密度汎関数法による奇核を含めた原子核質量の新しい計算法

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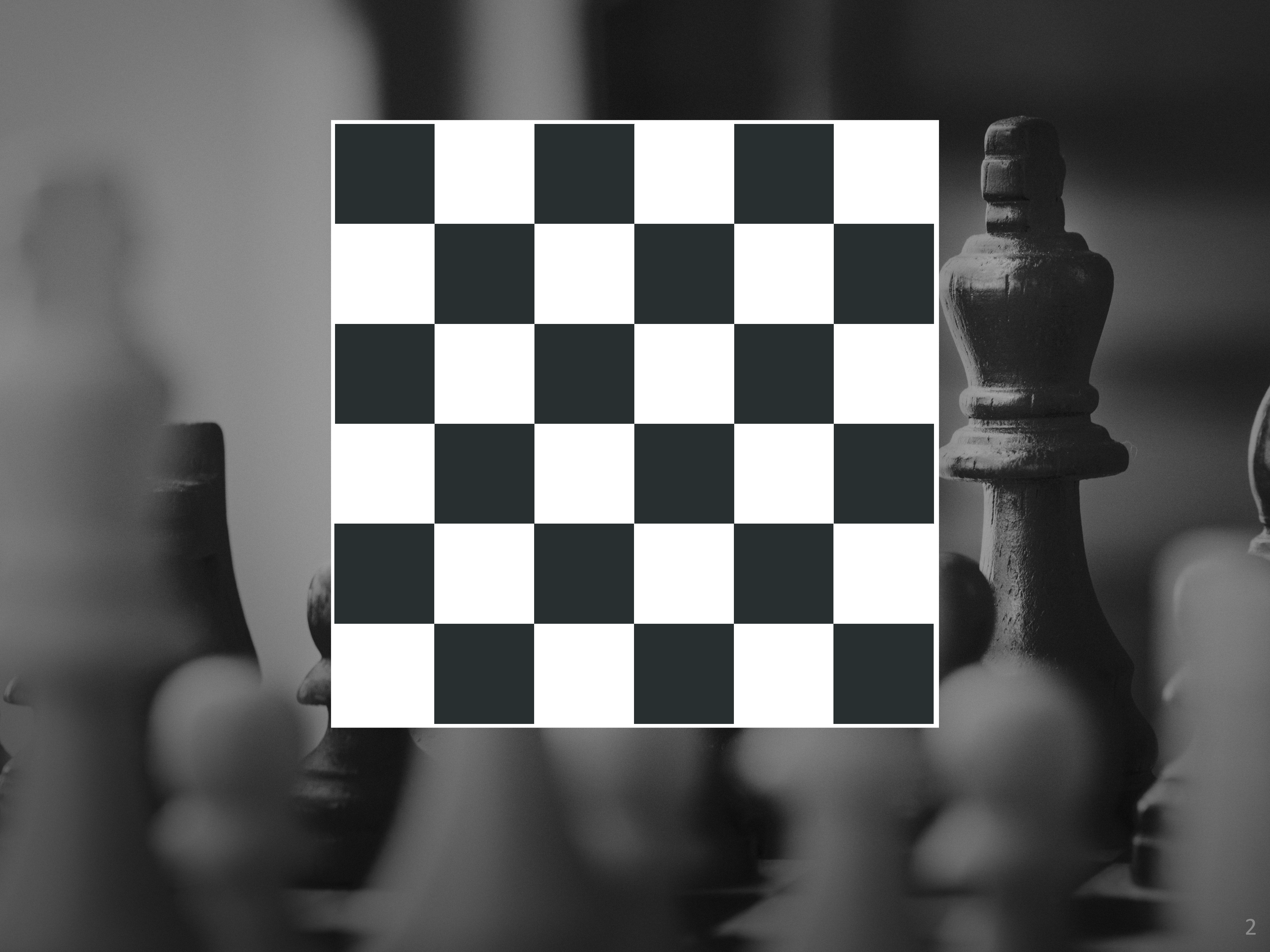
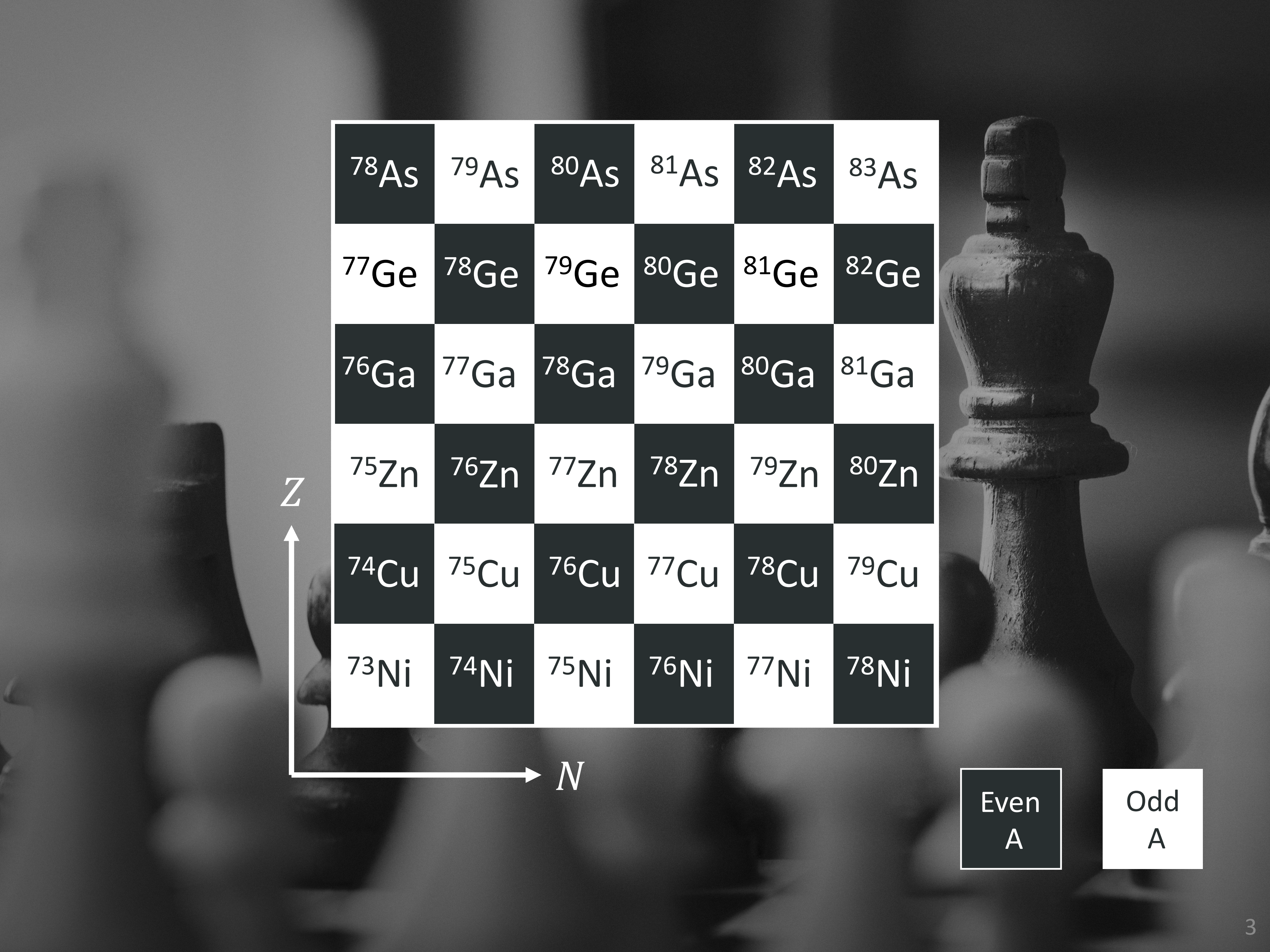
2019. 5. 23





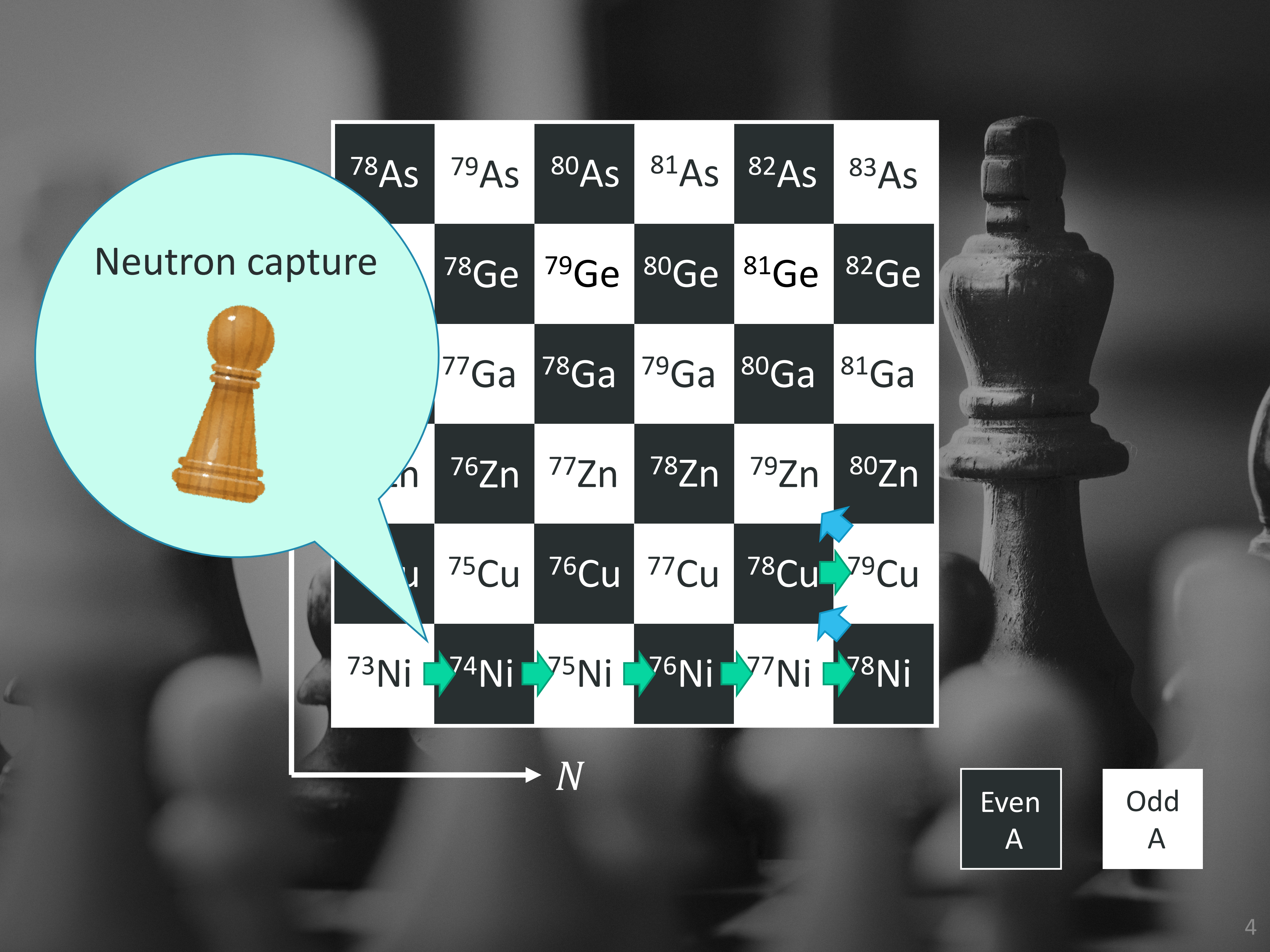
^{78}As	^{79}As	^{80}As	^{81}As	^{82}As	^{83}As
^{77}Ge	^{78}Ge	^{79}Ge	^{80}Ge	^{81}Ge	^{82}Ge
^{76}Ga	^{77}Ga	^{78}Ga	^{79}Ga	^{80}Ga	^{81}Ga
^{75}Zn	^{76}Zn	^{77}Zn	^{78}Zn	^{79}Zn	^{80}Zn
^{74}Cu	^{75}Cu	^{76}Cu	^{77}Cu	^{78}Cu	^{79}Cu
^{73}Ni	^{74}Ni	^{75}Ni	^{76}Ni	^{77}Ni	^{78}Ni

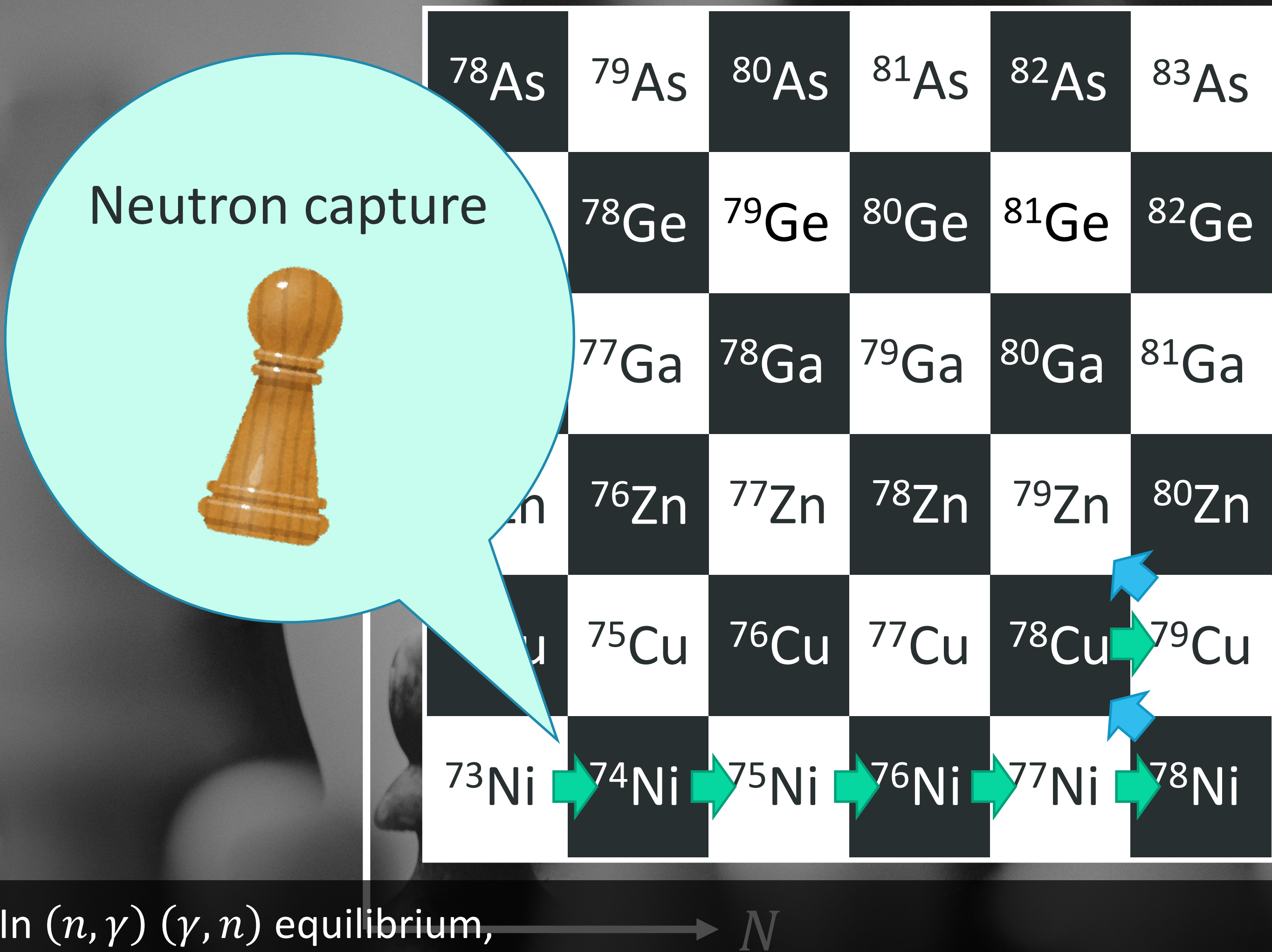
Z

N

Even A

Odd A


Neutron capture
^{78}As ^{79}As ^{80}As ^{81}As ^{82}As ^{83}As
^{78}Ge ^{79}Ge ^{80}Ge ^{81}Ge ^{82}Ge
^{77}Ga ^{78}Ga ^{79}Ga ^{80}Ga ^{81}Ga
^{76}Zn ^{77}Zn ^{78}Zn ^{79}Zn ^{80}Zn
^{75}Cu ^{76}Cu ^{77}Cu ^{78}Cu ^{79}Cu
^{73}Ni ^{74}Ni ^{75}Ni ^{76}Ni ^{77}Ni ^{78}Ni
N
Even A
Odd A



Even A

Odd A

In (n,γ) (γ,n) equilibrium,

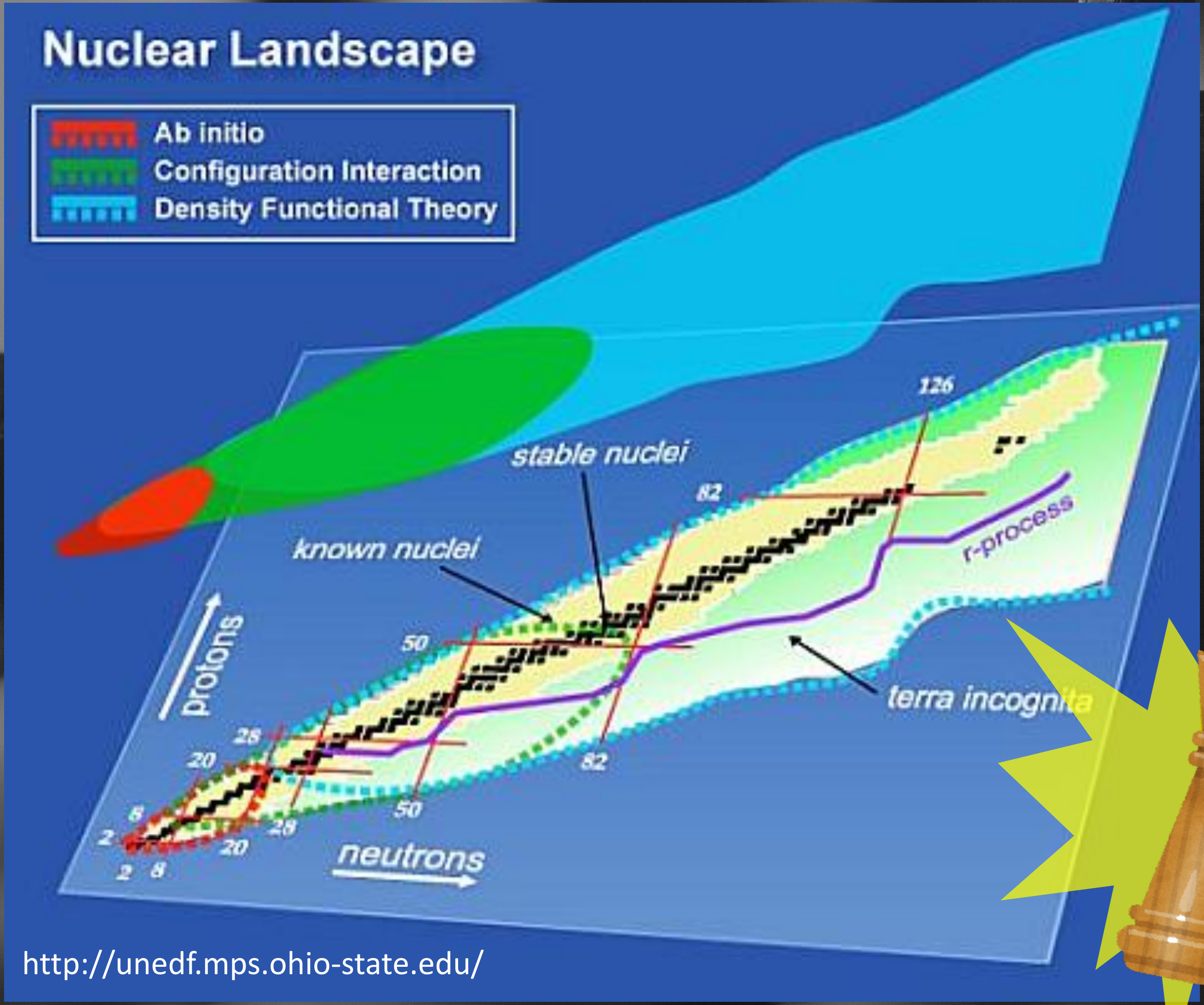
$$\frac{n(Z,A)}{n(Z,A+1)} \propto e^{-\beta S_n(Z,A+1)}$$

abundance ratio

$$S_n(Z,A+1) = B(Z,A+1) - B(Z,A)$$

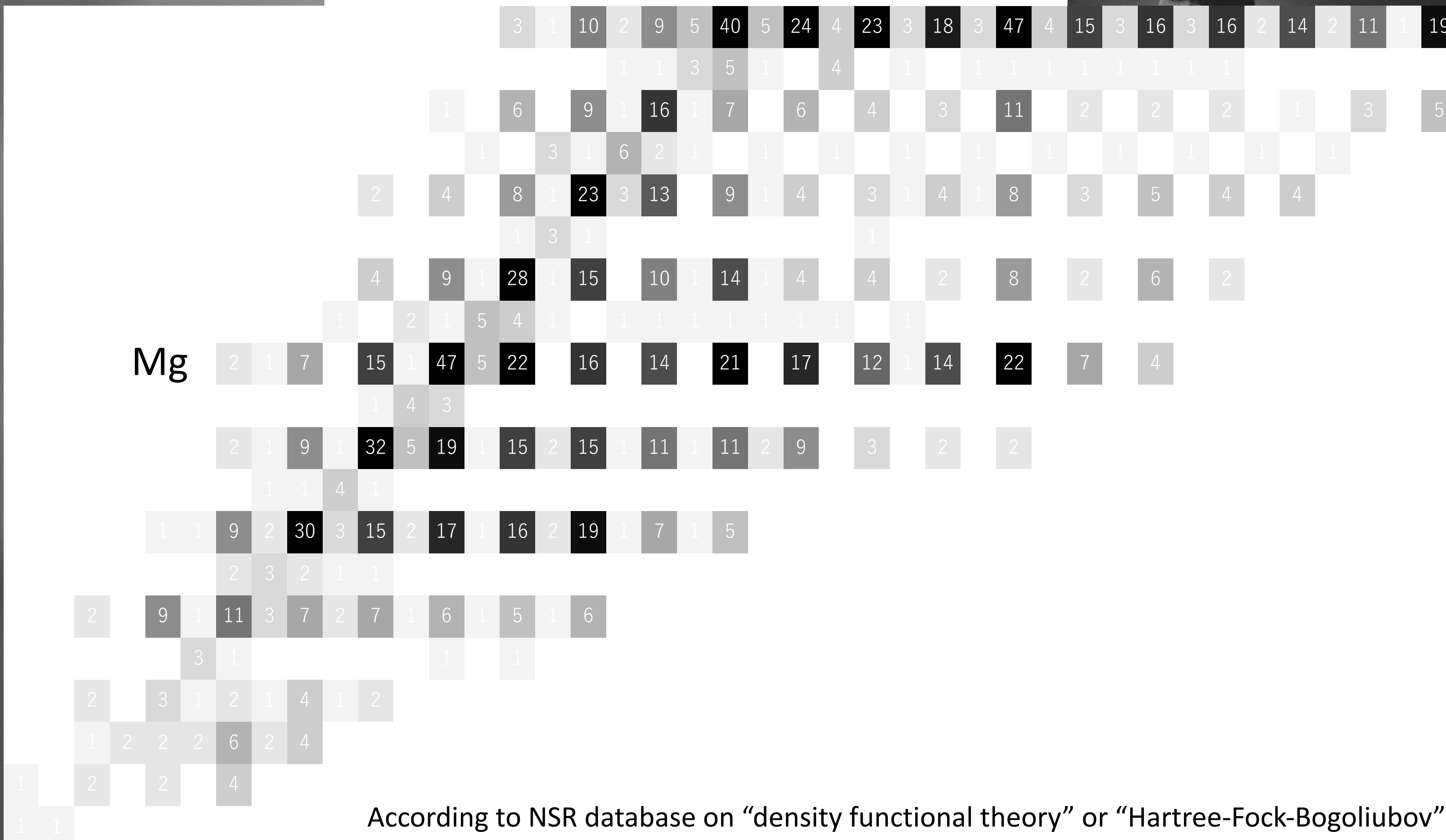
one-neutron separation energy

Density functional theory (DFT) is able to describe all the nuclei in a single framework.



While the nature of even-even nuclei has been studied a lot in a framework of DFT, there have been few DFT studies of odd (and odd-odd) nuclei.

Number of papers based on DFT (1969-2019)



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Density functional theory

$$\hat{N} = \sum_i c_i^\dagger c_i$$
$$\rho_{ij} = \langle c_j^\dagger c_i \rangle$$
$$\kappa_{ij} = \langle c_j \, c_i \rangle$$

Variation

$$\delta\left(E[\rho,\kappa] - \lambda\langle\hat{N}\rangle\right) = 0$$

HFB equation

Hartree-Fock-Bogoliubov

$$\begin{pmatrix} h - \lambda 1 & \Delta \\ -\Delta^* & -h^* + \lambda 1 \end{pmatrix}\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}\begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

$$h_{ij} = \frac{\delta E[\rho,\kappa]}{\delta \rho_{ji}} \quad \Delta_{\mathrm{ij}} = \frac{\delta E[\rho,\kappa]}{\delta \kappa_{ij}^*}$$

$$E = \begin{pmatrix} E_1 & & 0 \\ & E_2 & \\ 0 & & \ddots \end{pmatrix}$$

Number parity

[Ring and Schuck pp.249 – 250]

HFB equation

$$\begin{pmatrix} h-\lambda 1 & \Delta \\ -\Delta^* & -h^*+\lambda 1 \end{pmatrix}\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}\begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

Bloch-Messiah theorem: $\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix}\begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix}\begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}$

$$|\Phi\rangle = \prod_{k=1}^{N_1} a_k^\dagger \prod_{p=1}^{N_2} (u_p + v_p a_p^\dagger a_{\bar{p}}^\dagger)|0\rangle \quad \Rightarrow \quad \det\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = (-1)^{N_1}$$

HFB vacuum

number parity

$\det\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = +1 \quad \Longleftrightarrow$ Superposition of even-particle-number states

$\det\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = -1 \quad \Longleftrightarrow$ Superposition of odd-particle-number states

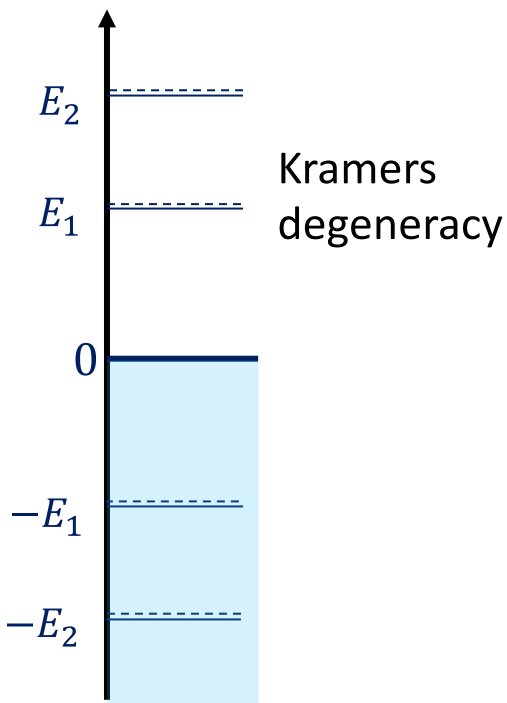
Blocking

[B. Banerjee, P. Ring, and H. J. Mang, Nucl. Phys. A221, 564 (1974).]

HFB equation

$$\begin{pmatrix} h-\lambda 1 & \Delta \\ -\Delta^* & -h^*+\lambda 1 \end{pmatrix}\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}\begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

A system with time-reversal symmetry: $\det\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = +1$ for the ground state



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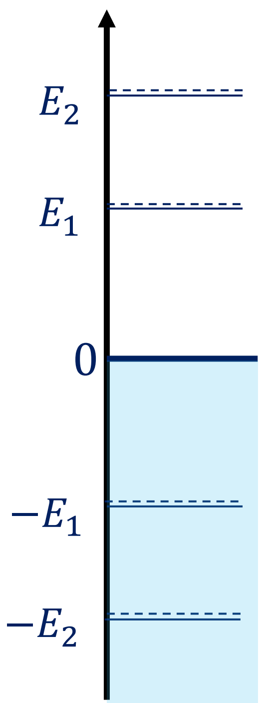
A system with time-reversal symmetry: $\det\begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = +1$ for the ground state

⇓ replace columns $\begin{pmatrix} U_k \\ V_k \end{pmatrix}$ and $\begin{pmatrix} V_k^* \\ U_k^* \end{pmatrix}$

$$\det\begin{pmatrix} U' & V'^* \\ V' & U'^* \end{pmatrix} = -1$$



Kramers degeneracy

Conventional method

An odd-number-parity state is obtained as a one-quasiparticle excited state by breaking a pair.

Variation under a time-odd external field

A system with a conserved symmetry $\hat{S}$ having time-odd character: $T\hat{s}T^{-1} = -\hat{s}$

$$\left(\hat{S} = \sum_{ij} \langle i|\hat{s}|j\rangle c_i^\dagger c_j \right)$$

Variation

$$\delta\left(E[\rho,\kappa] - \lambda\langle\hat{N}\rangle - \lambda_s\langle\hat{S}\rangle\right) = 0$$

HFB equation

$$\left[\begin{pmatrix} h-\lambda 1 & \Delta \\ -\Delta^* & -h^*+\lambda 1 \end{pmatrix} - \lambda_s\Omega_\mu \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]\begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = \left(E_\mu - \lambda_s\Omega_\mu\right)\begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}$$

Ω_μ: an eigenvalue of $\hat{S}$

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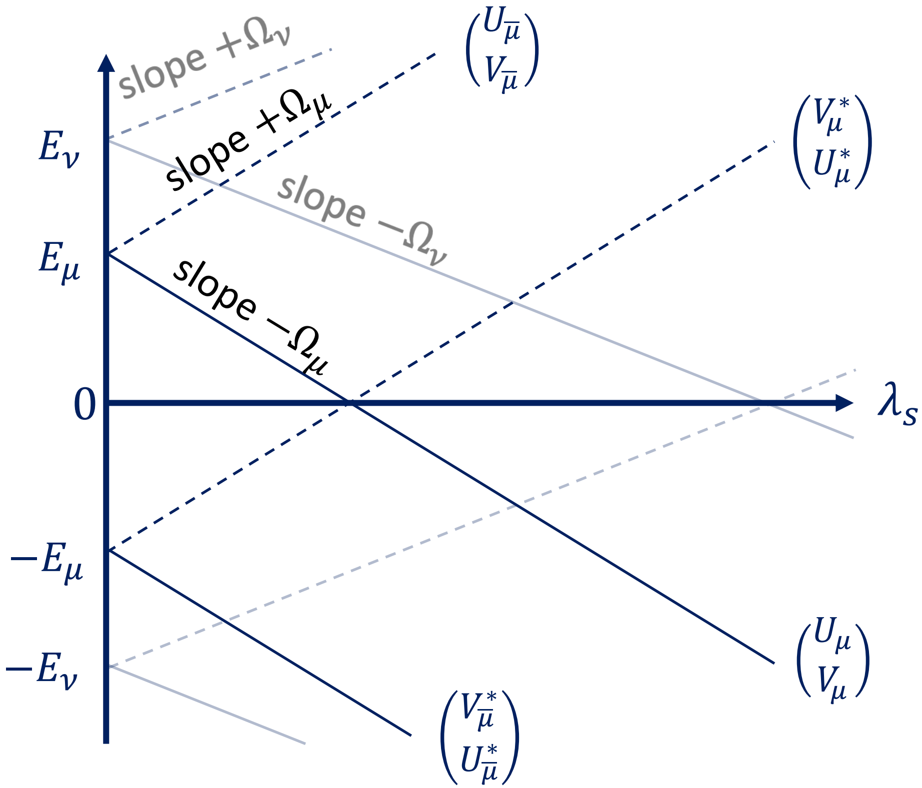

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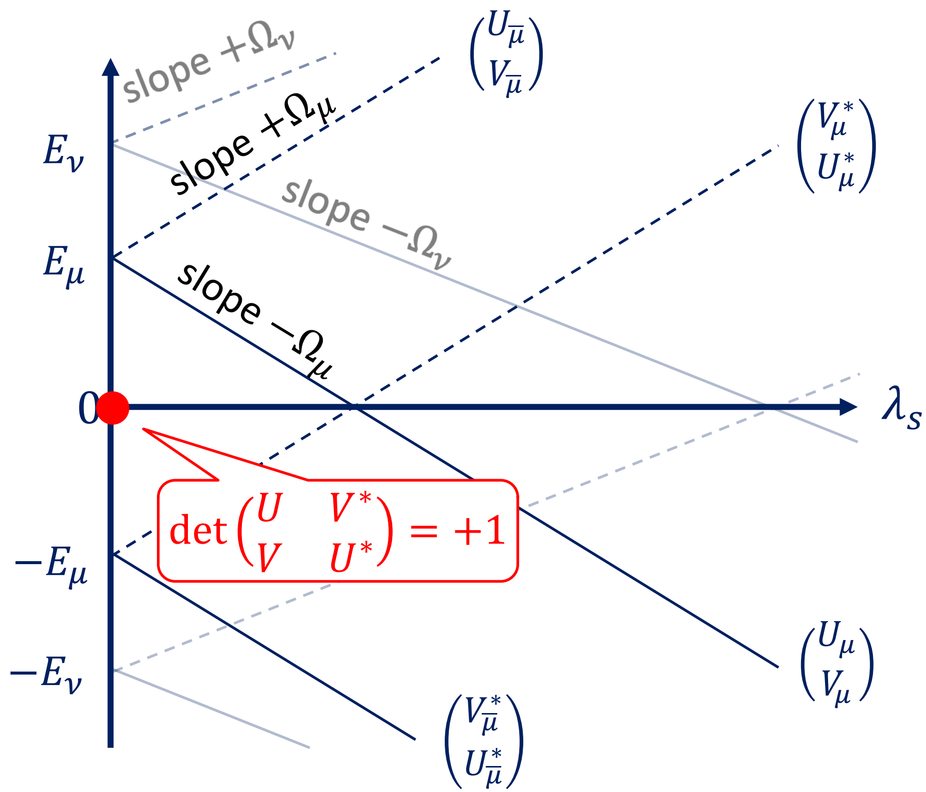

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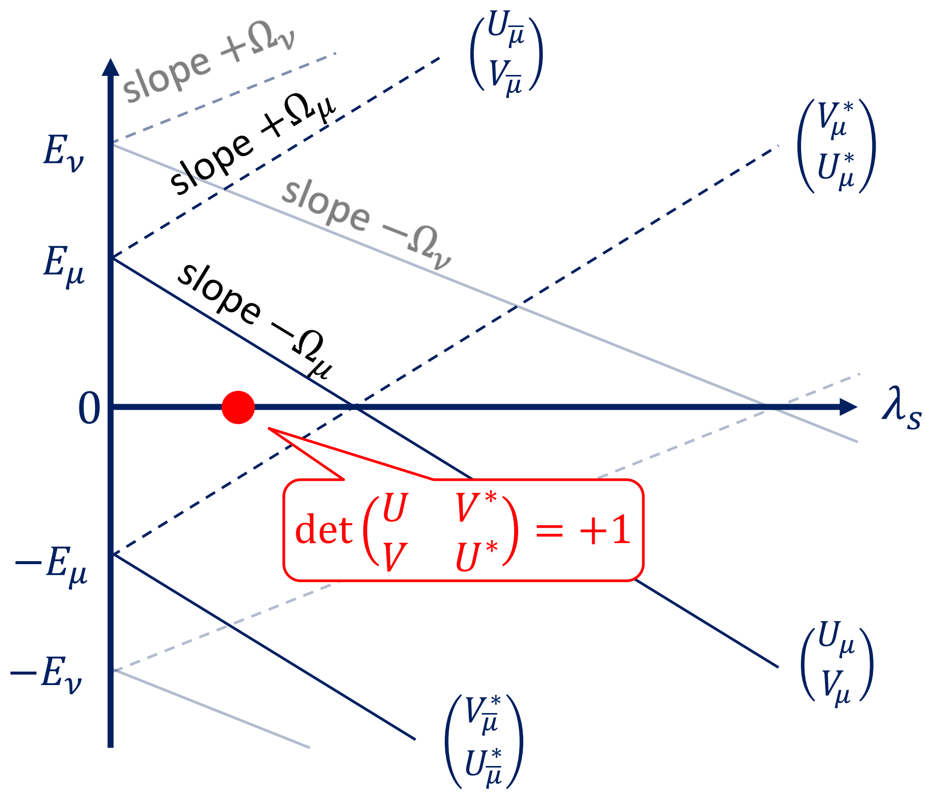

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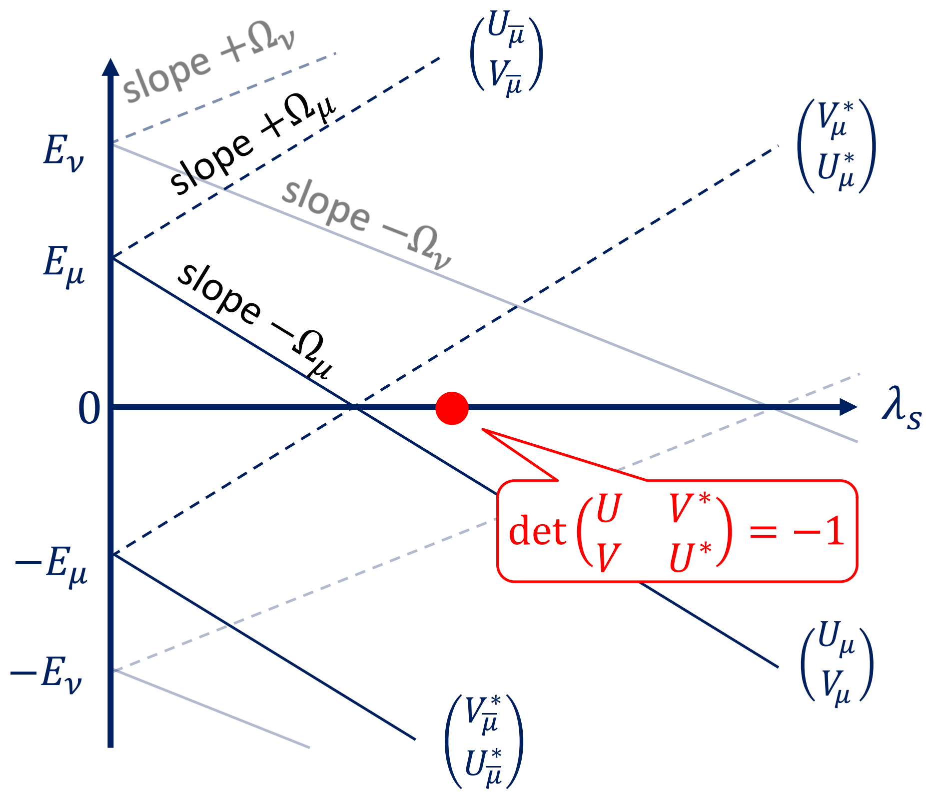
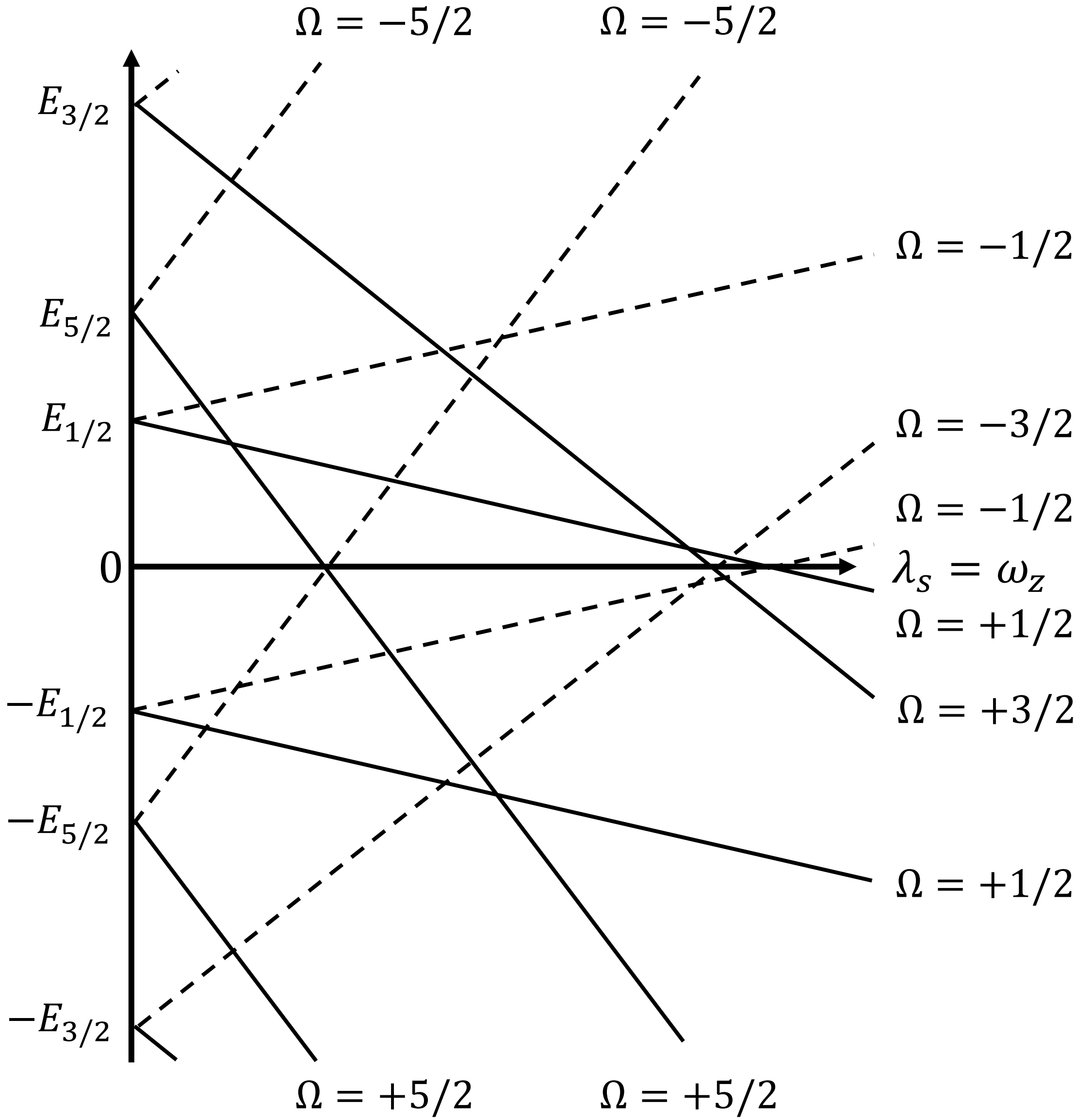


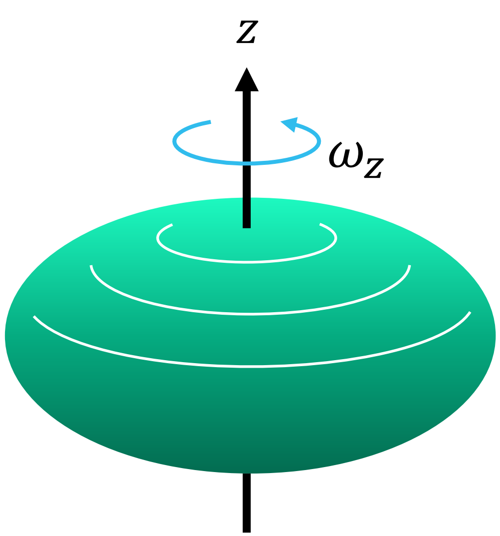
Our method

An odd-number-parity state is automatically obtained as the ground state under an appropriate external field by variation.

Example 1: $\hat{s} = J_z$



high-*K* state is preferably described

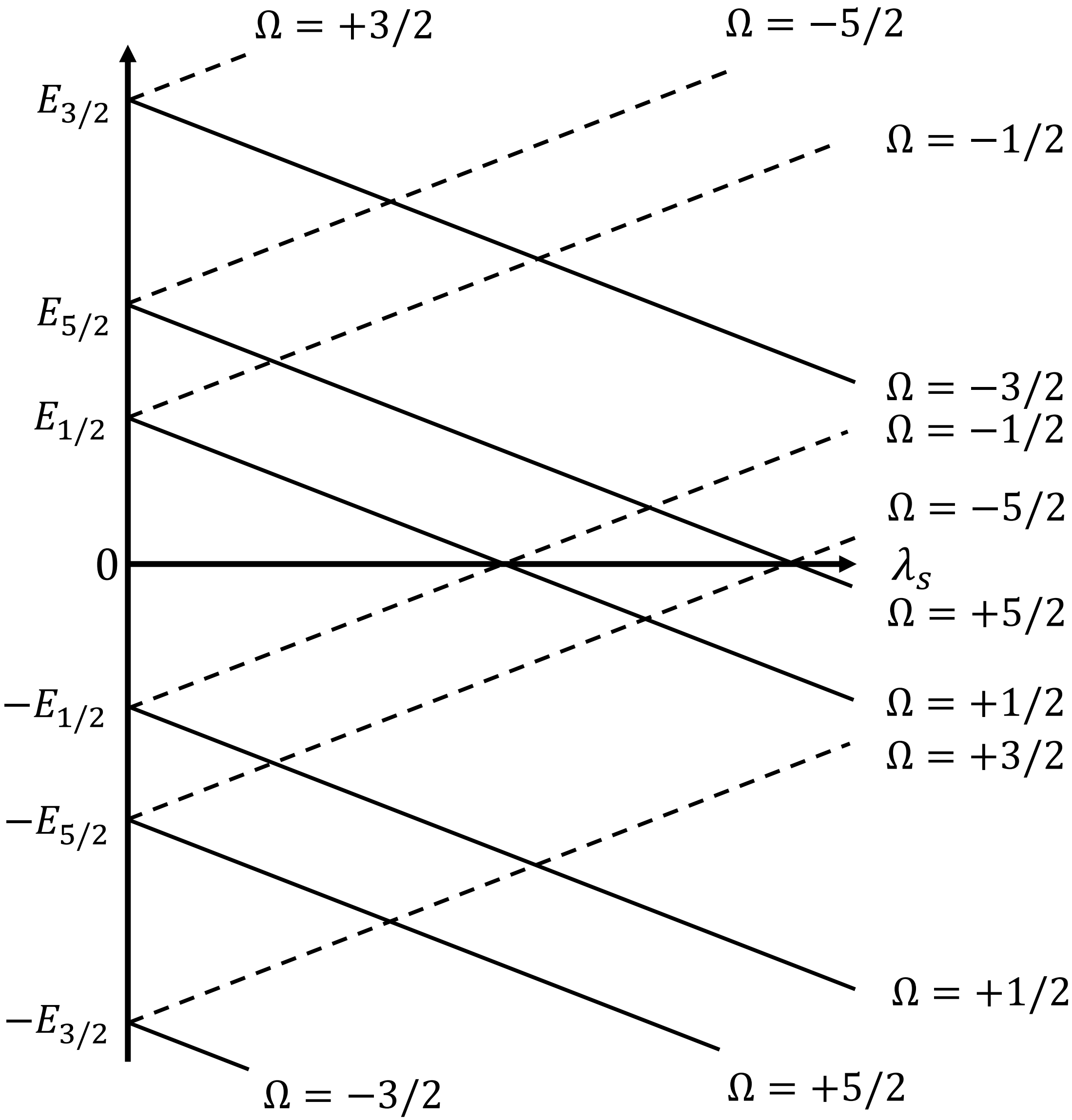


Noncollective cranking

Example 2: $\hat{s} = i\hat{R}_z$

Two-Fermi-level approach

[G. Bertsch, J. Dobaczewski, W. Nazarewicz and, J. Pei, Phys. Rev. A 79, 043602 (2009).]



Signature op. $\hat{R}_z = e^{-i\pi\hat{J}_z}$

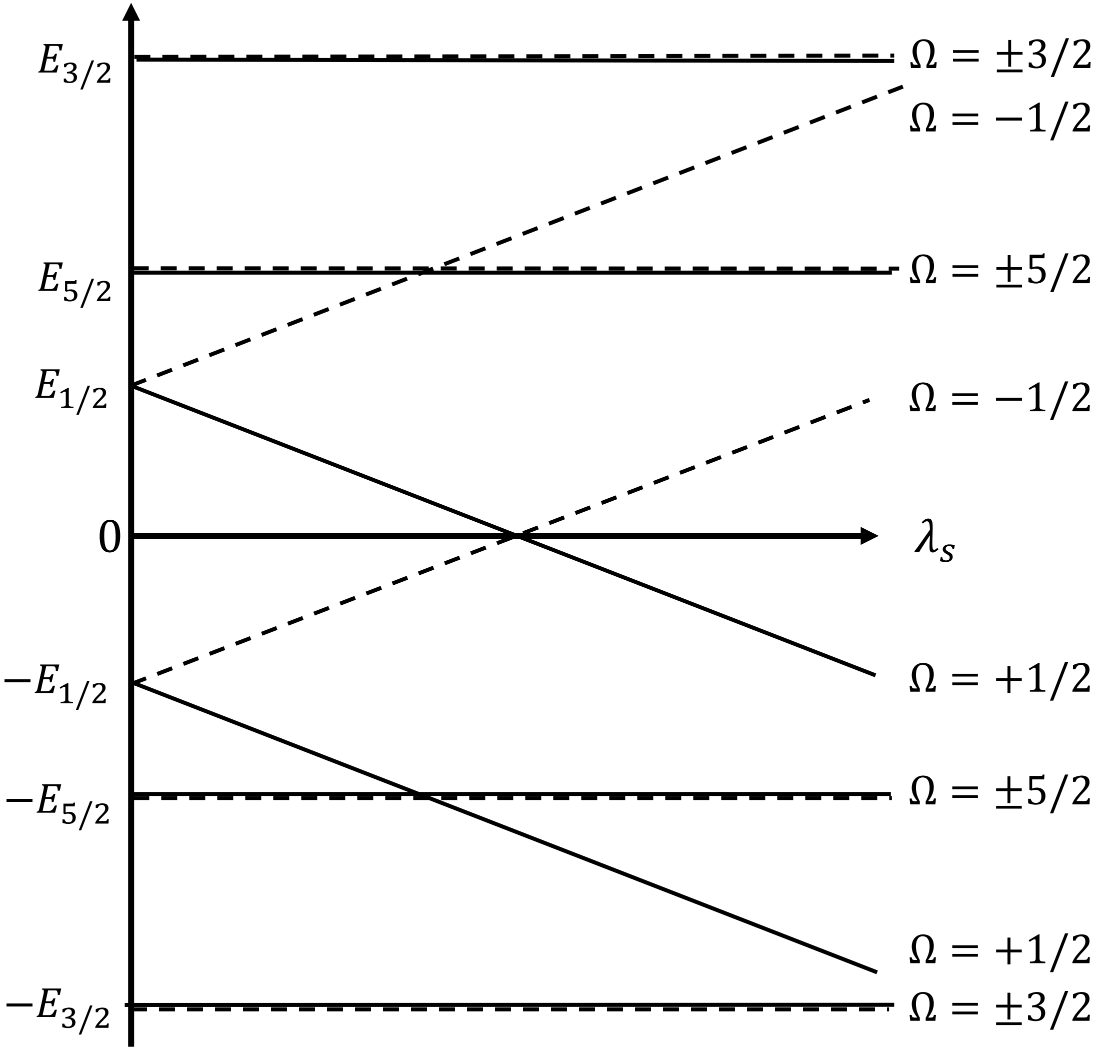
eigenvalue $r = \pm i$

low q.p. energy state is preferably described

if the density of state is high, hard to obtain the convergence

if levels are degenerate more than two, unable to obtain one q.p. state

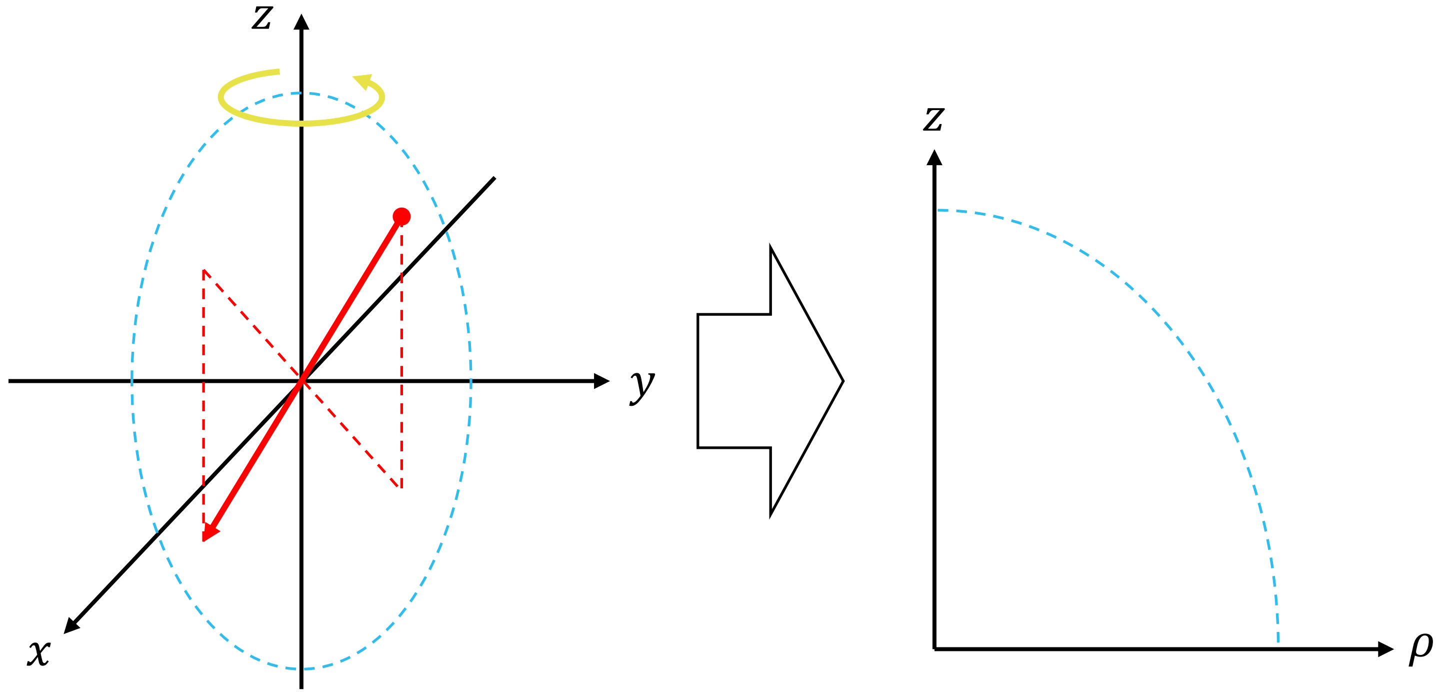
Example 2: $\hat{s} = |\Omega = 1/2\rangle\langle\Omega = 1/2| - |\Omega = -1/2\rangle\langle\Omega = -1/2|$



can select the state of interest

convenient for practical use

Axially deformed HFB code



Base	$\lvert \boldsymbol{r}\sigma\tau \rangle$
Symmetry	Axial, Parity
Interaction	Skyrme (SLy4) + density dependent delta pairing
Initial state	Nilsson (Non-isotropic HO+LS+ℓ^2)

Skyrme energy density functional

$$\langle\Phi|H|\Phi\rangle = \int d\boldsymbol{r}\,\left(H(\boldsymbol{r}) + \widetilde{H}(\boldsymbol{r})\right)$$

$$H(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\boldsymbol{r}) + \mathcal{H}_1(\boldsymbol{r})$$

$$\rho_0 = \rho_n + \rho_p$$

$$\rho_1 = \rho_n - \rho_p$$

$$\mathcal{H}_t(\boldsymbol{r}) = \mathcal{H}_t^{\mathrm{even}}(\boldsymbol{r}) + \mathcal{H}_t^{\mathrm{odd}}(\boldsymbol{r})$$ t=0,1

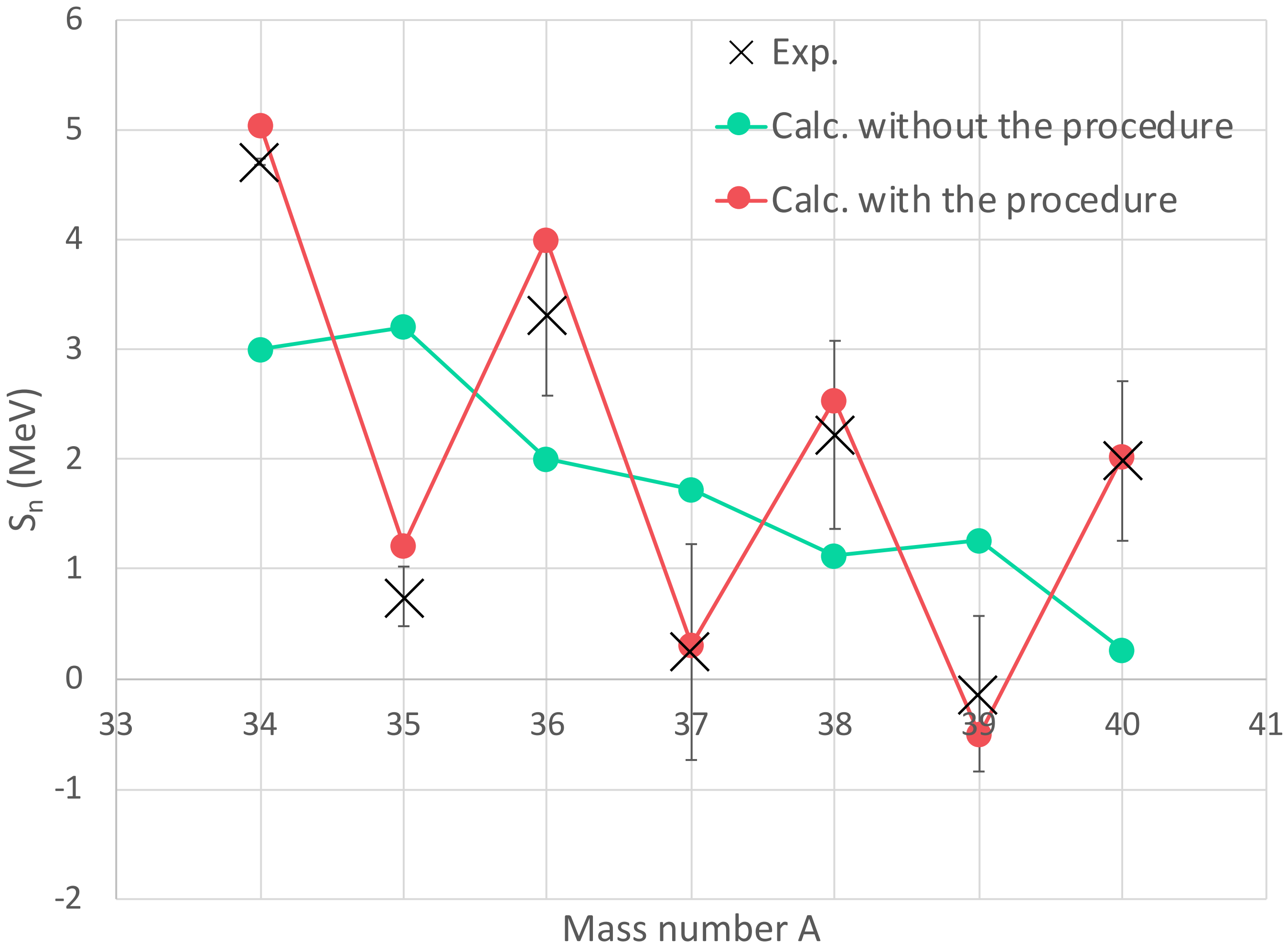
$$\mathcal{H}_t^{\mathrm{even}}(\boldsymbol{r}) = C_t^{\rho}[\rho_0]\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}\boldsymbol{J}_t^2 + C_t^{\nabla J}\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$$

$$\mathcal{H}_t^{\mathrm{odd}}(\boldsymbol{r}) = C_t^{s}[\rho_0]\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C_t^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t\cdot(\boldsymbol{\nabla}\times\boldsymbol{j}_t)$$

vanish in the case of even-even nuclei

$$\widetilde{H}(\boldsymbol{r}) = \frac{1}{2}V_0\left[1 - V_1\left(\frac{\rho_0}{\rho_{\mathrm{NM}}}\right)^{\gamma}\right]\sum_{q=p,n}\tilde{\rho}_q^2$$

Calculation results: one-neutron separation energy S_n for Mg isotopes

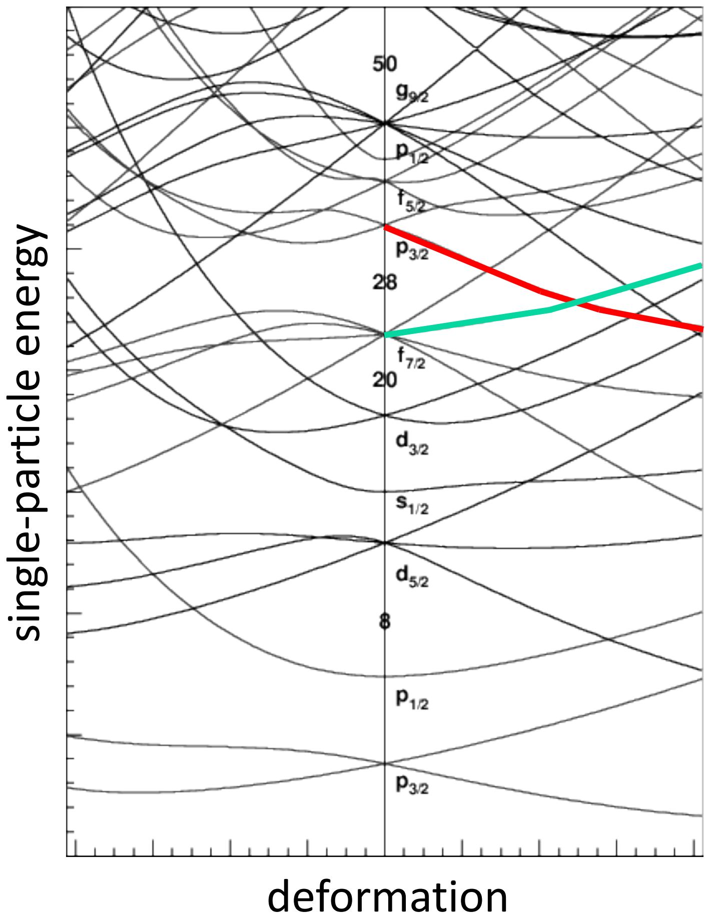


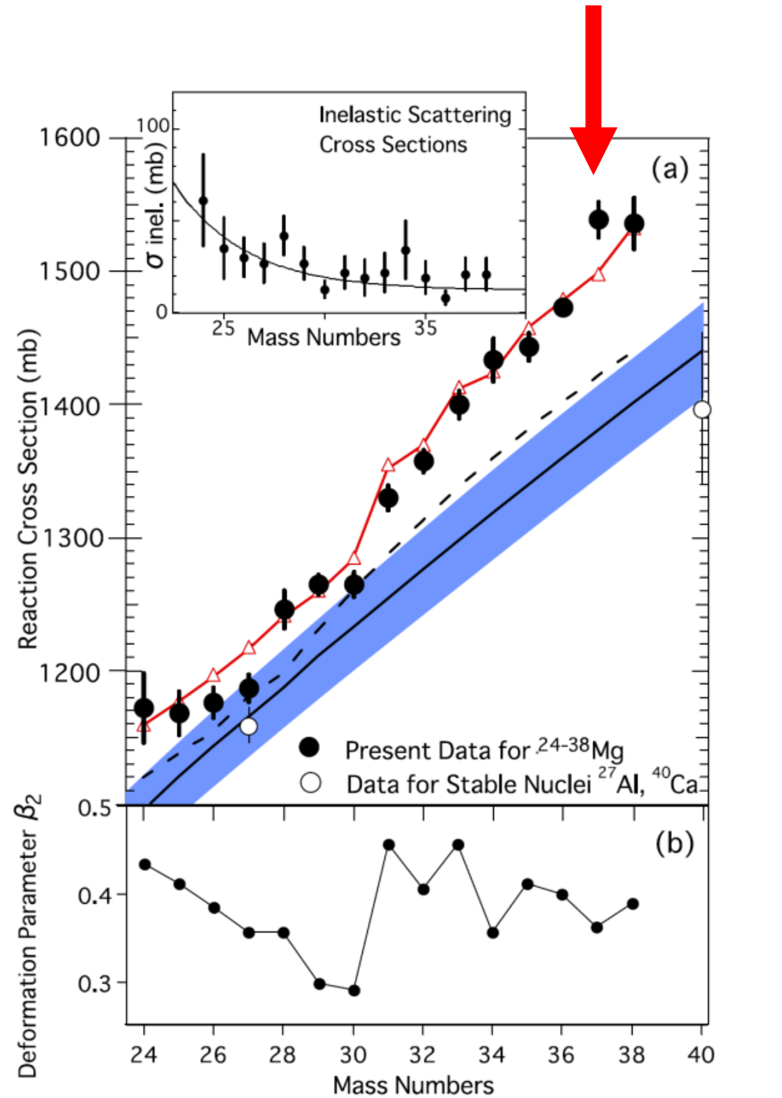
Calculation: deformed halo of ^{37}Mg

[M. Takechi et. al., Phys. Rev. C 90, 061305(R) (2014)]

Measurement of reaction cross section in RIBF suggests that ^{37}Mg has a large neutron radius that is considered to be derived from p-wave.

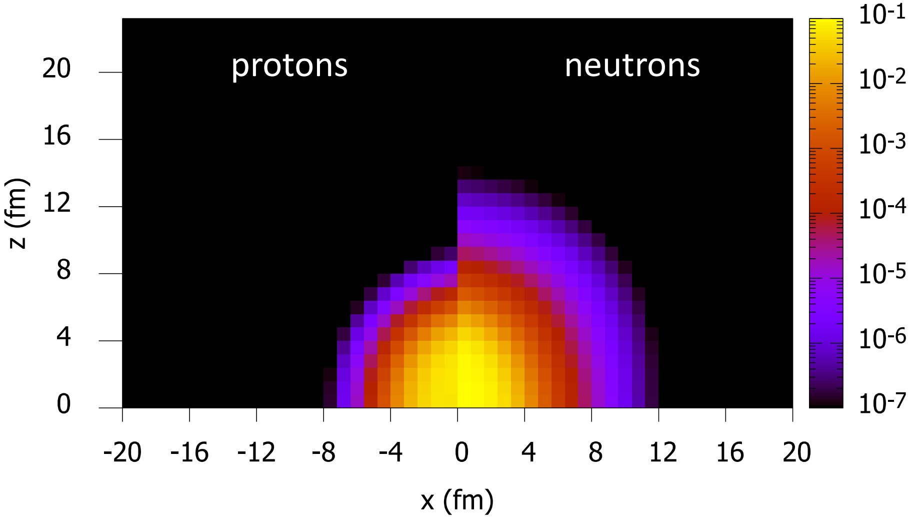
→deformed halo





Calculation: ^{37}Mg

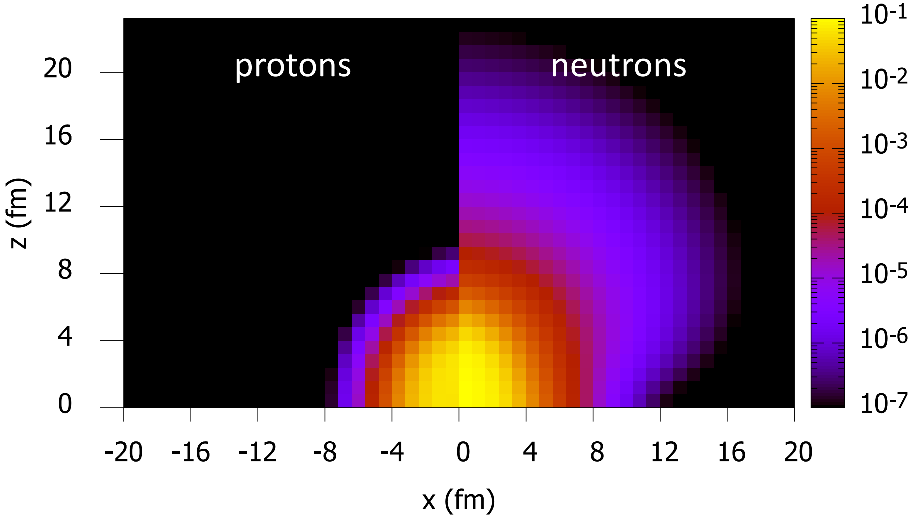
As an even-number-parity state
(superposition of ^{36}Mg and ^{38}Mg)



$$\sqrt{\langle r^2 \rangle_m} = 3.50 \text{ fm}$$

Matter radius

As an odd-number-parity state
(select $\Omega^\pi = 1/2^-$)

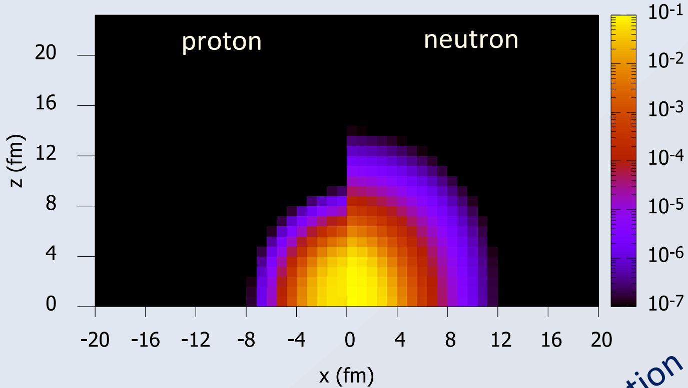


$$\sqrt{\langle r^2 \rangle_m} = 3.57 \text{ fm}$$

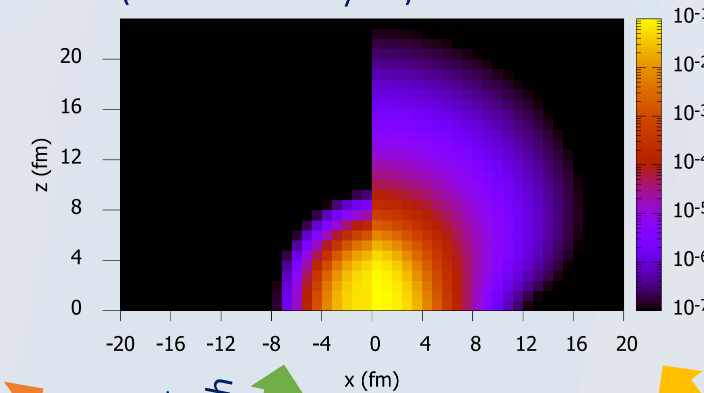
Experiment: $\sqrt{\langle r^2 \rangle_m} = 3.62 \pm 0.03 \text{ fm}$

Calculation results

As an even-number-parity state
(superposition of 36Mg and 38Mg)



As an odd-number-parity state
(select $\Omega^{\pi} = 1/2^{-}$)



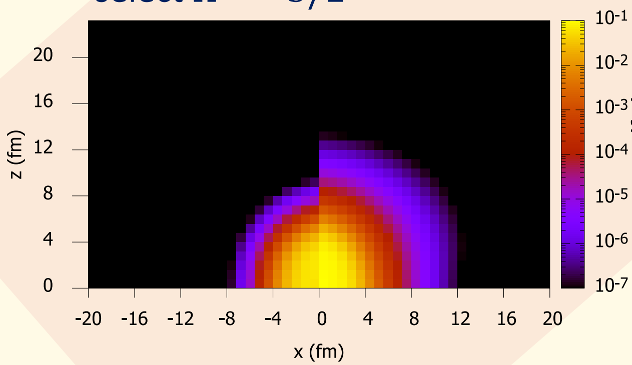
→variation as odd-number-particle system is necessary for emergence of halo

deformation: big / small

Pairing strength: weak / strong

Time-odd term in EDF: ON / OFF

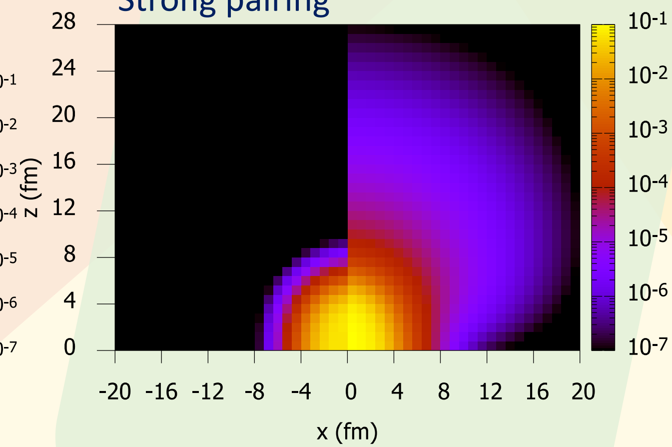
select $\Omega^{\pi} = 5/2^{-}$



→deformation is essential for the formation of halo

centrifugal barrier

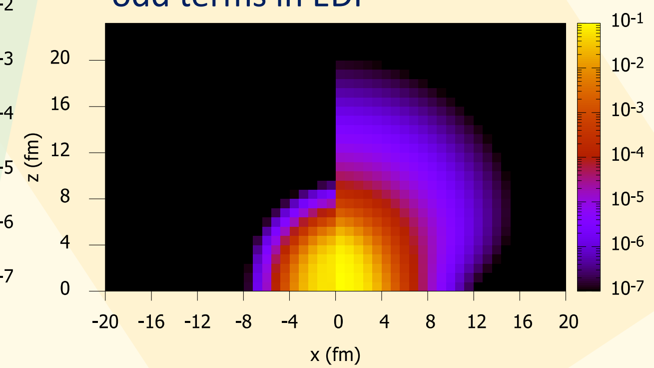
Strong pairing



→ superfluidity develops the halo structure

[Nakada, Takayama, PRC98, 011301 (2018)]

Zero for all coefficients of time-odd terms in EDF



→time-reversal symmetry breaking develops the halo structure

Conclusion

- **密度汎関数理論に基づき、時間反転反対称な拘束の下での最小エネルギー状態として奇核を記述する方法**を考案した。**奇核を偶々核と同様の手順で記述可能**であるので、**既存の偶々核のコードからの拡張が容易**であり、今後の奇核の研究の発展への貢献が期待される。

- **中性子過剰なMg同位体**に上の方法を適用し、原子核質量と一中性子分離エネルギーを計算した。奇核を奇数粒子系として記述することで実験値とよく合う値が得られた。

- 今後は、ｒプロセスに関わるような**より重い核**の計算や、得られた奇核の基底状態の上での**QRPA計算**をしてゆきたい。

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Densities

$$\rho(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = \langle\Phi|c^{\dagger}_{\boldsymbol{r}'\sigma'\tau'}c_{\boldsymbol{r}\sigma\tau}|\Phi\rangle$$

$$\tilde{\rho}(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = \langle\Phi|c_{\overline{\boldsymbol{r}'\sigma'\tau'}}c_{\boldsymbol{r}\sigma\tau}|\Phi\rangle$$

time even

$$\rho_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\langle\sigma'|1|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\tau_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \{\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|1|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$J_{q\,\mu\nu}(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \frac{1}{2i}\{(\nabla_\mu - \nabla'_\mu)\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|\sigma_\nu|\sigma\rangle\,\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\tilde{\rho}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \tilde{\rho}(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\langle\sigma'|1|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

time odd

$$\boldsymbol{s}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\langle\sigma'|\boldsymbol{\sigma}|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\boldsymbol{T}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \{\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|\boldsymbol{\sigma}|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\boldsymbol{j}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \frac{1}{2i}\{(\boldsymbol{\nabla} - \boldsymbol{\nabla}')\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|1|\sigma\rangle\,\delta(\boldsymbol{r}' - \boldsymbol{r})$$