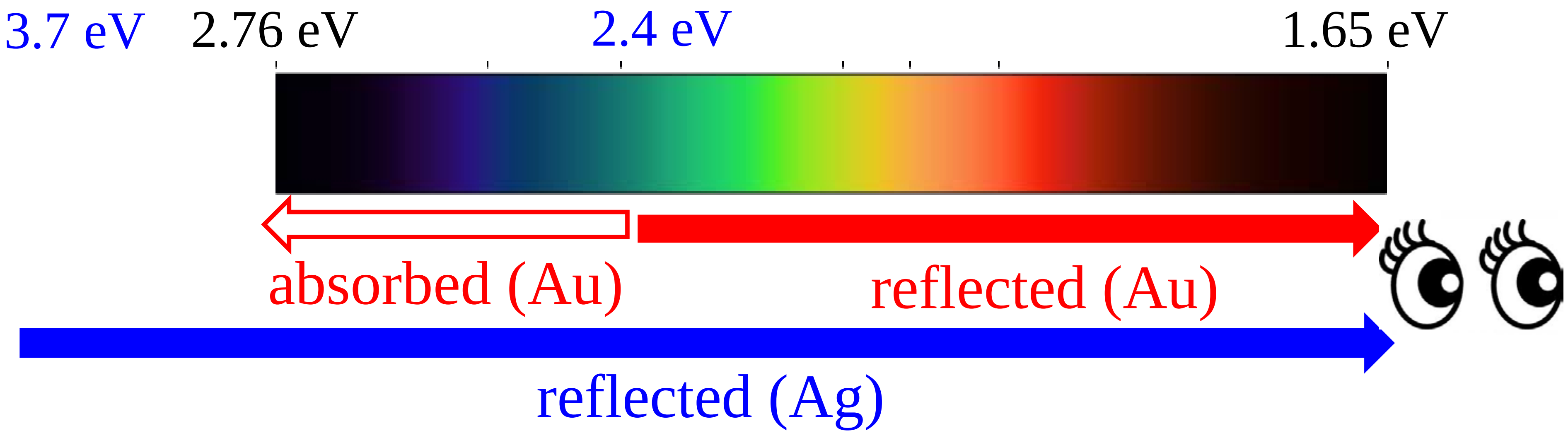
Gold (Au)

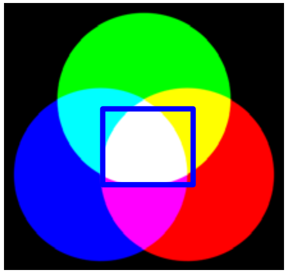
cf. visible spectrum



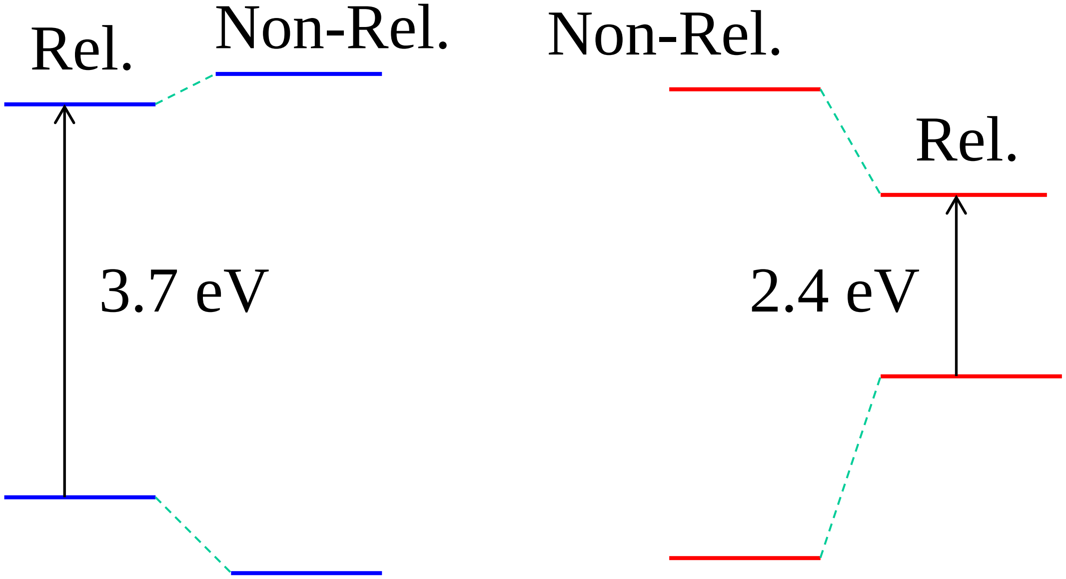


cf. visible spectrum





no color
absorbed



Rel.

Non-Rel.

3.7 eV

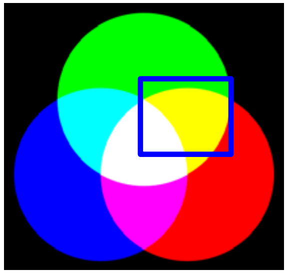
Non-Rel.

Rel.

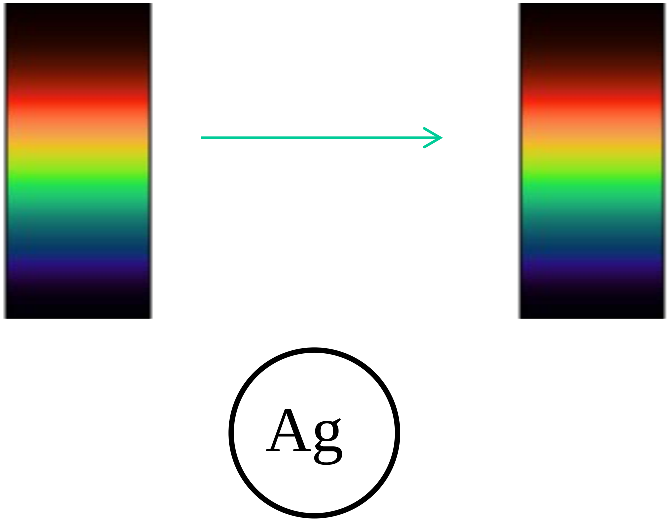
2.4 eV

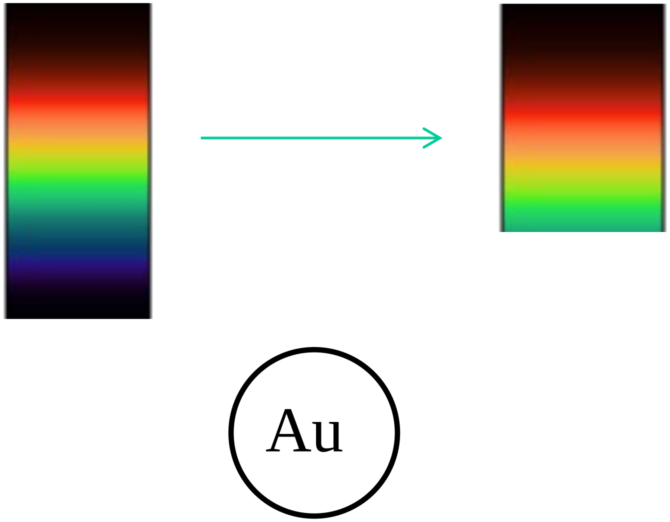
Silver (Ag)

Gold (Au)

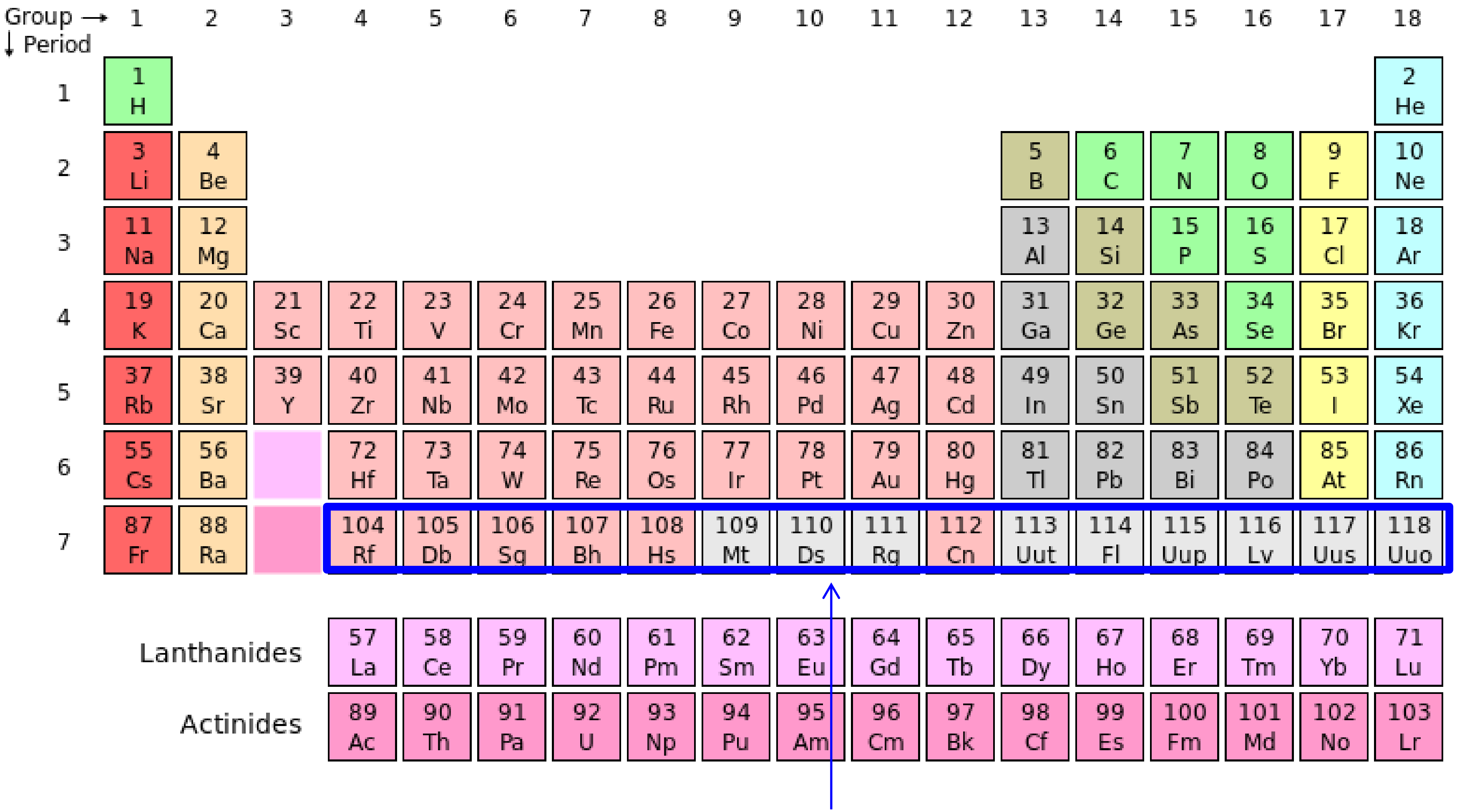


blue: absorbed





Chemistry of superheavy elements



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Lanthanides				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

How do the relativistic effects alter the periodic table for SHE?

⟶ a big open question

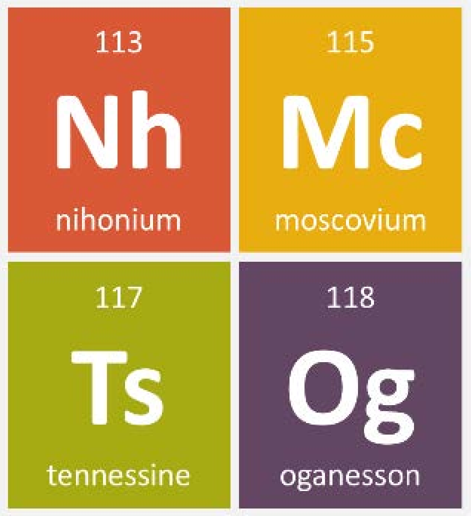
Summary

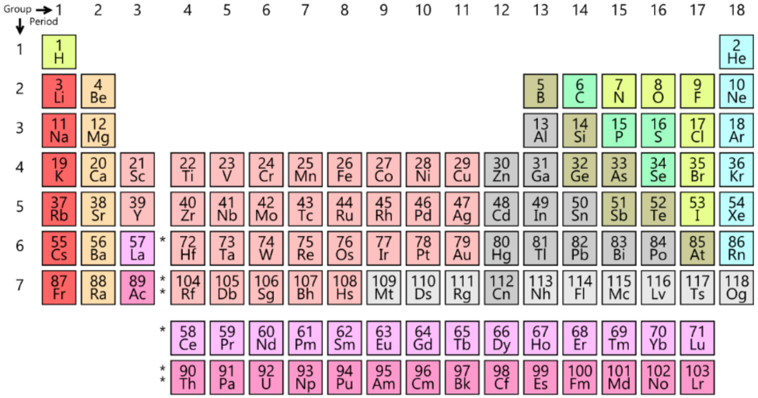
SHE: quantum many-body systems with a strong Coulomb field

physics

chemistry

astronomy





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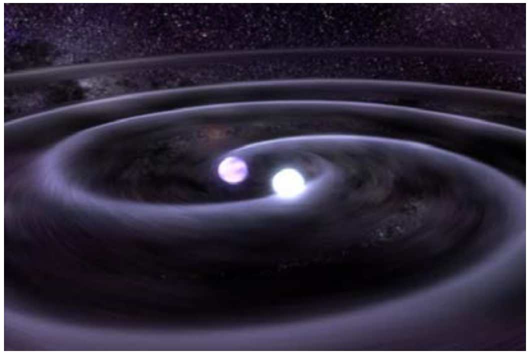
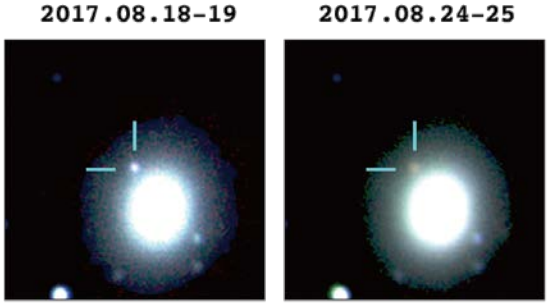
			*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
			**	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	





reaction dynamics

- ✓ quantum friction
- ✓ neutron-rich nuclei

2019 IYPT

International Year
of the Periodic Table
of Chemical Elements

- ✓ origin of elements
- ✓ r-process
- ✓ kilonova

interdisciplinary SHE science

New method for open quantum systems

M. Tokieda and K.H., Ann. of Phys., in press ('19)

$$H_{\rm tot} = \underbrace{H_S}_{\text{system}} + \underbrace{\sum_i \hbar\omega_i a_i^\dagger a_i}_{\text{environment}} + \underbrace{h(q)\sum_i d_i(a_i^\dagger + a_i)}_{\text{coupling}}$$

naiive coupled-channels equations:

$$\Psi_{\rm tot}(q,t) = \sum_{\{n_i\}} \psi_{\{n_i\}}(q,t)\,|\{n_i\}\rangle; \quad |\{n_i\}\rangle = \prod_i \frac{1}{\sqrt{n_i!}}\left(a_i^\dagger\right)^{n_i}|0\rangle$$

$$\Longrightarrow \quad \langle\{n_i\}|i\hbar\frac{\partial}{\partial t}|\Psi_{\rm tot}\rangle = \langle\{n_i\}|H_{\rm tot}|\Psi_{\rm tot}\rangle$$

⟶ coupled-channels eqs. for $\psi_{\{n_i\}}(q,t)$

difficult when the number of environmental osc. modes is large

$$H_{\mathrm{tot}} = H_S + \sum_i \hbar\omega_i a_i^\dagger a_i + h(q) \sum_i d_i (a_i^\dagger + a_i)$$

➡ introduce more efficient basis

$$e^{-i\omega t} \sim \sum_{k=1}^{K} \underbrace{\eta_k(\omega)}_{\text{exp. coef.}} \underbrace{u_k(t)}_{\text{basis}}$$

cf. correlation function

$$L(t) = \int_{-\infty}^{\infty} d\omega \, \frac{J(\omega)}{1 - e^{-\beta\hbar\omega}} e^{-i\omega t}$$

cf. 階層型運動方程式

Y. Tanimura and R. Kubo,
J. Phys. Soc. Jpn 58 (’89)101

➡

$$\boxed{b_k^\dagger = \sum_i \frac{d_i}{\hbar} \eta_k(\omega_i) a_i^\dagger}$$

cf. Lanczos method

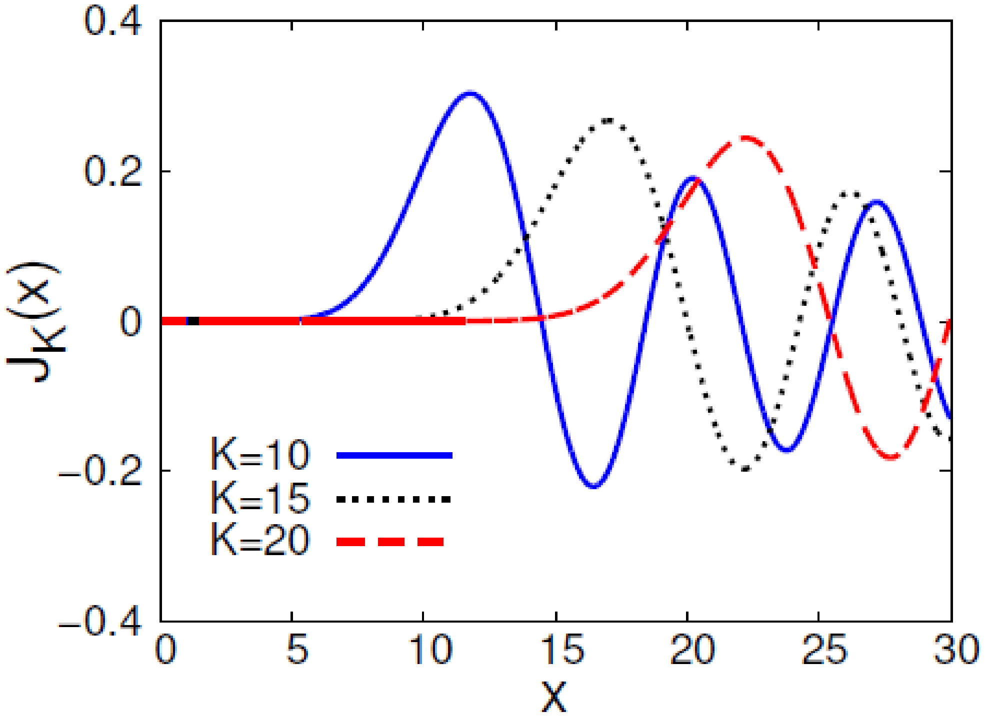
$$\Psi_{\mathrm{tot}}(q,t) = \sum_{\{\tilde{n}_k\}} \tilde{\psi}_{\{\tilde{n}_k\}}(q,t) \, |\{\tilde{n}_k\}\rangle; \quad |\{\tilde{n}_k\}\rangle = \prod_{k=1}^{K} \frac{1}{\sqrt{\tilde{n}_k!}} \left(b_k^\dagger\right)^{\tilde{n}_k} |0\rangle$$

$$e^{-i\omega t} \sim \sum_{k=1}^{K} \eta_k(\omega) u_k(t) \quad \Longrightarrow \quad b_k^\dagger = \sum_i \frac{d_i}{\hbar}\eta_k(\omega_i) a_i^\dagger$$

in actual calc.: expansion with Bessel function (Jacobi-Anger identity):

$$e^{-i\omega t} = J_0(\Omega t) + 2\sum_{k=1}^{\infty} (-i)^k \underline{T_k\left(\frac{\omega}{\Omega}\right)} J_k(\Omega t)$$

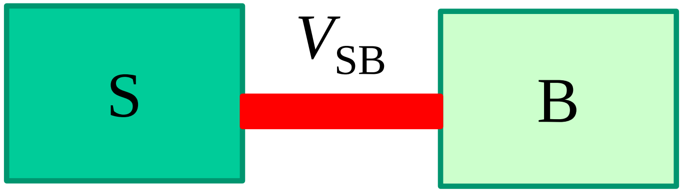
Chebyshev polynomials



large *k:* does not contribute when *t* is small

$$J_k(x) = \sum_{s=0}^{\infty} \frac{(-1)^2}{s!(s+k)!}\left(\frac{x}{2}\right)^{k+2s}$$

modelling of open quantum systems



i) system + bath

$$H = H_S + H_B + V_{SB}$$

✓ Caldeira-Leggett
✓ Feynmann-Vernon

solution:

a) eliminate B (bath)
→ eff. action for S
(influence functional)

b) $\rho_S = Tr_B[\rho]$

$$\to i\hbar\dot{\rho}_S = \cdots$$

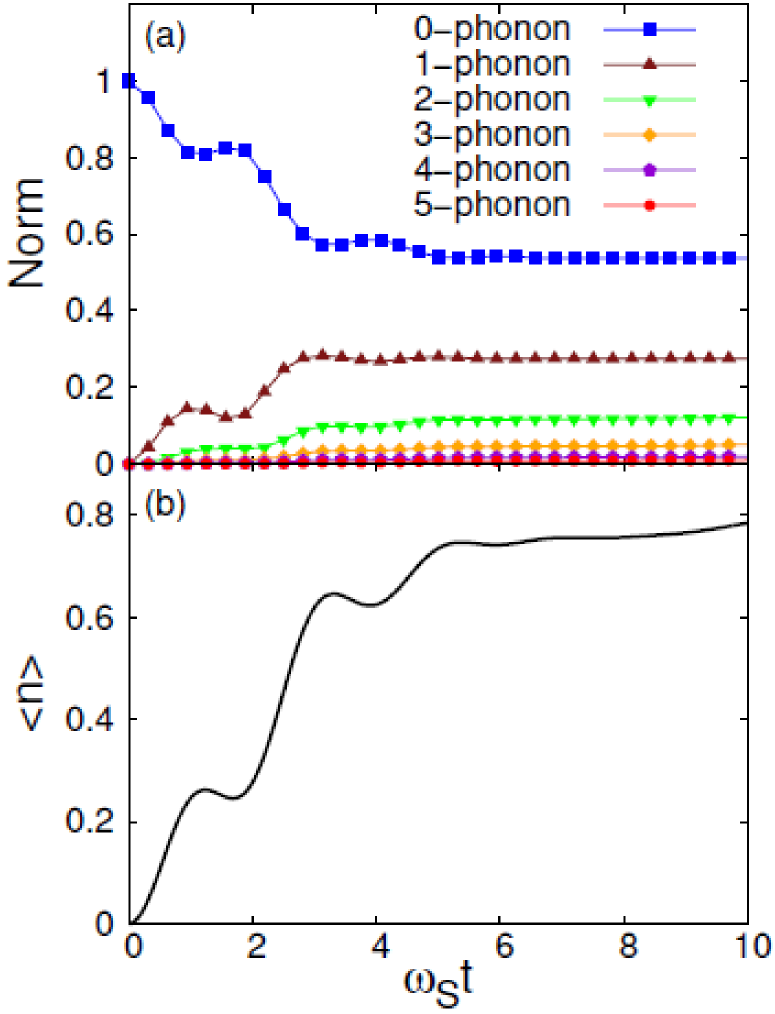
Markovian approximation
→ Lindblad equation

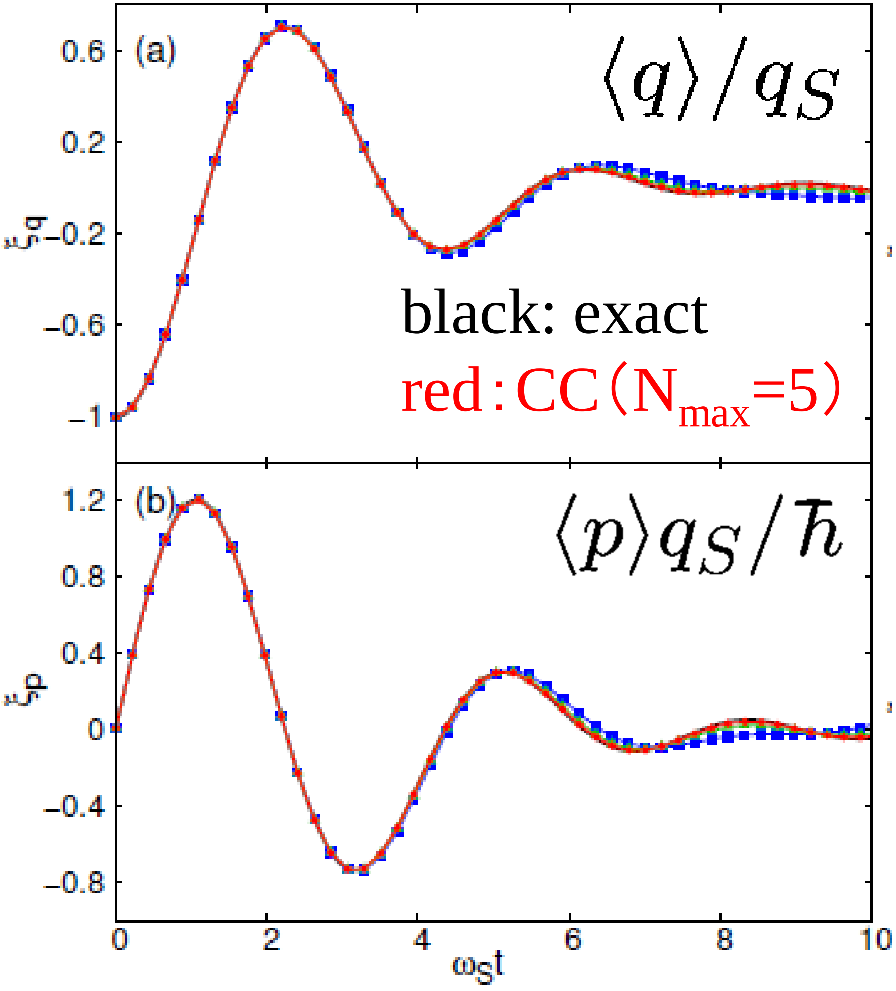
c) expand the tot. wf with the eigen states of H_B (coupled-channels eq.)

M. Tokieda and K.H.,
Ann. of Phys. 412 (‘20) 168005.
Front. in Phys. 8 (‘20) 8.

application to damped oscillation: HO + environment (conti. spectrum)

expansion with Bessel functions up to K=20





black: exact

red：CC（N_{max}=5）

M. Tokieda and K. Hagino, Ann. of Phys. 412 (‘20) 168005

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- microscopic
- but, hard to solve

ii) quantum friction model

construct a Hamiltonian which leads to

$$\frac{d}{dt}\langle p\rangle = -\langle V'(x)\rangle - \gamma\langle p\rangle$$

- ✓ E. Kanai, PTP 3 (‘48)
- ✓ M.D. Kostin, JCP 57 (‘72)
- ✓ K. Albrecht, PLB56 (‘75)
- ✓ K.-K. Kan & J.-J. Griffin, PLB50 (‘74)
- ✓ A. Bulgac, S. Jin, and I. Stetcu, PRC100, 014615 (2019)

Quantum friction

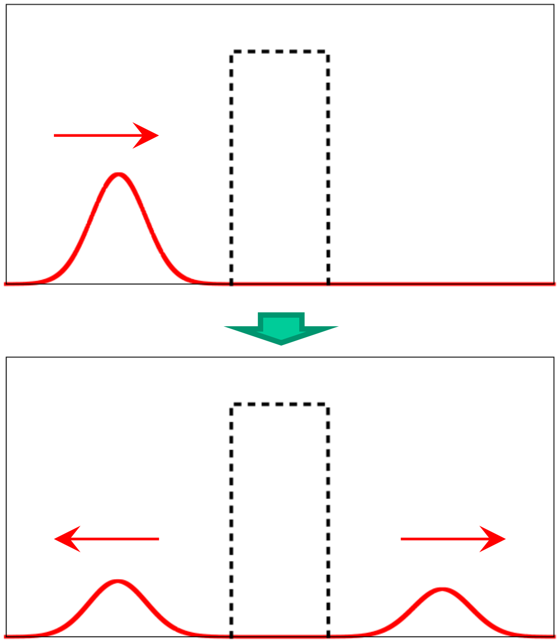
classical eq. of motion $\dot{p} = -V'(x) - \gamma p$

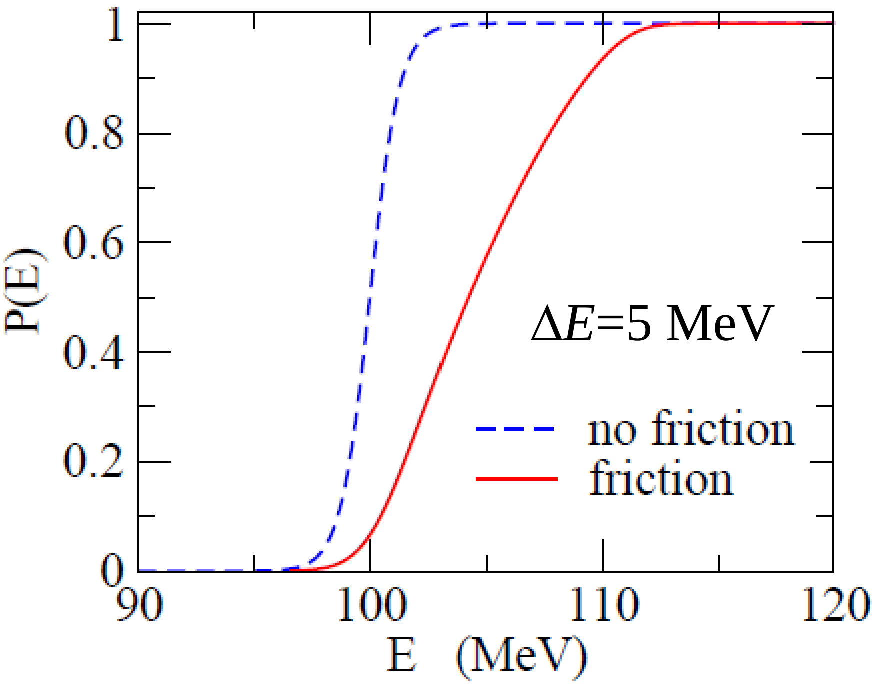
a quantization: Kanai model E. Kanai, PTP 3 (1948) 440

$$\boxed{H = \frac{p^2}{2m} + V(x) \to \frac{\pi^2}{2m} e^{-\gamma t} + e^{\gamma t} V(x) \qquad (\pi = e^{\gamma t} p)}$$

$$\Rightarrow \frac{d}{dt}\langle p \rangle = -\langle V'(x) \rangle - \gamma \langle p \rangle$$

time-dep. wave packet approach





M. Tokieda and K.H., PRC95 ('17) 054604

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