Self-consistent multiparticle-multihole configuration mixing description of nuclei

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Introduction

Self-consistent Multiparticle-Multihole Configuration Mixing Method (MPMH):

★ Method applied in atomic physics and quantum chemistry:
↠ Multi-Configuration Hartree-Fock (MCHF), Multi-Configuration Self-Consistent Field (MCSCF)

★ Based on the determination of a Configuration Interaction (CI) wave function ➡ allows:

- explicit symmetry preservations (particle number, spherical symmetry, Pauli principle),
- indiscriminate treatment of long-range correlations,
- treatment of ground and excited states in even-even, odd-even & odd-odd nuclei on the same footing.

★ The underlying mean-field and the single-particle states evolve with the correlations of the system

➡ **fully self-consistent approach**

Outline

- Formalism of the MPMH method

  → *role and interpretation of the orbital optimization*

- Applications with the Gogny D1S interaction

  - Numerical algorithm
    → *doubly iterative convergence process*

  - Description of even-even sd-shell nuclei
    → *Effect of the orbital optimization on ground and excited states properties: Charge radii, excitation energies, transition probabilities, inelastic electron and proton scattering…*

- *Towards an "ab-initio" theory*

  → *implementation of a chiral interaction: preliminaries*

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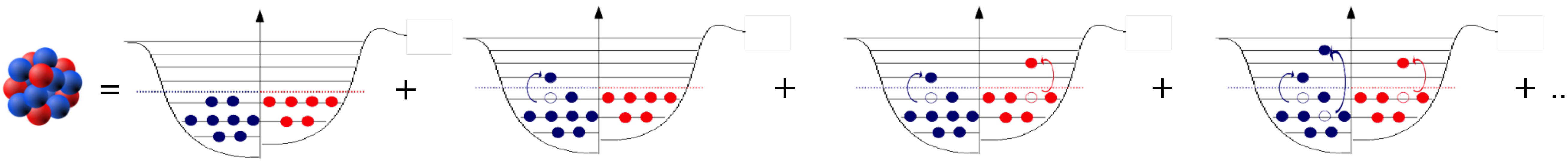
MPMH method: Formalism

* **Trial wave function $|\Psi\rangle$ = superposition of Slater determinants**

$$|\Psi\rangle = A_{0p0h}|\Phi_{0p0h}\rangle + \sum_{1p1h} A_{1p1h}|\Phi_{1p1h}\rangle + \sum_{2p2h} A_{2p2h}|\Phi_{2p2h}\rangle + \sum_{3p3h} A_{3p3h}|\Phi_{3p3h}\rangle + \ldots$$



$$|\Phi_{0p0h}\rangle = \prod_i a_i^\dagger |0\rangle$$

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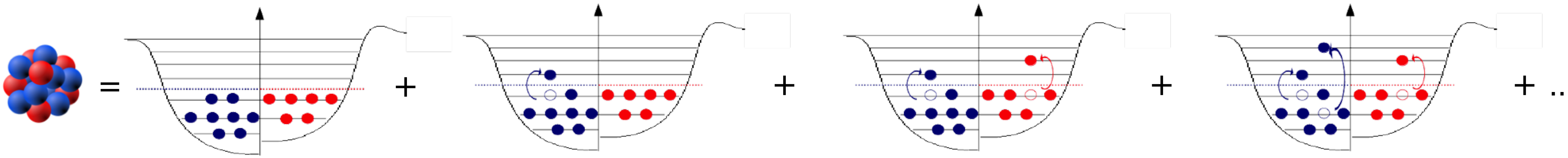

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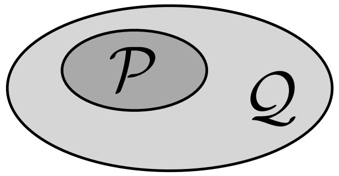
Combinatorial growth of the number of configurations $\Longrightarrow$ select the most relevant ones

Possible truncation schemes:

- *Core + Valence space*
- *Excitation order (Np-Nh)*
- *Excitation energy*
- *etc (symmetry-constrained)*

→ *defines subspace $\mathcal{P}$ of Hilbert space*

$\mathcal{H} =$ 

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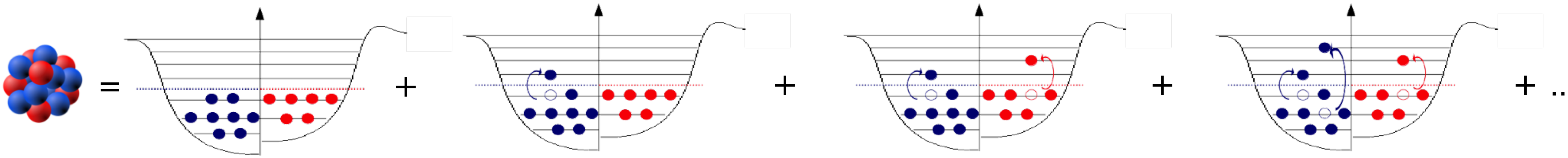

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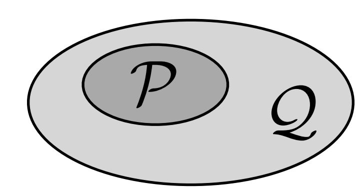
$\mathcal{H} =$ 

Unknowns?

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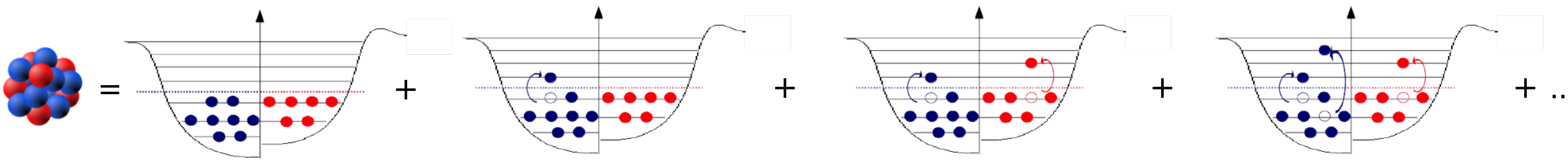

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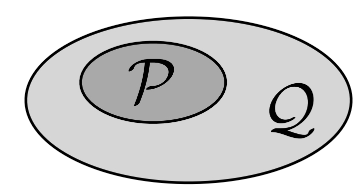
$\mathcal{H} =$ 

Unknowns? $\Big\{$ The mixing coefficients $\{A_\alpha\}$

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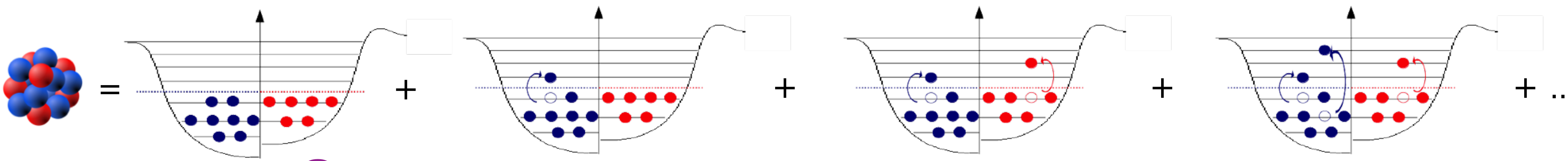

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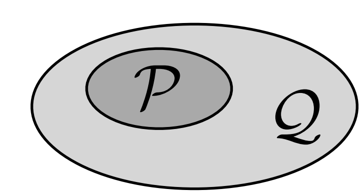
$\mathcal{H} =$ 

Unknowns?

- The mixing coefficients $\{A_\alpha\}$
- The single-particle states $\{\varphi_i\}$

MPMH method: Formalism

✱ ***Variational principle applied to the energy of the system:*** $\mathcal{E}[\Psi] = \langle\Psi|\hat{H}|\Psi\rangle = 0$

➡ Two *coupled* equations to solve:

$$\begin{cases} \delta\mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0 \\ \delta\mathcal{E}[\Psi]_{/\{\varphi^*_i\}} = 0 \end{cases}$$

Note: formalism shown here for a 2-body Hamiltonian

derivations for 2-body density-dependent or 3-body interaction available
in *C.R., N. Pillet, D. Peña Arteaga & J.-F. Berger, PRC 93, 024302 (2016).*

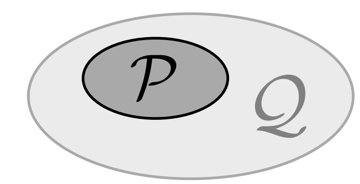
MPMH method: Formalism

Usual
CI diagonalization

★ ***1st variational equation: The mixing coefficients***

$$\delta\mathcal{E}[\Psi]_{/\{A_\alpha^*\}} = 0 \;\Rightarrow\; \sum_\beta A_\beta \langle \phi_\alpha | \hat{H} | \phi_\beta \rangle = E A_\alpha$$

$$\begin{pmatrix} & & \\ & H & \\ & & \end{pmatrix} \begin{pmatrix} \\ A \\ \\ \end{pmatrix} = E \begin{pmatrix} \\ A \\ \\ \end{pmatrix}$$



➡ introduces explicit correlations in restricted configuration space $\mathcal{P}$

All types of long-range correlations are treated at the same time:

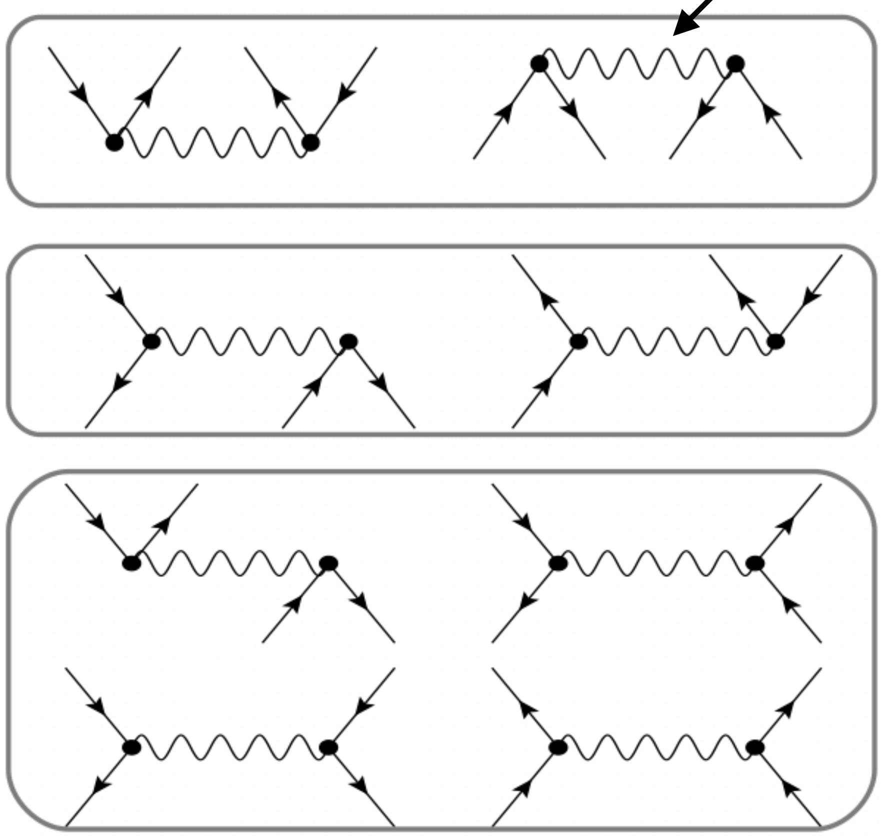
Interaction vertex $\langle \phi_\alpha | \hat{V} | \phi_\beta \rangle$

Excitation order of the configuration

$|n_\alpha - n_\beta| = 2$

$|n_\alpha - n_\beta| = 1$

$|n_\alpha - n_\beta| = 0$



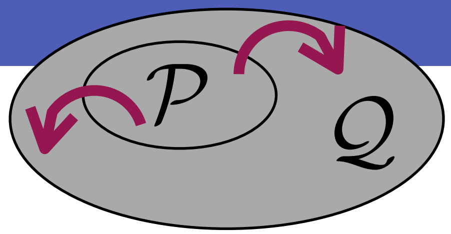
RPA, pairing

Particle-vibration coupling

RPA

Pairing

MPMH method: Formalism



★ 2nd variational equation: The single-particle states

✦ variation of the single-particle states:

$$a_i^\dagger \to e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}} \quad \Rightarrow \delta a_i^\dagger = i\left[\hat{T}, a_i^\dagger\right]$$

T = hermitian 1-body operator

✦ 1st order variation of the many-body wave function:

$$|\delta\Psi\rangle = i\hat{T}|\Psi\rangle_{\mathcal{P}}$$
$$= |\delta\Psi\rangle_{\mathcal{P}} + |\delta\Psi\rangle_{\mathcal{Q}}$$

↠ <u>*Note:*</u> $\delta\mathcal{E}[\Psi]_{/\{\varphi_i^*\}} = {}_{\mathcal{P}}\langle\Psi|\hat{H}|\delta\Psi\rangle + \langle\Psi|\hat{H}|\delta\Psi\rangle_{\mathcal{P}}$

$$= {}_{\mathcal{P}}\langle\Psi|\hat{P}\hat{H}\hat{P}|\delta\Psi\rangle_{\mathcal{P}} + {}_{\mathcal{P}}\langle\Psi|\hat{P}\hat{H}\hat{P}|\delta\Psi\rangle_{\mathcal{P}} + {}_{\mathcal{P}}\langle\Psi|\hat{P}\hat{H}\hat{Q}|\delta\Psi\rangle_{\mathcal{Q}} + {}_{\mathcal{Q}}\langle\Psi|\hat{Q}\hat{H}\hat{P}|\delta\Psi\rangle_{\mathcal{P}}$$

↠ the orbital optimization takes into account the coupling H_{PQ}/H_{QP} between P and Q spaces (however not H_{QQ})

$$\delta\mathcal{E}[\Psi]_{/\{\varphi_i^*\}} = \langle\Psi|\left[\hat{H}, \hat{T}\right]|\Psi\rangle = 0 \quad \Longleftrightarrow \quad \left[\hat{h}(\rho), \hat{\rho}\right] = \hat{G}(\sigma)$$

"Generalized Brillouin condition"

Generalized mean-field equation

MPMH method: Formalism

Generalized mean-field equation

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MPMH method: Formalism

Generalized mean-field equation

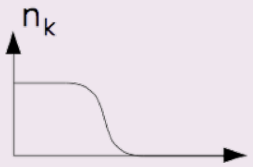
$$\left[\hat{h}(\rho), \hat{\rho}\right] = \hat{G}(\sigma)$$

correlated one-body density

$$\rho_{ki} = \langle \Psi | a_i^\dagger a_k | \Psi \rangle$$

➡ "natural" basis

➡ occupation numbers



MPHM method: Formalism

Generalized mean-field equation

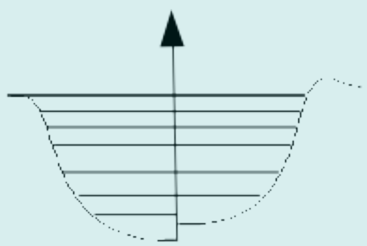
$$\left[\hat{h}(\rho), \hat{\rho}\right] = \hat{G}(\sigma)$$

general mean field

$$h_{ij}(\rho) = K_{ij} + \sum_{kl} \langle ik|\widetilde{V}|jl\rangle \rho_{lk}$$

contribution from particles & holes

➡ single-particle energies



$$\varepsilon_a = \sum_N |\langle \Psi_N^{A+1}|a_a^\dagger|\Psi\rangle|^2 (E_N^{A+1} - E)$$
$$+ \sum_M |\langle \Psi_M^{A-1}|a_a|\Psi\rangle|^2 (E - E_M^{A-1})$$

= centroid of one-nucleon separation energies
= "most unambiguous definition of single-particle energies"

(Baranger (1970), Duguet & Hagen (2012)...)

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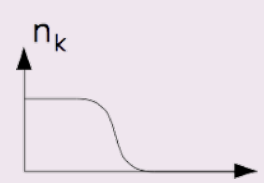

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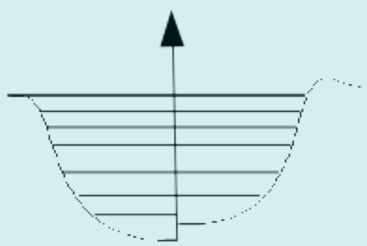

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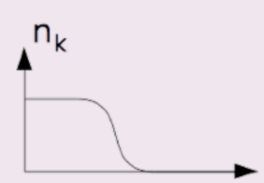

source term

$$G_{ij}(\sigma) = \frac{1}{2} \sum_{klm} \left(\widetilde{V}_{kmjl}\sigma_{kiml} - \widetilde{V}_{kiml}\sigma_{jlkm} \right)$$

σ = two-body correlation matrix

$$\sigma_{kiml} = \langle \Psi | a_i^\dagger a_m^\dagger a_l a_k | \Psi \rangle - (\rho_{ki}\rho_{lm} - \rho_{km}\rho_{li})$$

MPMH method: Formalism

Generalized mean-field equation

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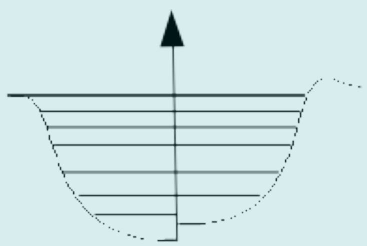

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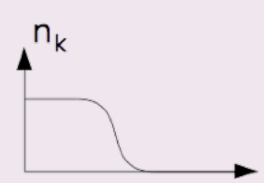

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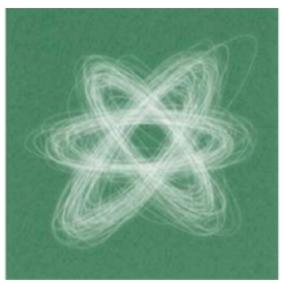
single-particle orbitals *used to build the many-body configurations*



MPMH method: Formalism

★ *Interpretation of the orbital equation:*

General equation in physics:

1-body GF $\mathcal{G}^{(1)}$

Connected 2-body GF $\mathcal{G}_C^{(2)}$

Equation of motion for the one-body Green's function (at equal times) $\Rightarrow$

$$\boxed{\left[h(\rho),\rho\right] = G(\sigma)}$$

$\Rightarrow$ Renormalization of the one-body propagator

—

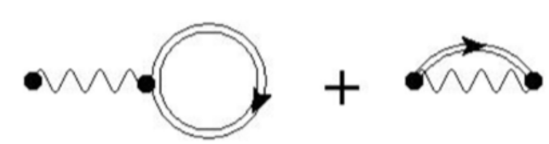
equivalent to solving a Dyson equation

Self-energy: $\Sigma(t_1 - t_2) = \Sigma^{(0)}\delta(t_1 - t_2) + \Sigma^{(dyn)}(t_1 - t_2)$

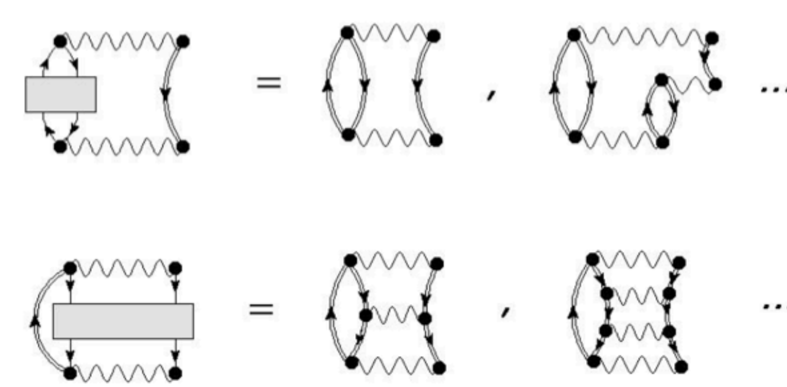
Static part

Dynamical part

- $\Gamma_{ij}(\rho) = \sum_{kl} \langle ik|\widetilde{V}|jl\rangle \rho_{kl} = \Sigma^{(0)}_{ij}$



- $G(\sigma) = \lim_{t_2 \to t_1^+} \int dt \left[\mathcal{G}^{(1)}(t - t_2), \Sigma^{(dyn)}(t_1 - t)\right]$



➡ ***Consistency between correlations and single-particle picture***

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Application to sd-shell nuclei with the Gogny force

★ Gogny D1S interaction *(Dechargé, Gogny PRC 21, 1568 (1980)):*

$$V[\rho] = \sum_{j=1,2} (W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau)\, e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{\mu_j^2}}$$
$$+t_3(1+x_0 P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)$$
$$+\, iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\times\overleftarrow{\nabla}_{12}(\sigma_1+\sigma_2)$$
$$+\,(1+2\tau_{1z})(1+2\tau_{2z})\frac{e^2}{|\vec{r}_1-\vec{r}_2|}$$

Central part: two gaussians (two ranges μ=0.7 fm and μ=1.2 fm)

Density-dependent term (zero-range, α=1/3)

(many-body effects …)

Spin-Orbit (zero-range)

Coulomb

$$\rightarrow\ \mathcal{E}[\Psi] = \langle\Psi|\hat{H}[\rho]|\Psi\rangle$$

correlated density

Application to sd-shell nuclei with the Gogny force

➡ modified coupled equations to solve:

1) $$\boxed{\delta\mathcal{E}[\Psi]_{/A^*_\alpha} = 0 \Leftrightarrow \sum_\beta A_\beta \langle \phi_\alpha | \hat{H}[\rho] + \hat{\mathcal{R}}[\rho,\sigma] | \phi_\beta \rangle = \lambda A_\alpha}$$

- where $\hat{\mathcal{R}}[\rho,\sigma] = \int d^3r \langle\Psi| \frac{\delta V[\rho]}{\delta\rho(\vec{r})} |\Psi\rangle \hat{\rho}(\vec{r})$

- ρ and σ-dependency ➡ non-linear equation

rearrangement terms

2) $$\boxed{\delta\mathcal{E}[\Psi]_{/\varphi^*_i} = 0 \Leftrightarrow \left[\hat{h}(\rho,\sigma), \hat{\rho}\right] = \hat{G}(\sigma)}$$

- where $h_{ij}(\rho,\sigma) = K_{ij} + \sum_{kl} \langle ik|\widetilde{V}|jl\rangle \rho_{lk} + \frac{1}{4}\sum_{klmn} \langle kl| \frac{\partial \widetilde{V}}{\partial|\rho_{ji}} |mn\rangle \langle\Psi| a^\dagger_k a^\dagger_l a_n a_m |\Psi\rangle$

  ➡ explicit dependence on σ

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MPHM method: Numerical algorithm

The full solution requires a doubly-iterative algorithm:

starting point: Hartree-Fock orbitals

Solve 1st equation

$$\sum_\beta A_\beta \langle \phi_\alpha | \hat{H}[\rho] + \hat{\mathcal{R}}[\rho,\sigma] | \phi_\beta \rangle = \lambda A_\alpha$$

$\Rightarrow$ Mixing coefficients $\{A_\alpha\}$

Calculation of the densities and source term

- $\rho_{ki} = \langle \Psi | a_i^\dagger a_k | \Psi \rangle$
- $\sigma_{kiml} = \langle \Psi | a_i^\dagger a_m^\dagger a_l a_k | \Psi \rangle - (\rho_{ki}\rho_{lm} - \rho_{km}\rho_{li})$

$\Rightarrow G(\sigma)$

Solve 2nd equation

$$\left[\hat{h}(\rho,\sigma), \hat{\rho}\right] = \hat{G}(\sigma)$$

$\Rightarrow$ single-particle orbitals $\{\varphi_i\}$

... until convergence

C.R., N. Pillet, D. Peña Arteaga & J.-F. Berger, PRC 93, 024302 (2016).

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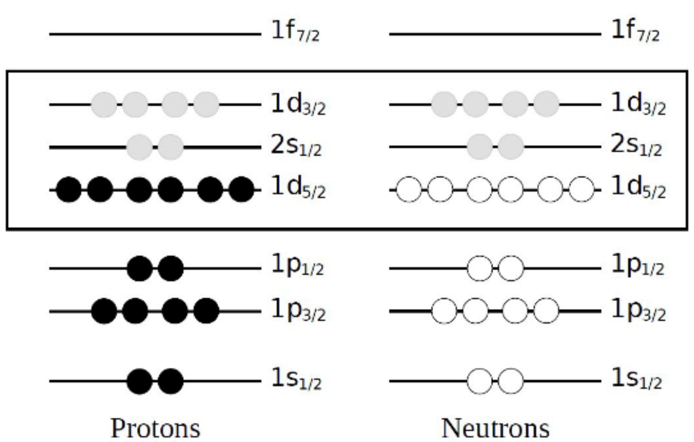
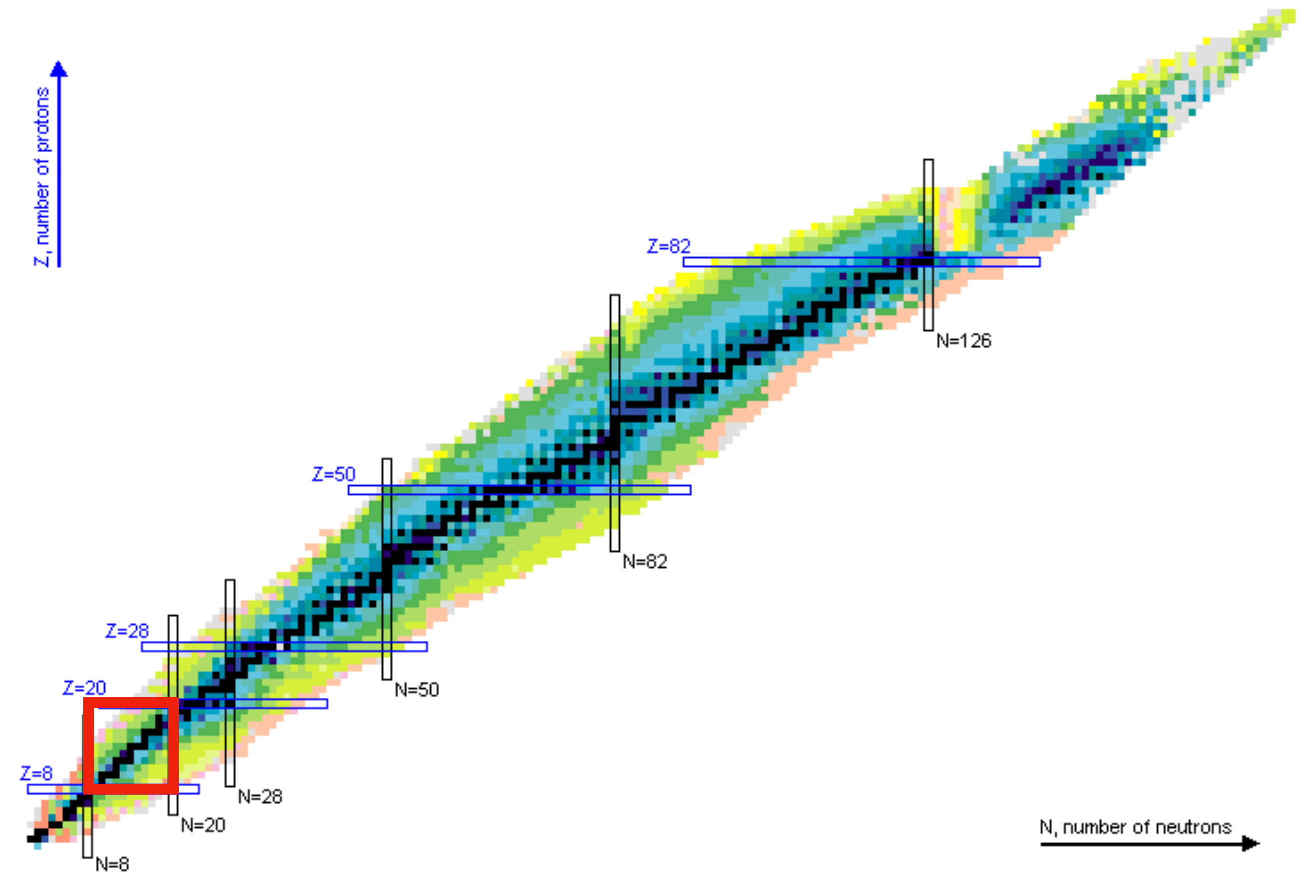
Application to sd-shell nuclei with the Gogny force

Framework

- Even-even nuclei with $10 \leqslant (Z, N) \leqslant 18$
- truncation scheme: **core of ^{16}O + valence space**
- 9 major oscillator shells

Ex: ^{28}Si → 12p-12h





nndc.bnl.gov

Calculation of ground- and excited-state properties:

- Binding and separation energies, charge radii
- Excitation energies
- Magnetic dipole moments and quadrupole spectroscopic moments
- Transition probabilities B(E2), B(M1)…

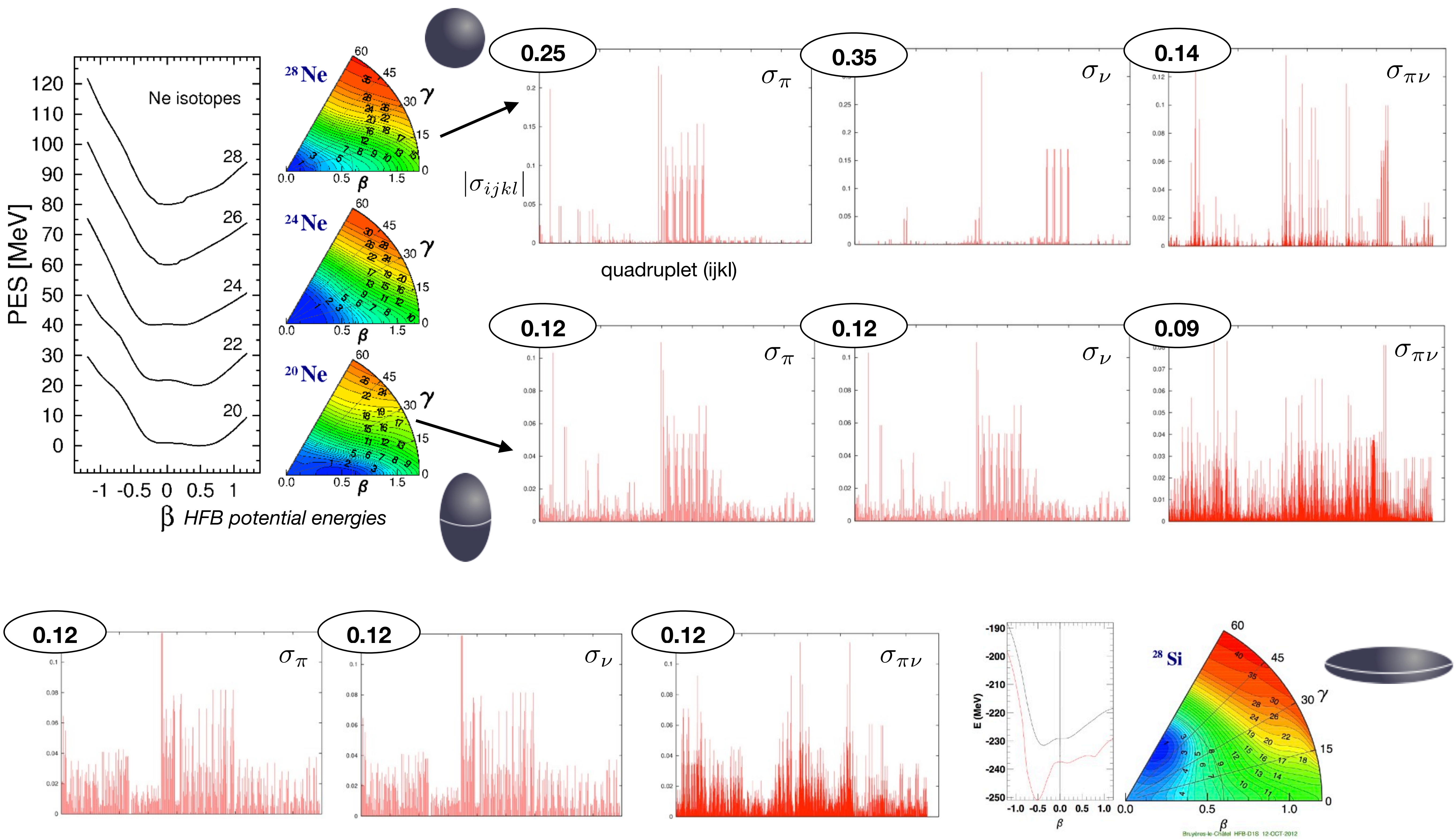
➡ How are these observables impacted by the optimization of orbitals?

C. Robin, N. Pillet, M. Dupuis, J. Le Bloas, D. Peña Arteaga and J.F. Berger, PRC 95 044315 (2017).

Application to sd-shell nuclei with the Gogny force

Symmetry-preserving scheme

➡ The information about deformation is contained in the two-body correlation matrices σ :

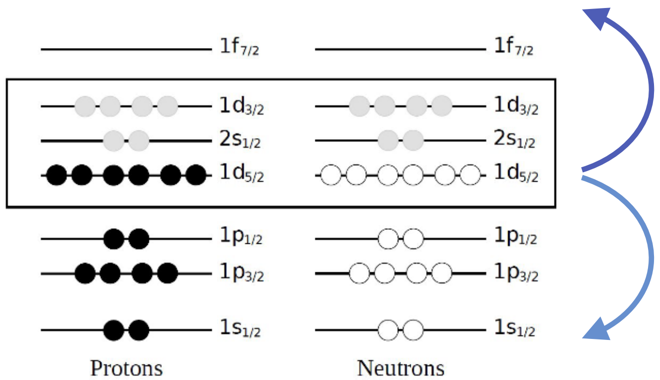


Application to sd-shell nuclei with the Gogny force

Source term of the orbital equation:

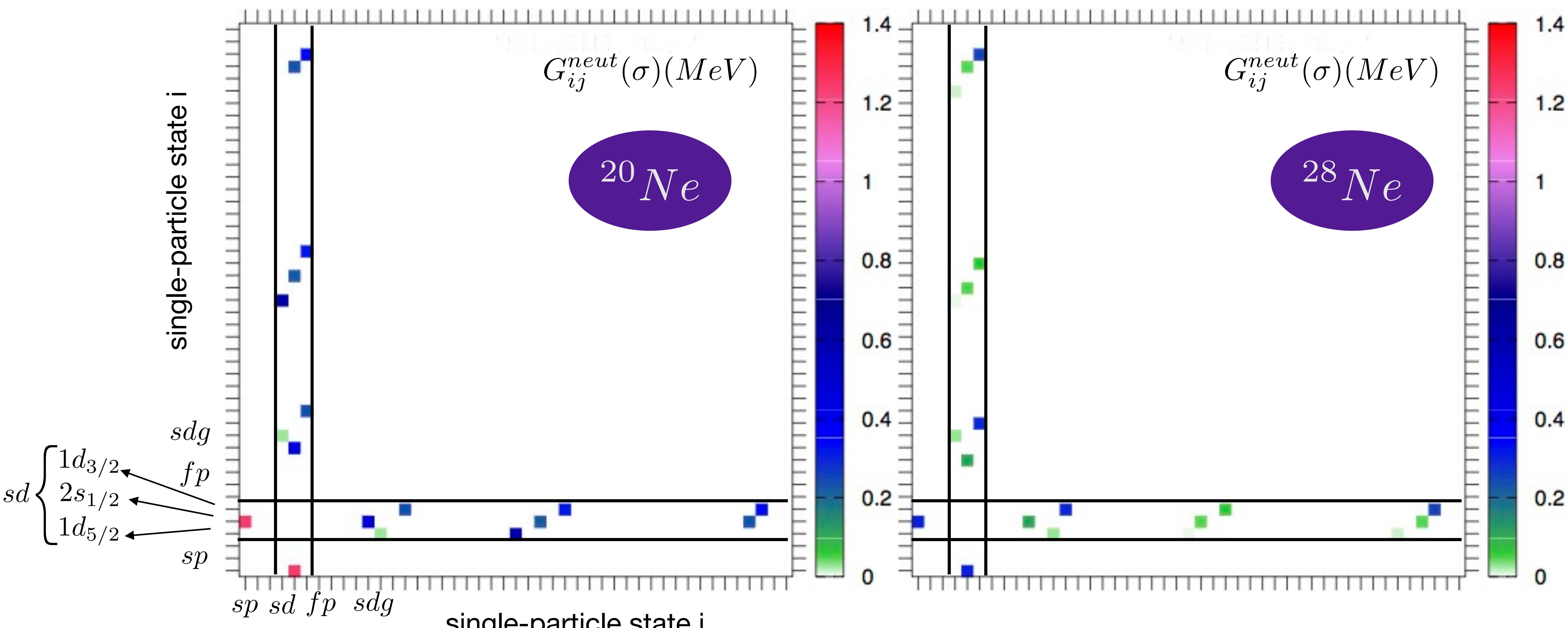
$$G_{ij}(\sigma) = \frac{1}{2}\sum_{klm} \widetilde{V}_{kmjl}\,\sigma_{kiml} - \frac{1}{2}\sum_{klm} \widetilde{V}_{kiml}\,\sigma_{jlkm}$$

$\in$ whole basis $\in$ valence space



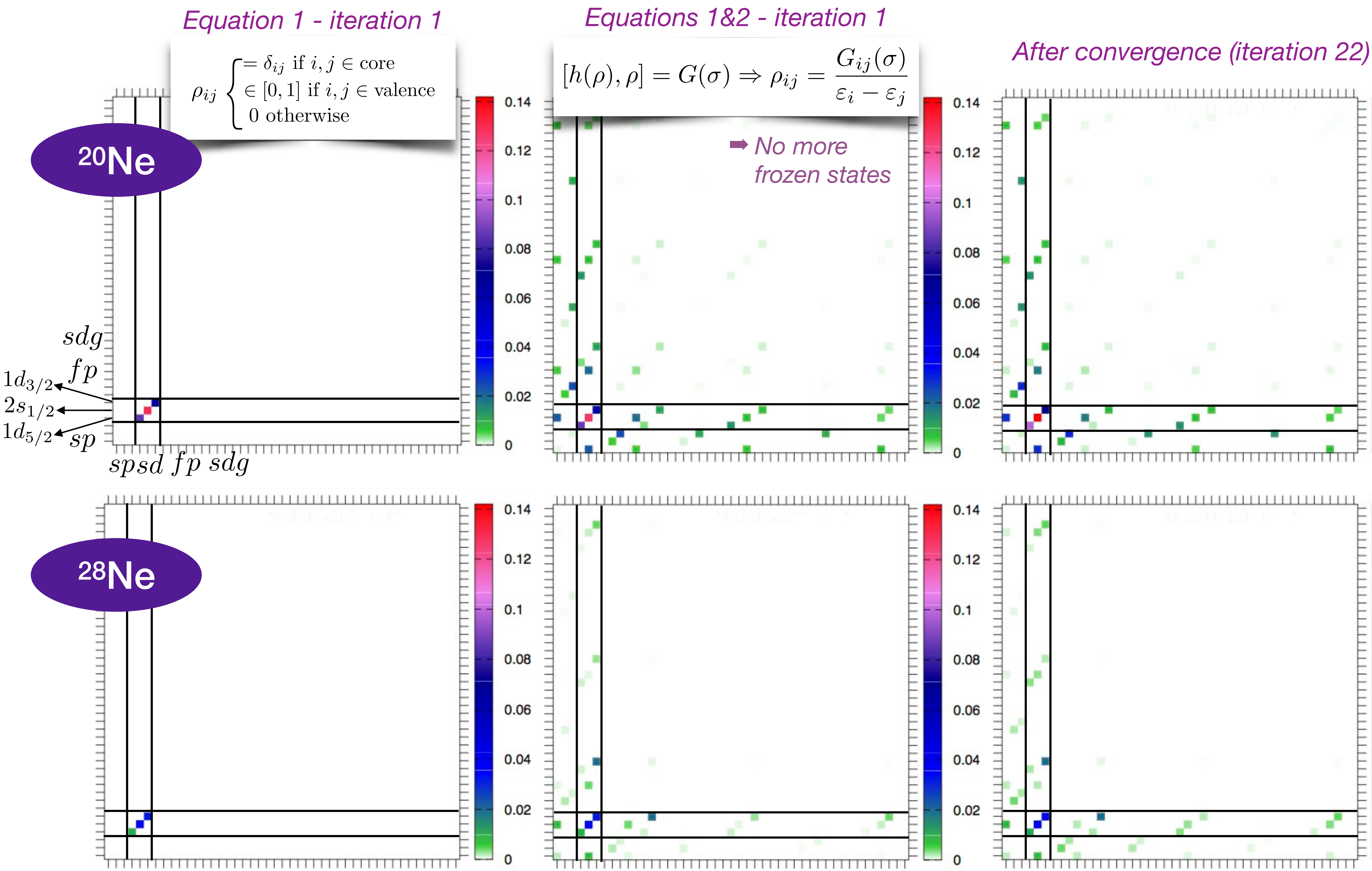
$\Longrightarrow$ Introduces couplings between the valence space and the rest of the single-particle basis.

At iteration #1:



Application to sd-shell nuclei with the Gogny force

One-body density matrix (neutrons): Representation of $\Delta\rho = |\rho - \rho^{(0)}_{HF}|$ in the HF basis:

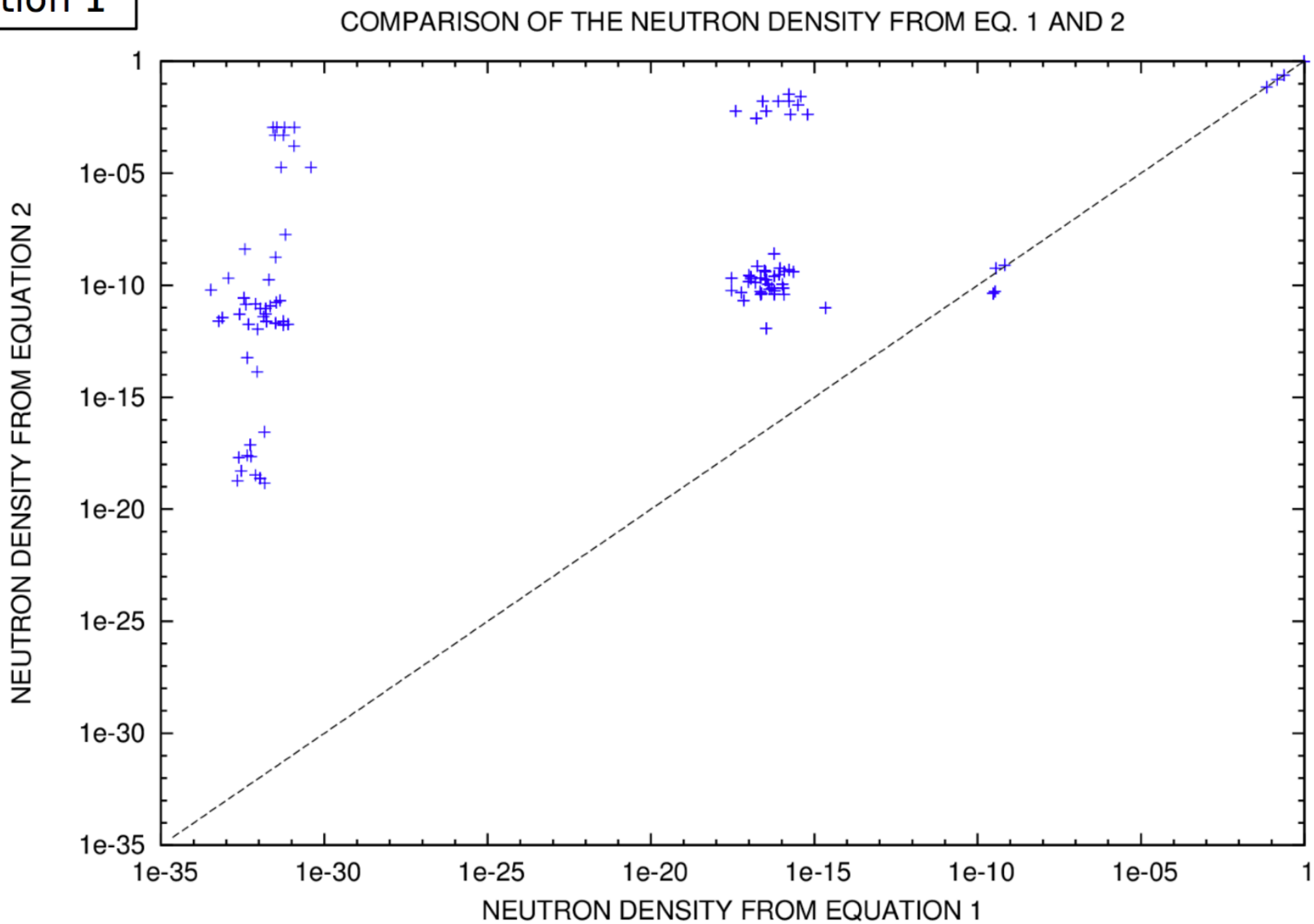


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

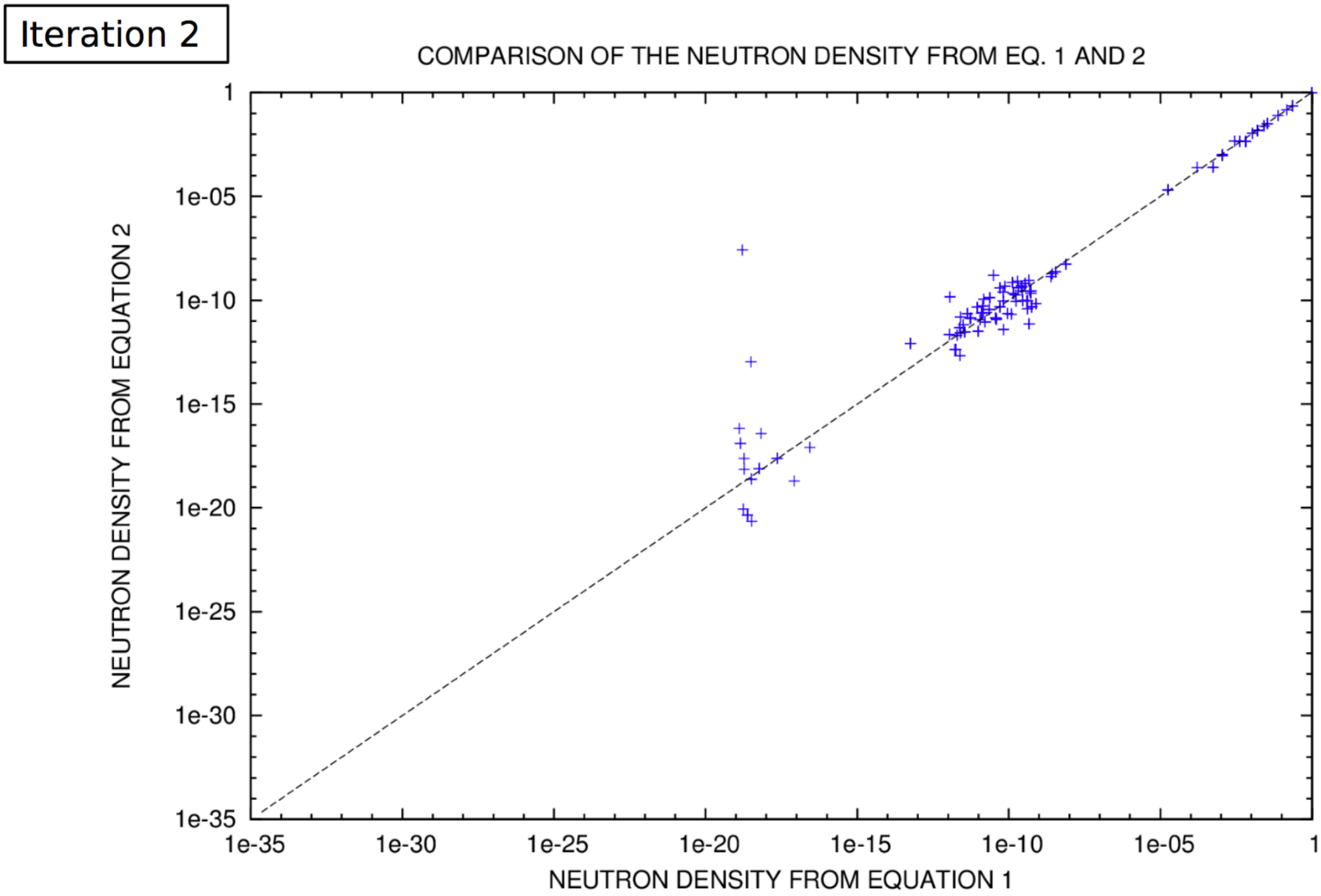
Iteration 1



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

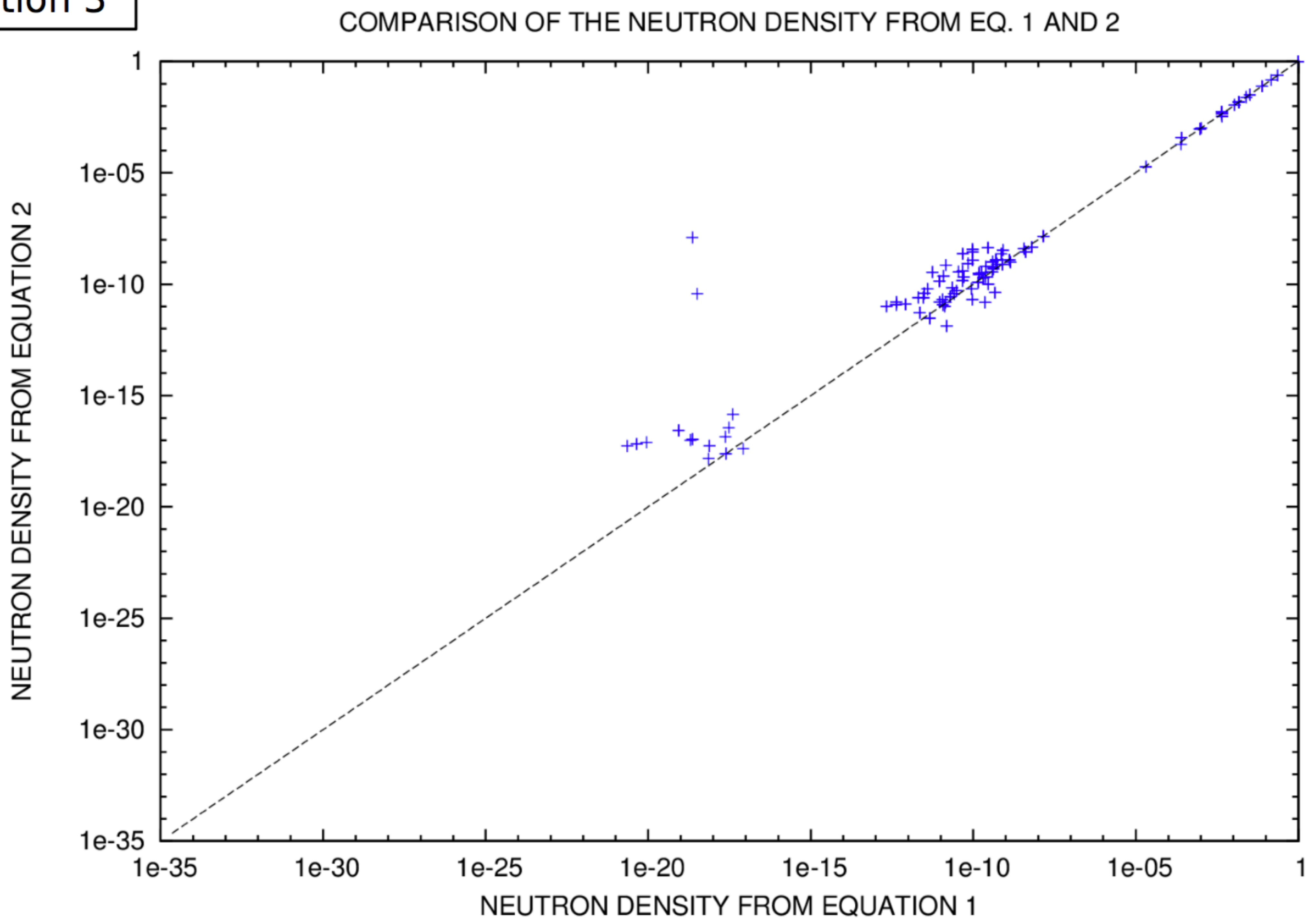


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

Iteration 3

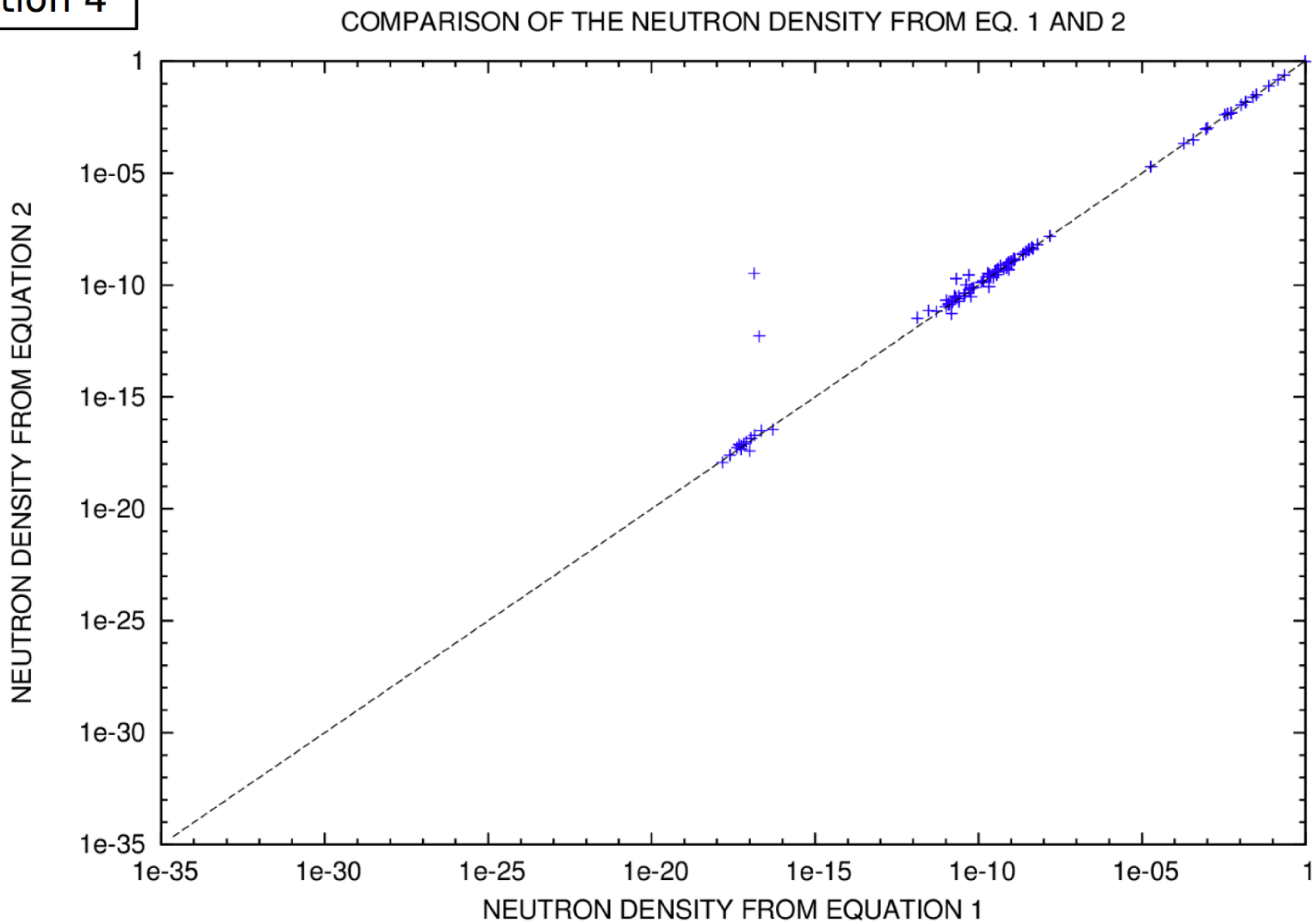


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

Iteration 4

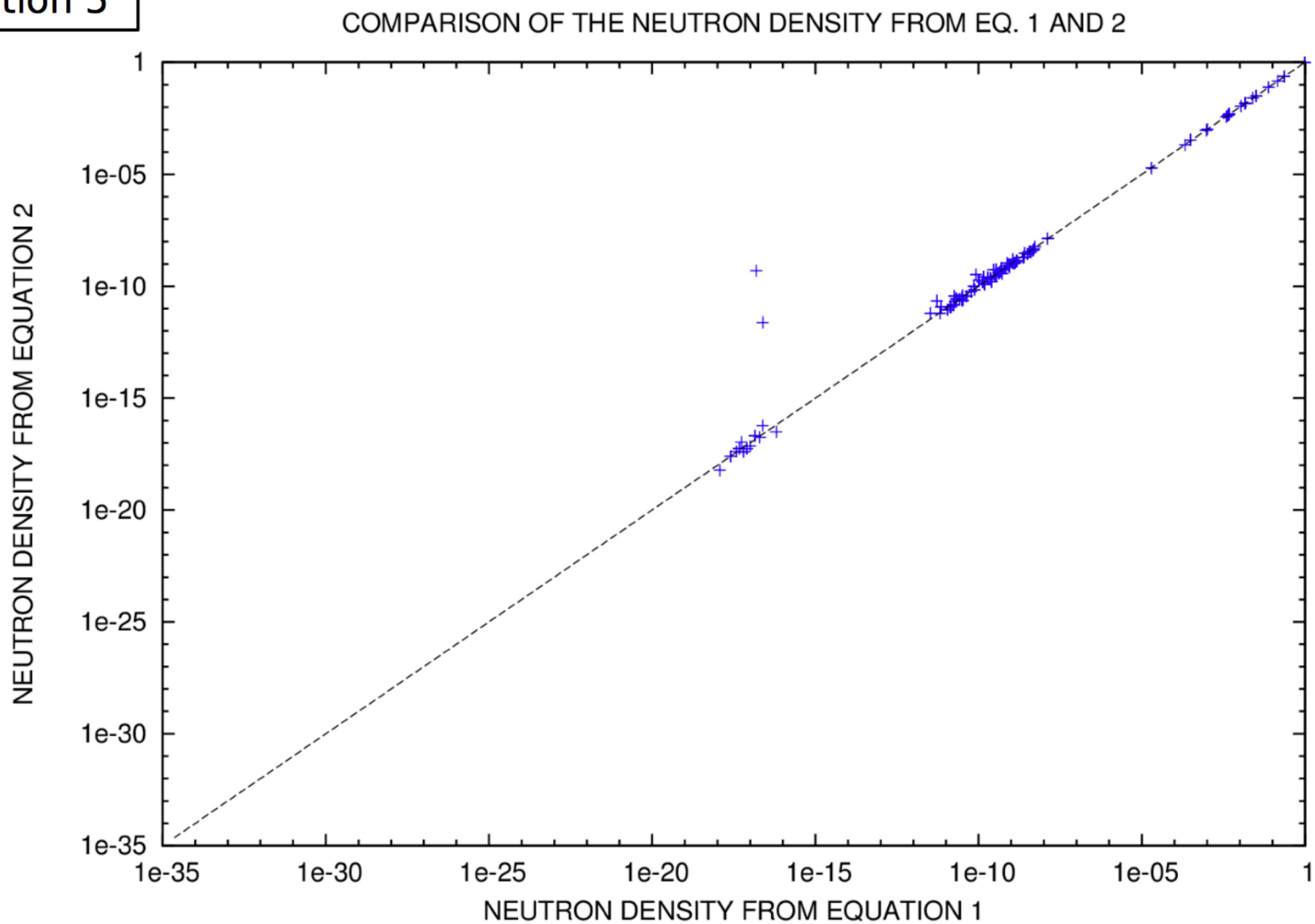


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

Iteration 5

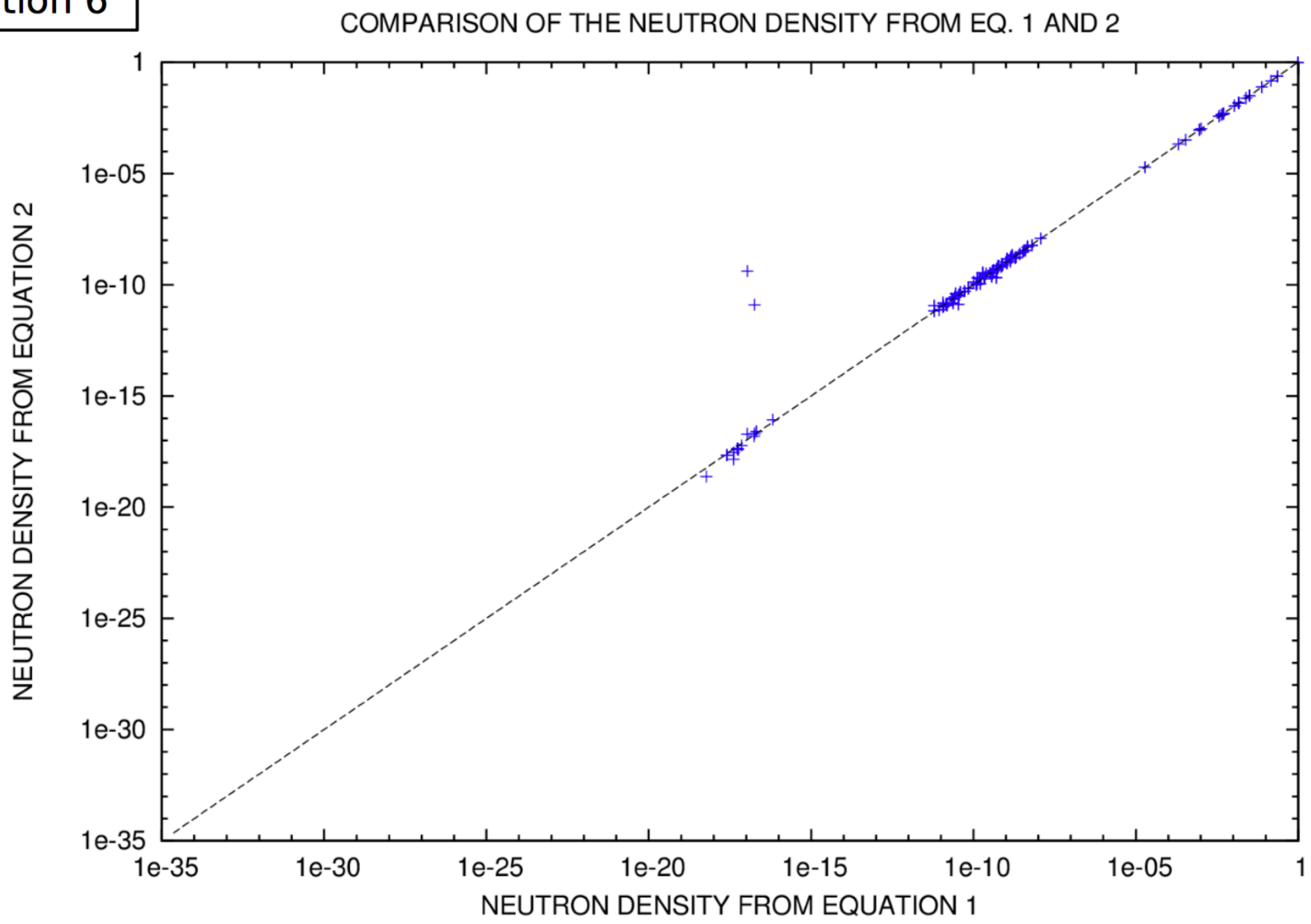


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

Iteration 6

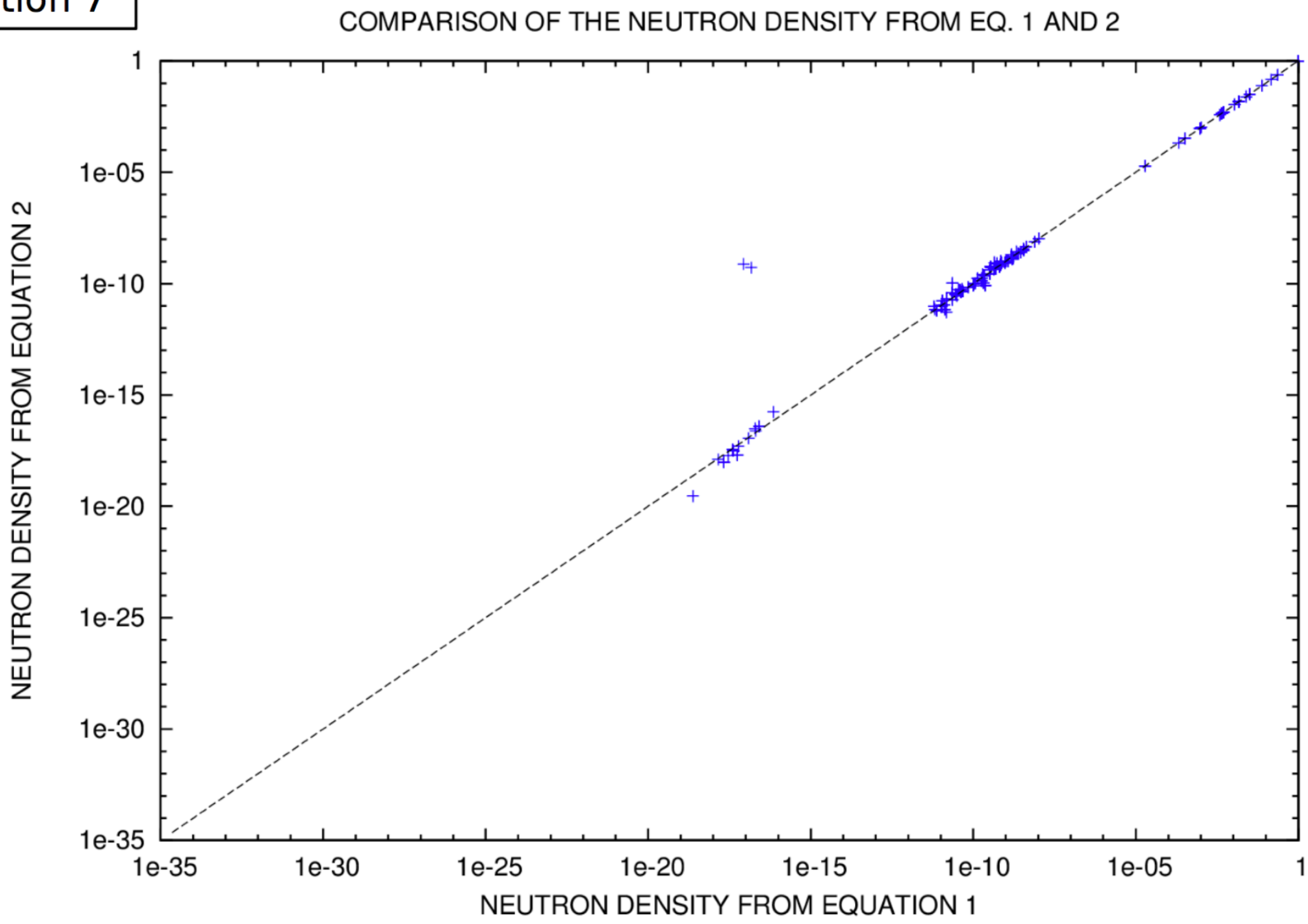


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

Iteration 7

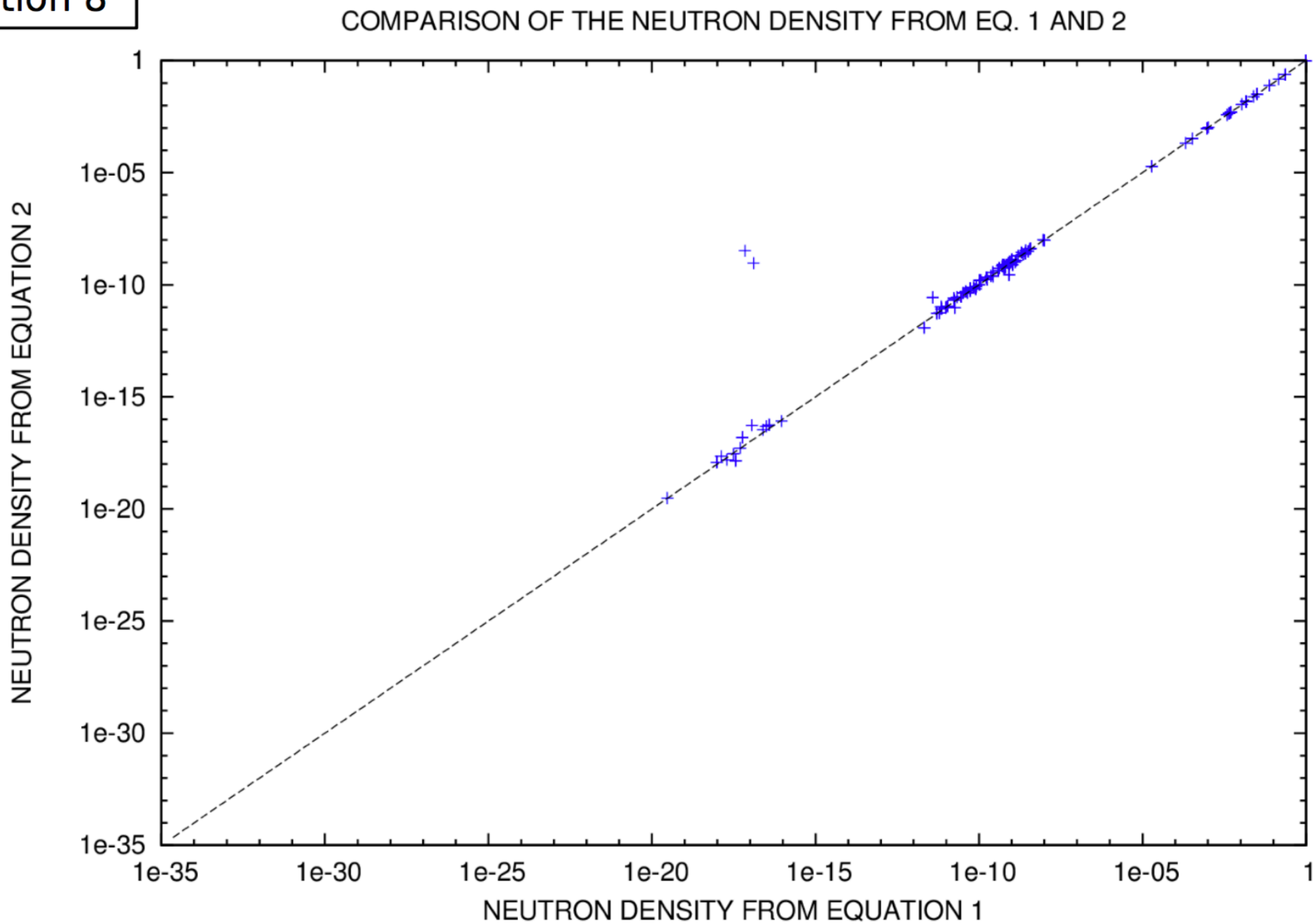


Application to sd-shell nuclei

* **_Convergence of the one-body density matrix (neutrons):_**

^{20}Ne

Iteration 8

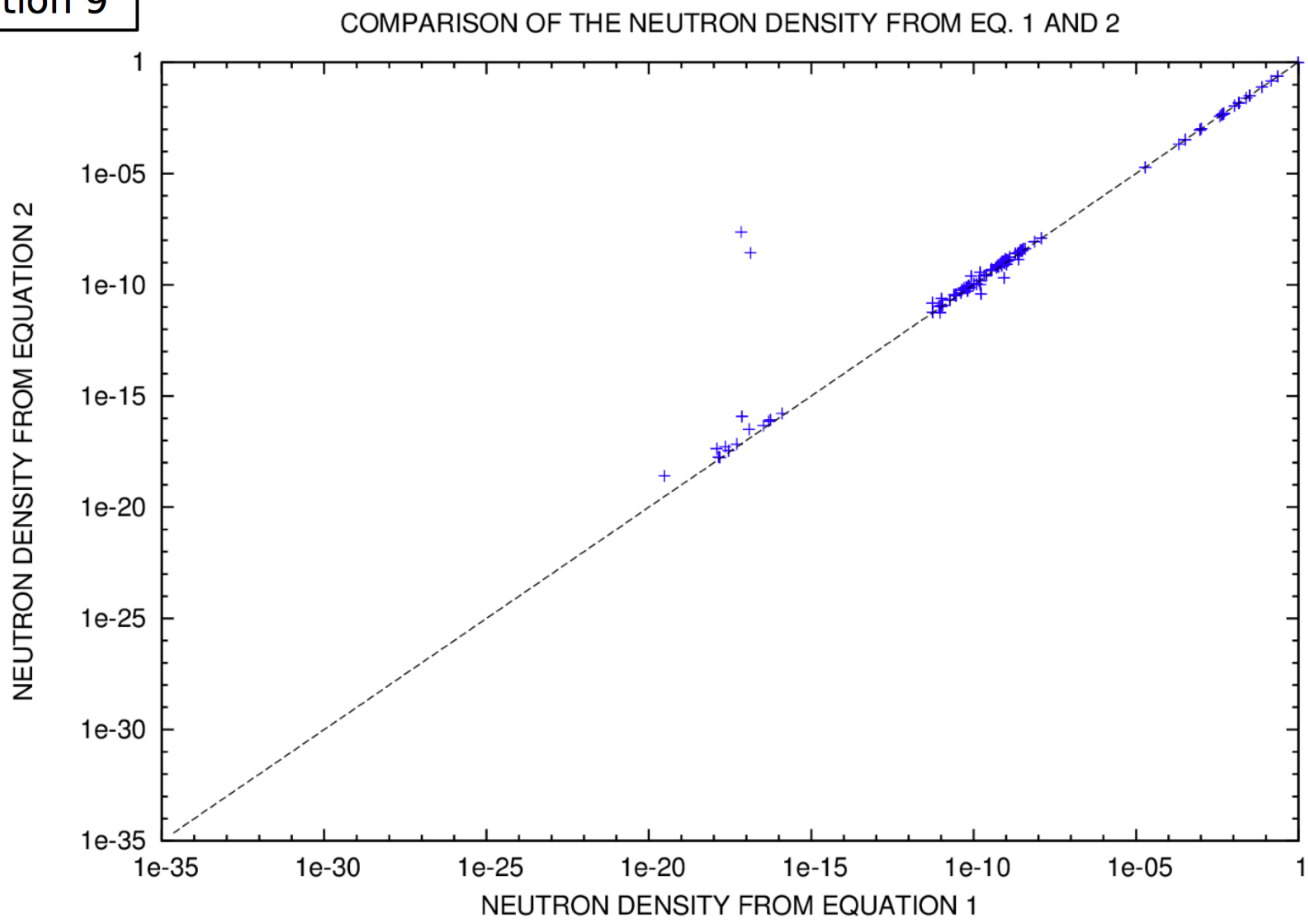


Application to sd-shell nuclei

✱ ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

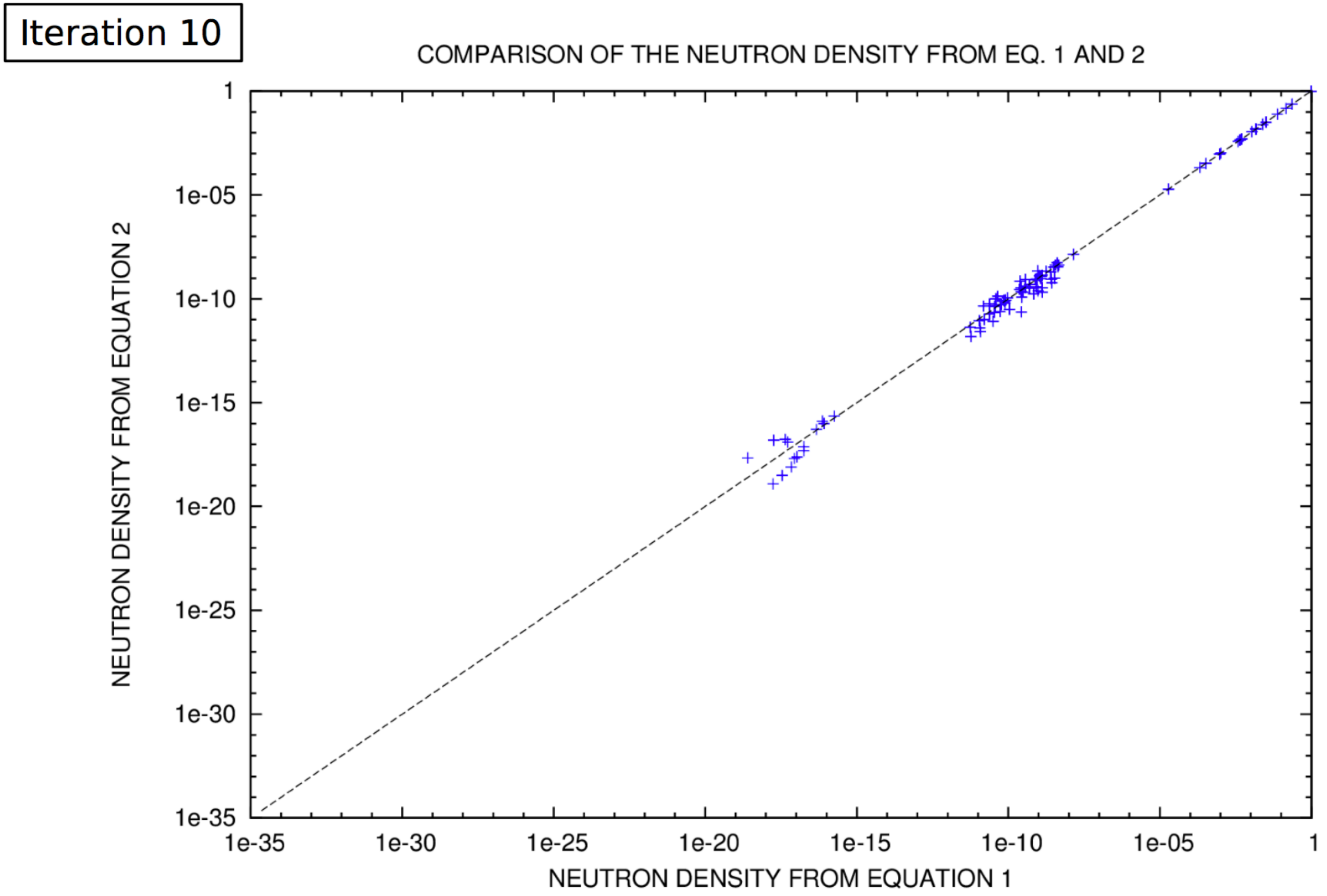
Iteration 9



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

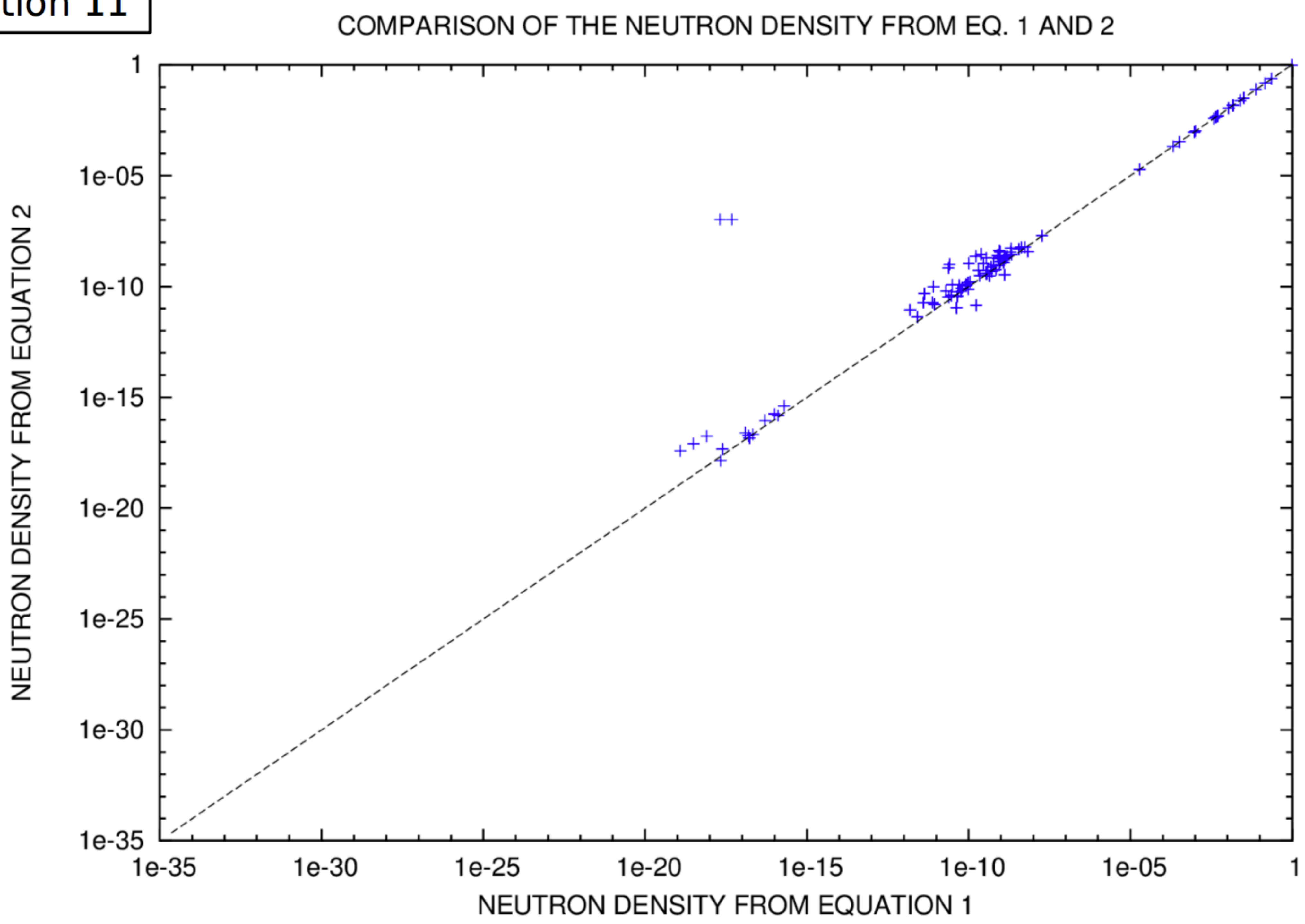


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

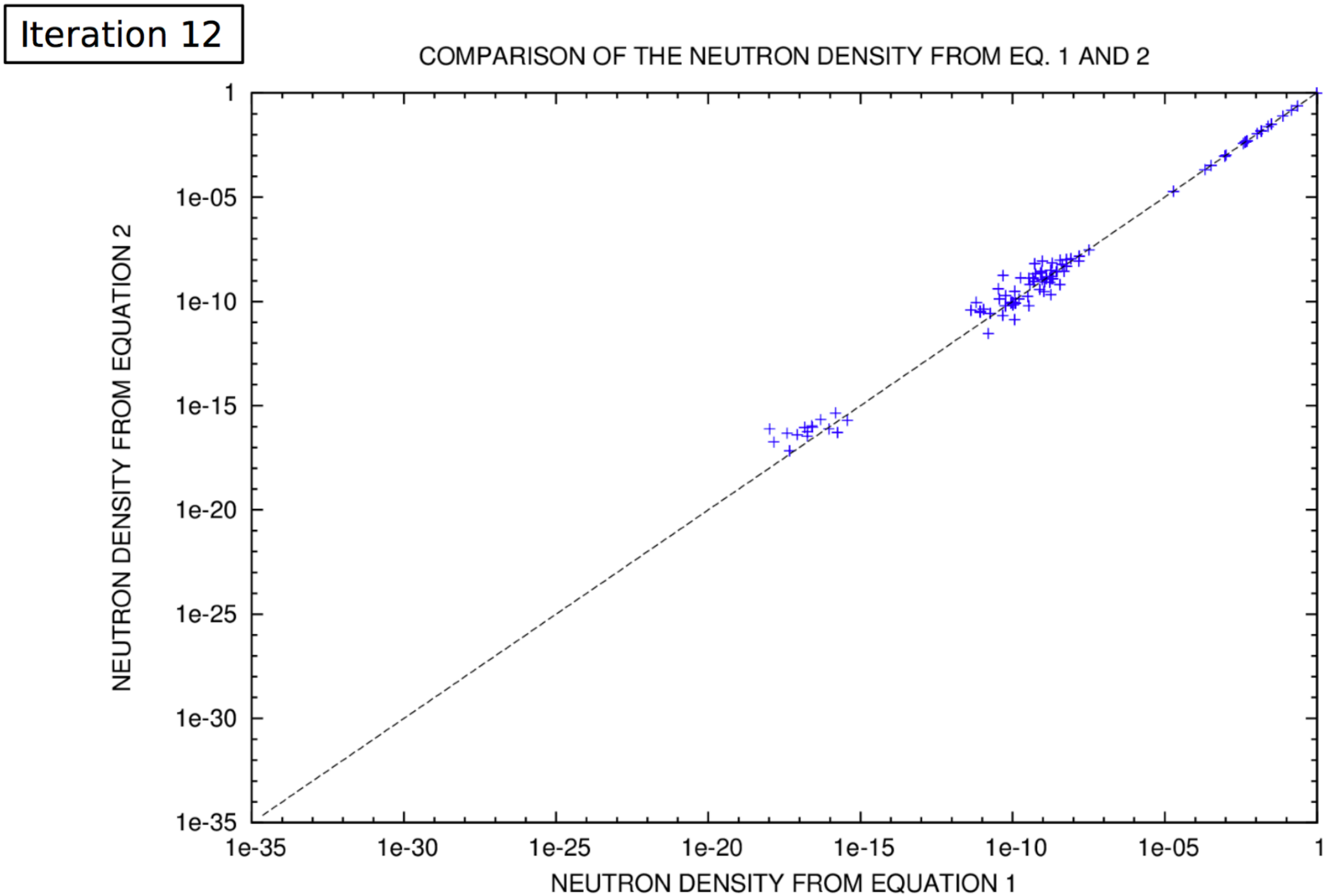
Iteration 11



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

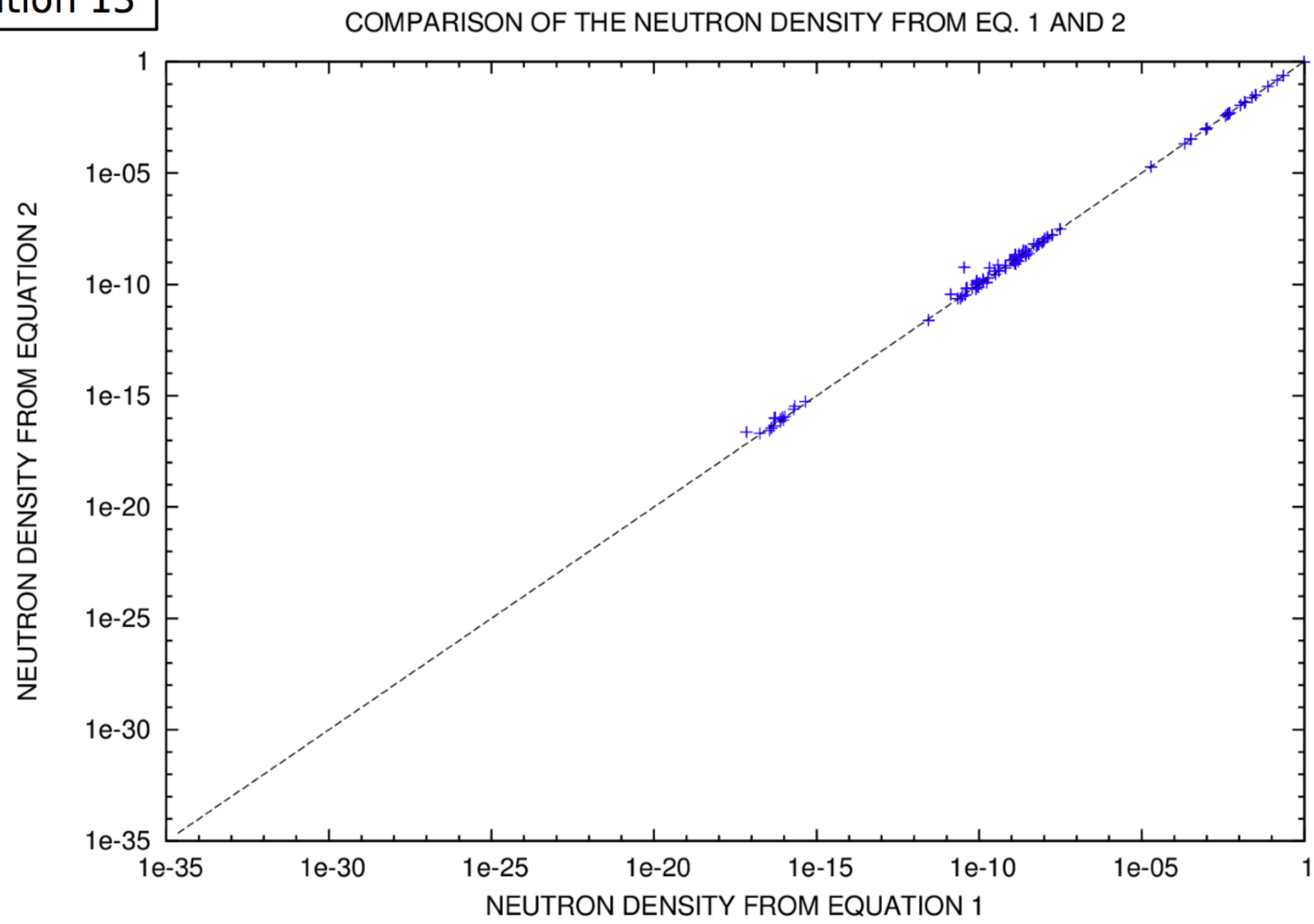


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

Iteration 13

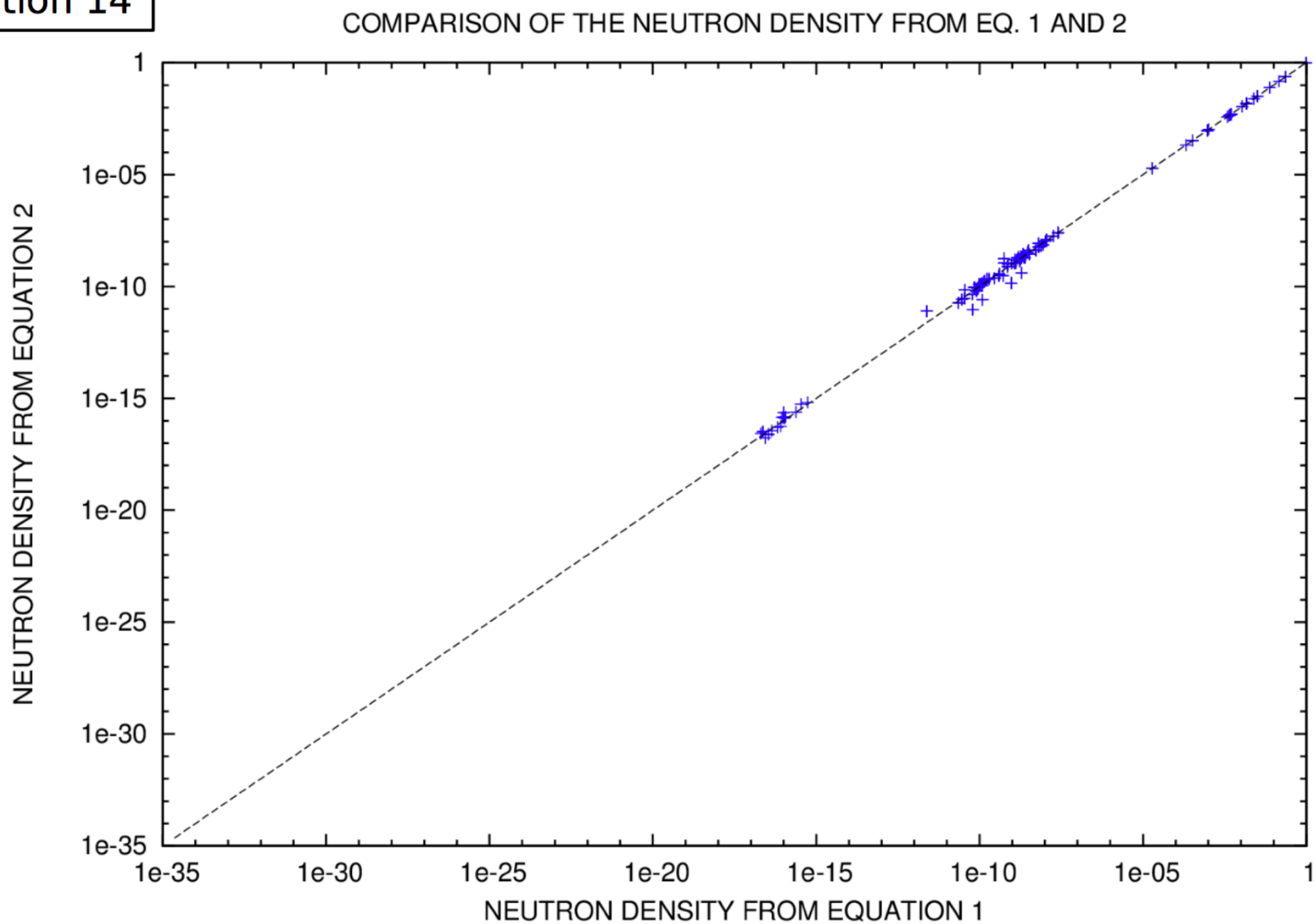


Application to sd-shell nuclei

Convergence of the one-body density matrix (neutrons):

^{20}Ne

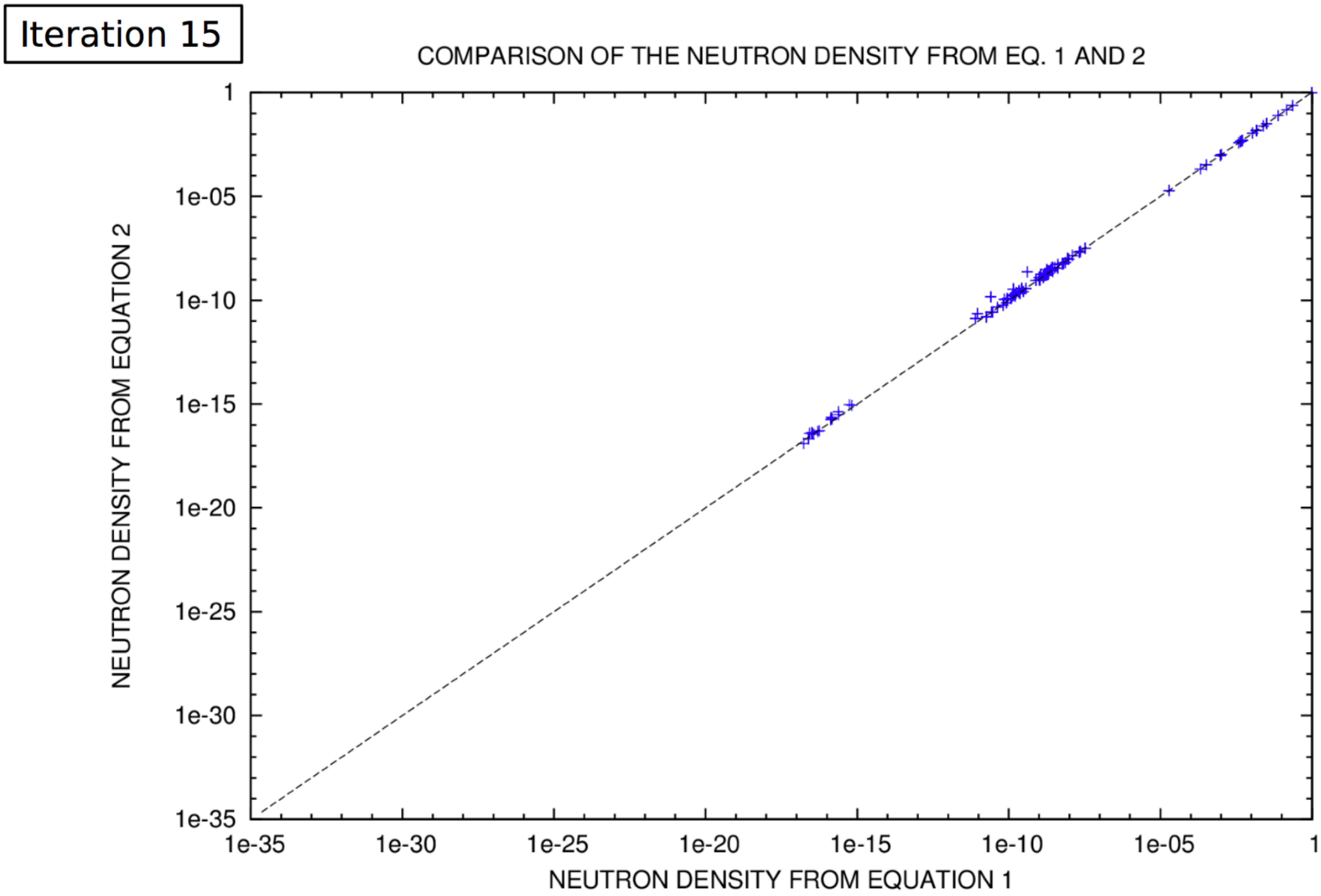
Iteration 14



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

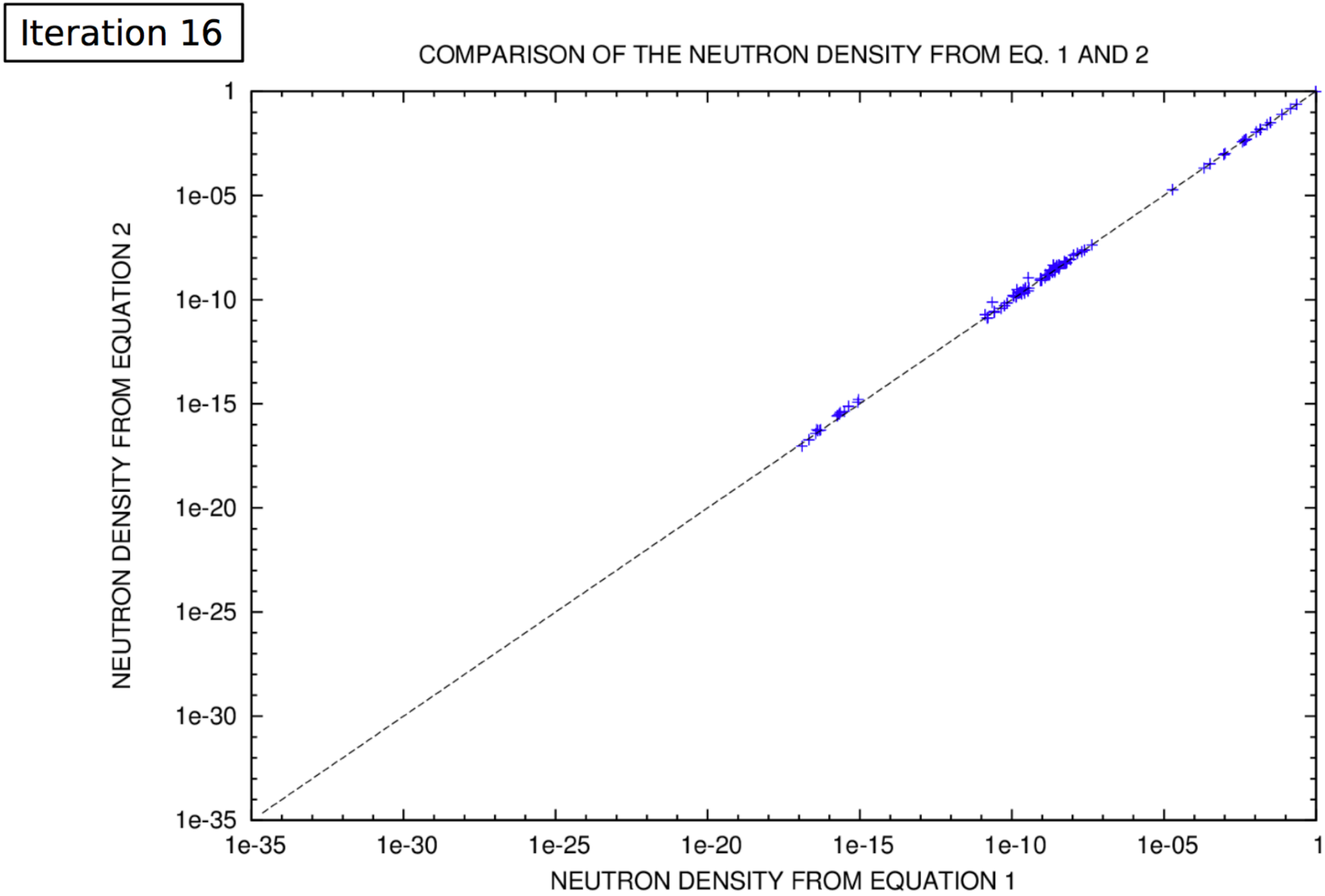
^{20}Ne



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

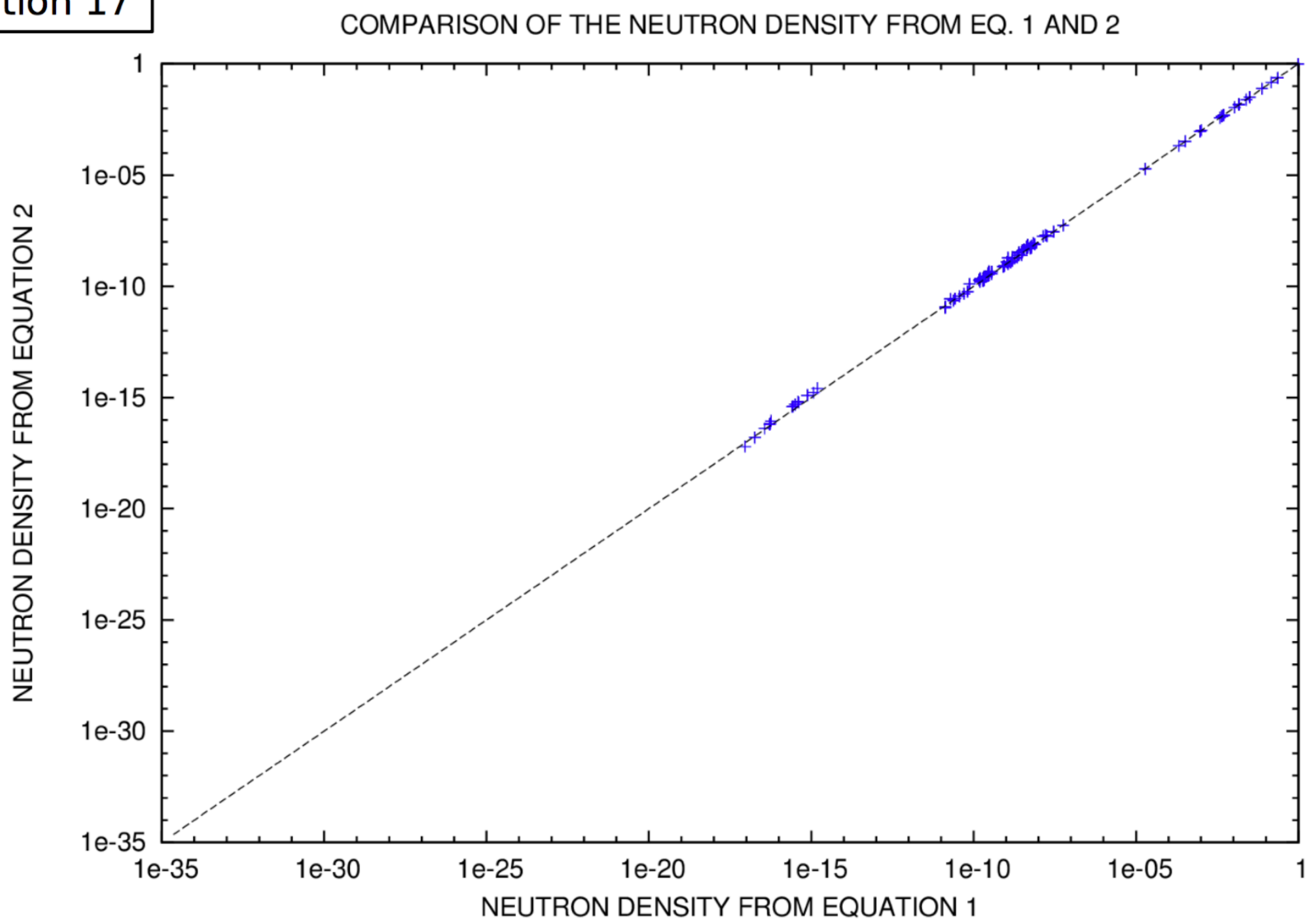


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

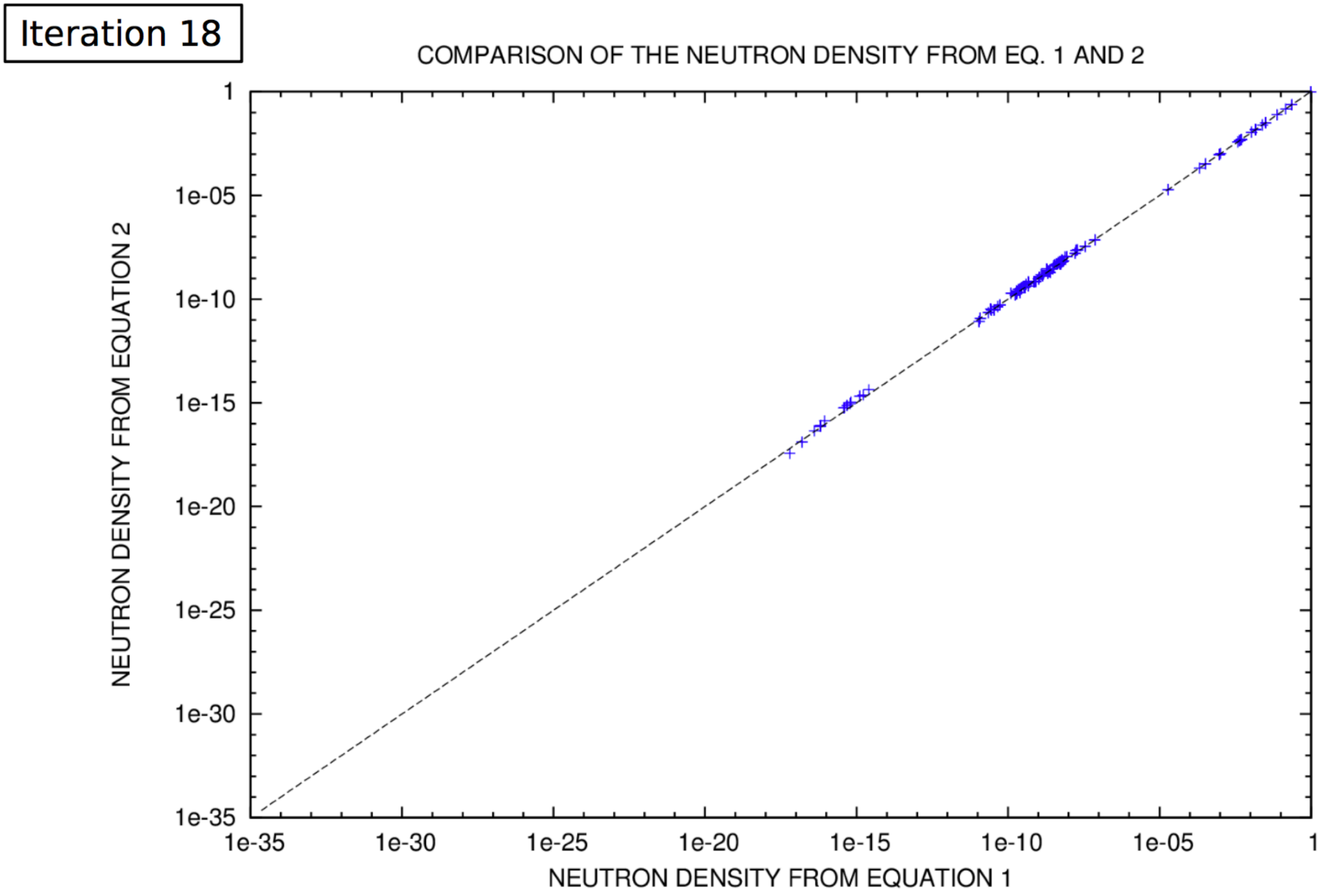
Iteration 17



Application to sd-shell nuclei

* **_Convergence of the one-body density matrix (neutrons):_**

^{20}Ne

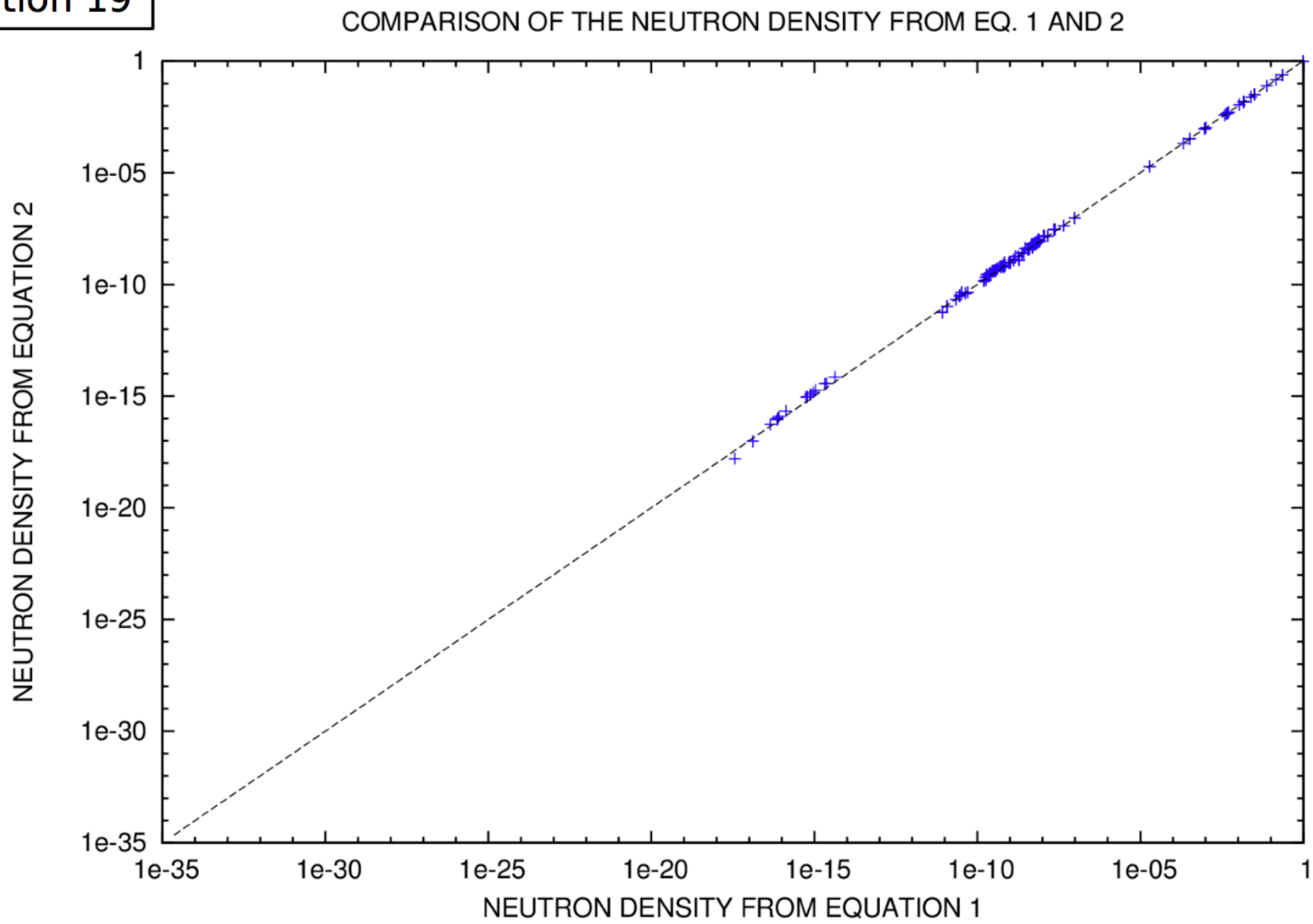


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

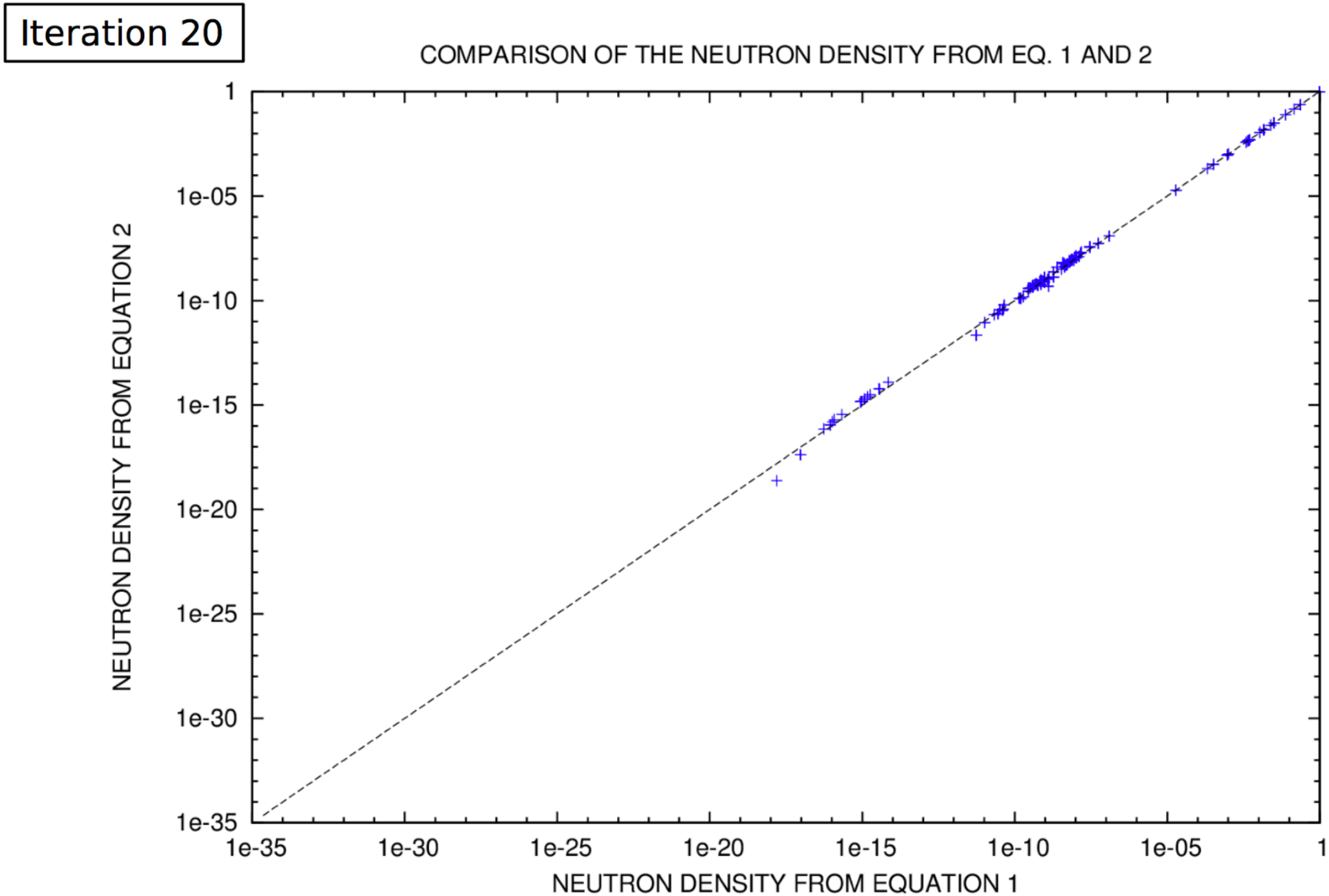
Iteration 19



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

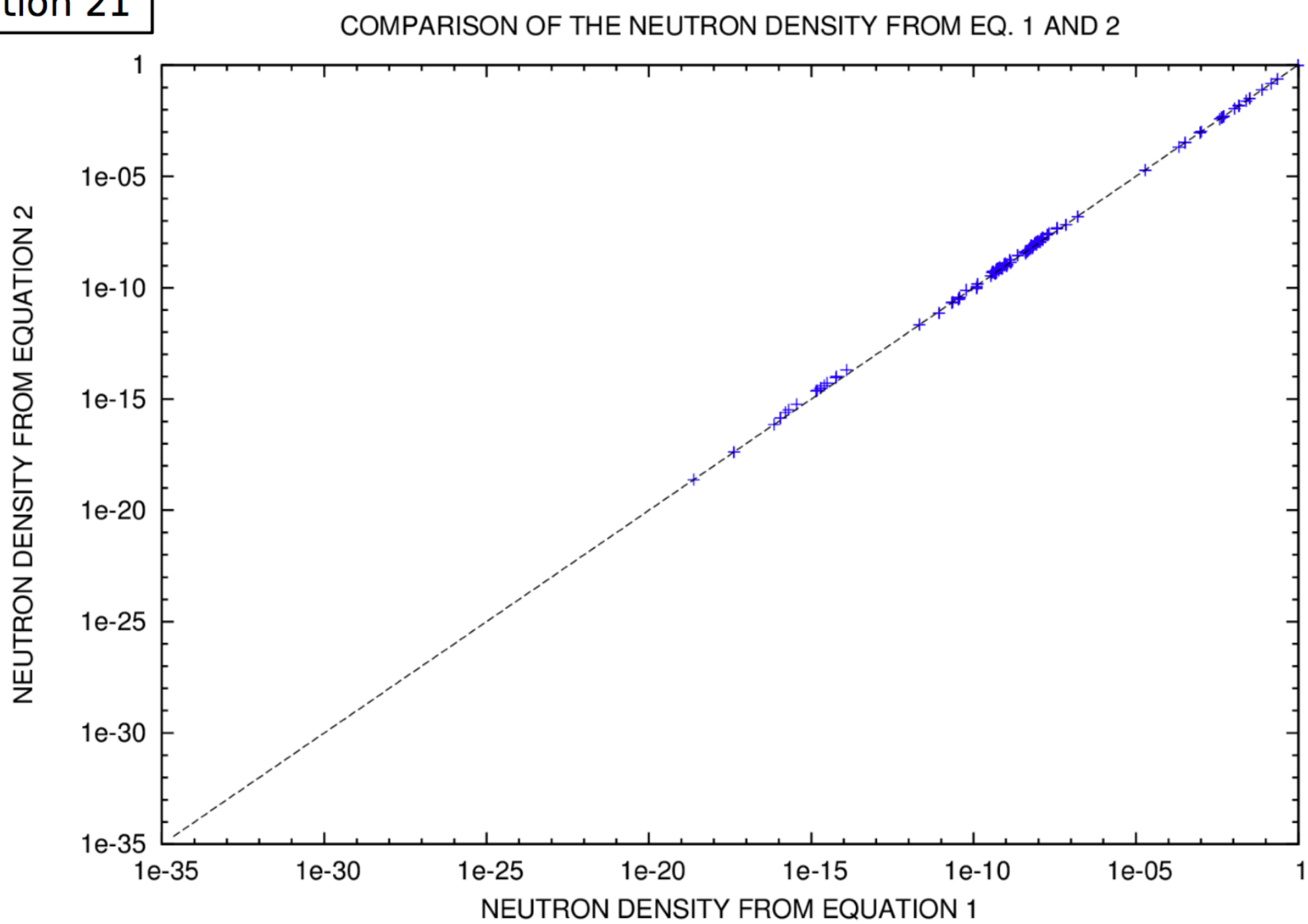


Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

^{20}Ne

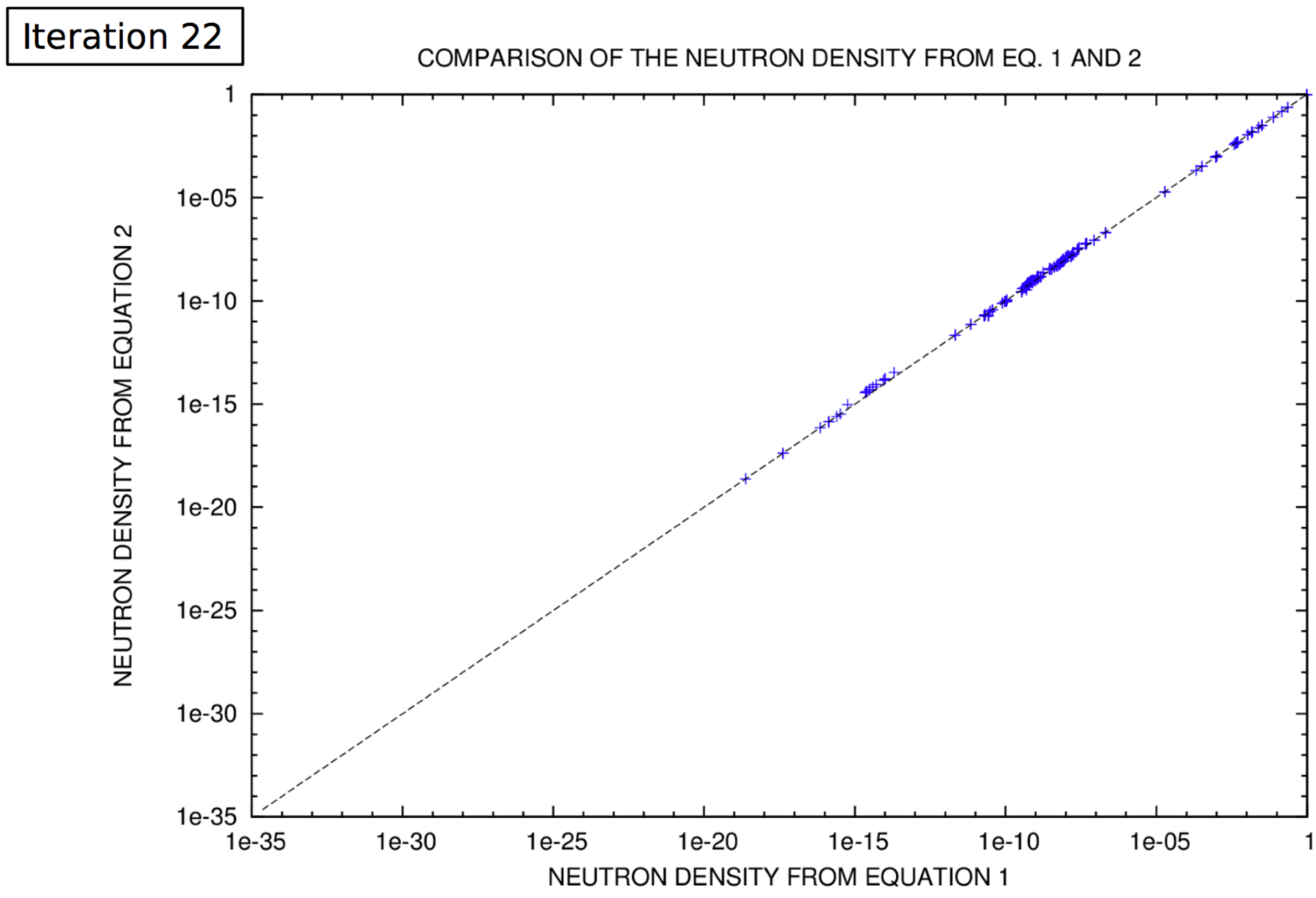
Iteration 21



Application to sd-shell nuclei

* ***Convergence of the one-body density matrix (neutrons):***

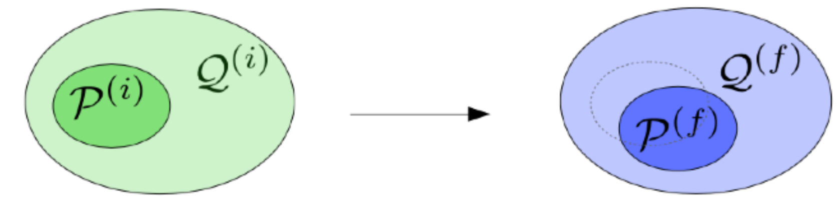
^{20}Ne



Application to sd-shell nuclei with the Gogny force

Effect on the many-body wave function:

Orbital transformation: $b_i^\dagger = e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}}$



$$|\Psi^{(f)}\rangle = \sum_{\alpha \in \mathcal{P}^{(f)}} A_\alpha^{(f)} |\phi_\alpha^{(f)}\rangle$$

$$= \sum_{\beta \in \mathcal{P}^{(i)}} A_\beta^{(i)} |\phi_\beta^{(i)}\rangle + \sum_{\beta \in \mathcal{Q}^{(i)}} A_\beta^{(i)} |\phi_\beta^{(i)}\rangle$$

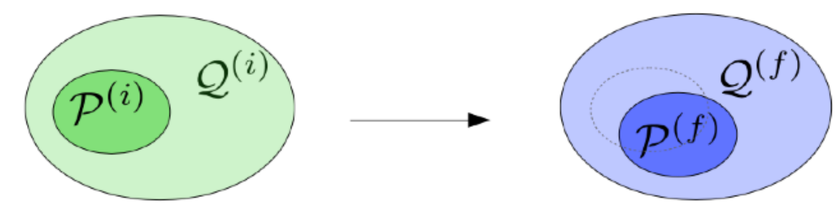
How big?

	1st equation only		1st+2nd equations Starting from HF orbitals	
nucleus	Weight of $P^{(i)}$	Weight of $Q^{(i)}$	Weight of $P^{(i)}$	Weight of $Q^{(i)}$
^{20}Ne	100%	0%	98%	2%
^{24}Mg	100%	0%	97%	3%
^{28}Si	100%	0%	95%	4%
^{32}S	100%	0%	93%	7%
^{28}Ne	100%	0%	85%	15%

Application to sd-shell nuclei with the Gogny force

✱ ***Effect on the many-body wave function:***

Orbital transformation: $b_i^\dagger = e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}}$



$$|\Psi^{(f)}\rangle = \sum_{\alpha\in\mathcal{P}^{(f)}} A_\alpha^{(f)} |\phi_\alpha^{(f)}\rangle$$

$$= \sum_{\beta\in\mathcal{P}^{(i)}} A_\beta^{(i)} |\phi_\beta^{(i)}\rangle + \sum_{\beta\in\mathcal{Q}^{(i)}} A_\beta^{(i)} |\phi_\beta^{(i)}\rangle$$

How big?

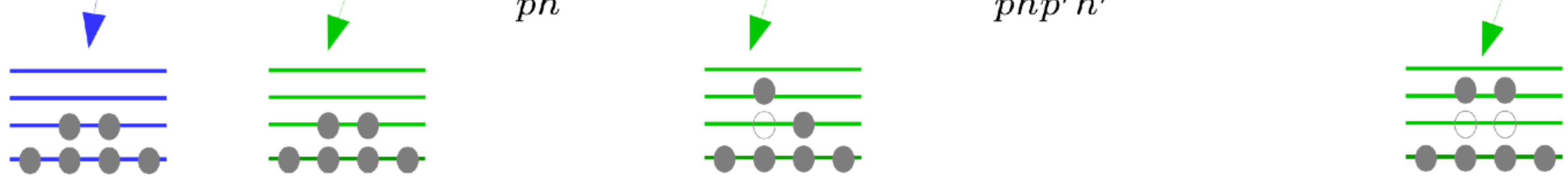
	1st equation only		1st+2nd equations Starting from HF orbitals		1st+2nd equations Starting from HO orbitals	
nucleus	Weight of P(i)	Weight of Q(i)	Weight of P(i)	Weight of Q(i)	Weight of P(i)	Weight of Q(i)
^{20}Ne	100%	0%	98%	2%	66%	34%
^{24}Mg	100%	0%	97%	3%	61%	39%
^{28}Si	100%	0%	95%	4%	55%	45%
^{32}S	100%	0%	93%	7%	61%	39%
^{28}Ne	100%	0%	85%	15%	78%	22%

The weight of the initial Q space increases when starting further from the final solution

Application to sd-shell nuclei with the Gogny force

✱ ***Effect on the many-body wave function:*** Orbital transformation: $b_i^\dagger = e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}}$

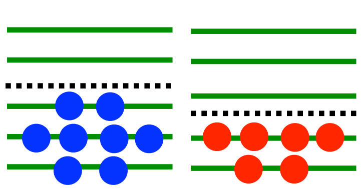
$$|\phi^{(f)}\rangle = e^{iT}\,|HF\rangle$$
$$= |HF\rangle + i\sum_{ph} T_{ph}\, a_p^\dagger a_h |HF\rangle - \frac{1}{2}\sum_{php'h'} T_{ph}T_{p'h'}\, a_p^\dagger a_h a_{p'}^\dagger a_{h'} |HF\rangle + \ldots$$



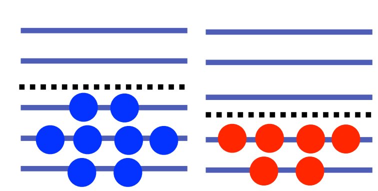
➡ final reference state = superposition of mpmh excitations on the initial HF reference state = richer

Pure Hartree-Fock component in correlated ground state		
nucleus	1st equation only	1st + 2nd equations
^{26}Ne	71%	62%
^{28}Si	60%	24%
^{32}S	58%	39%
^{34}S	39%	17%

New reference-state component
1st + 2nd equations
69%
26%
47%
18%



➡ Pure HF component decreases: self-consistent procedure appears to fragment the wave function

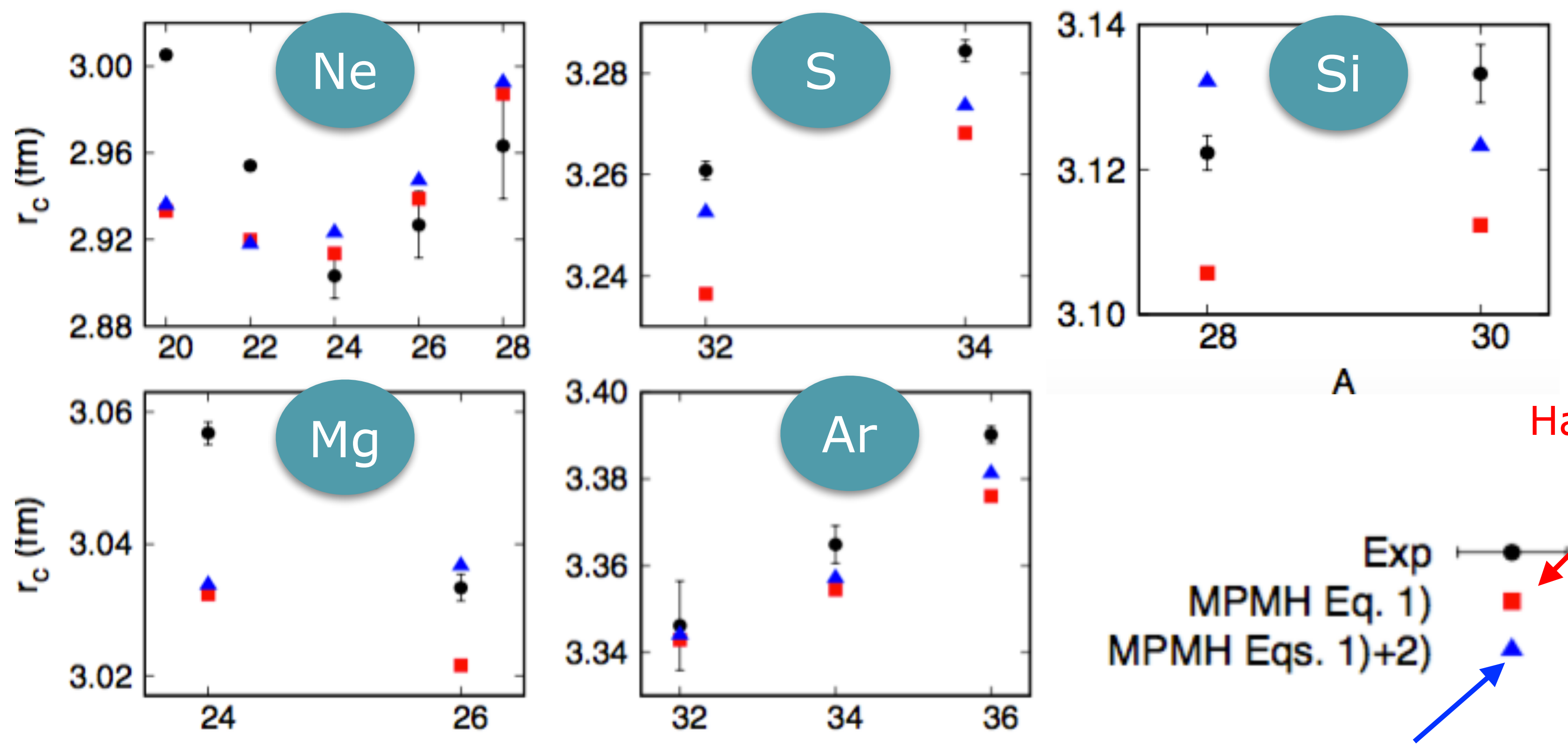


Reference state built on optimized orbitals

➡ "better" than HF state

Application to sd-shell nuclei with the Gogny force

Charge radii:



- *Average difference:*

$$\langle \Delta r_c \rangle = 0.021 \text{ fm} \rightarrow 0.018 \text{ fm}$$

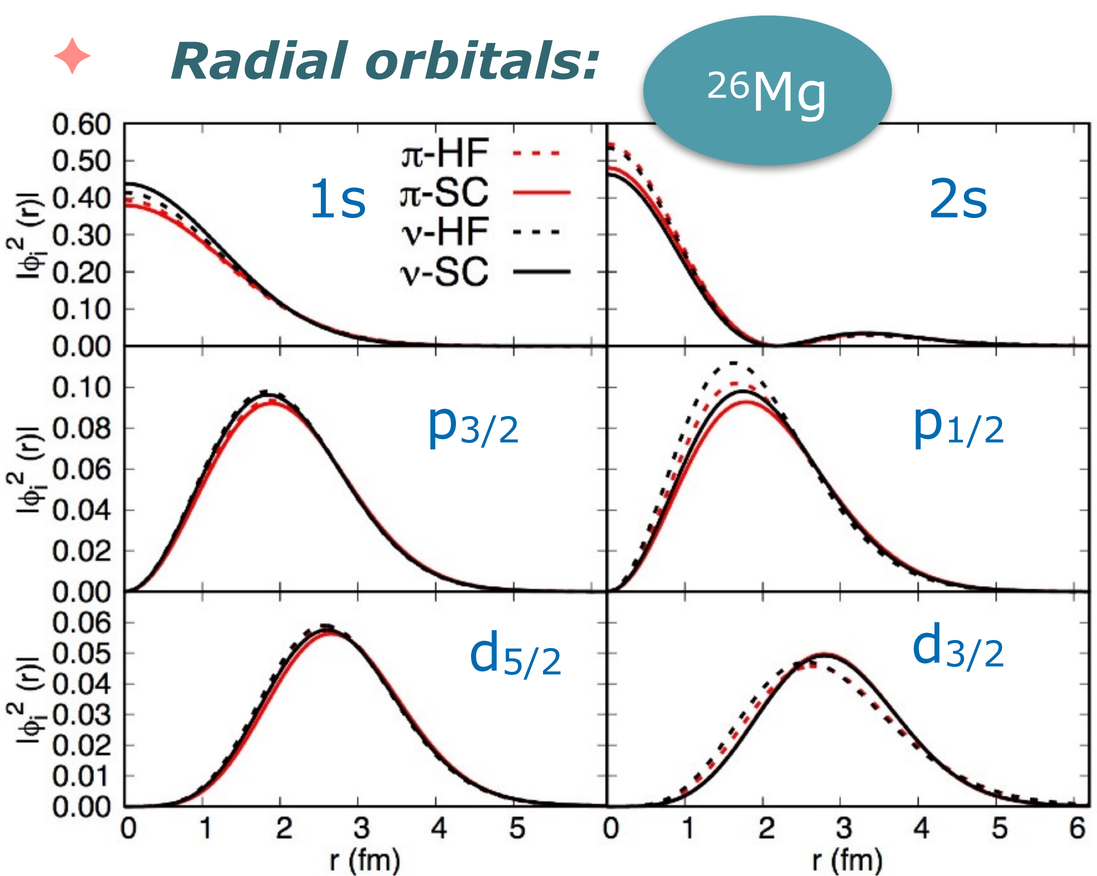
- *Standard deviation*:

$$\sigma(\Delta r_c) = 0.017 \text{ fm} \rightarrow 0.018 \text{ fm}$$

Hartree-Fock orbitals

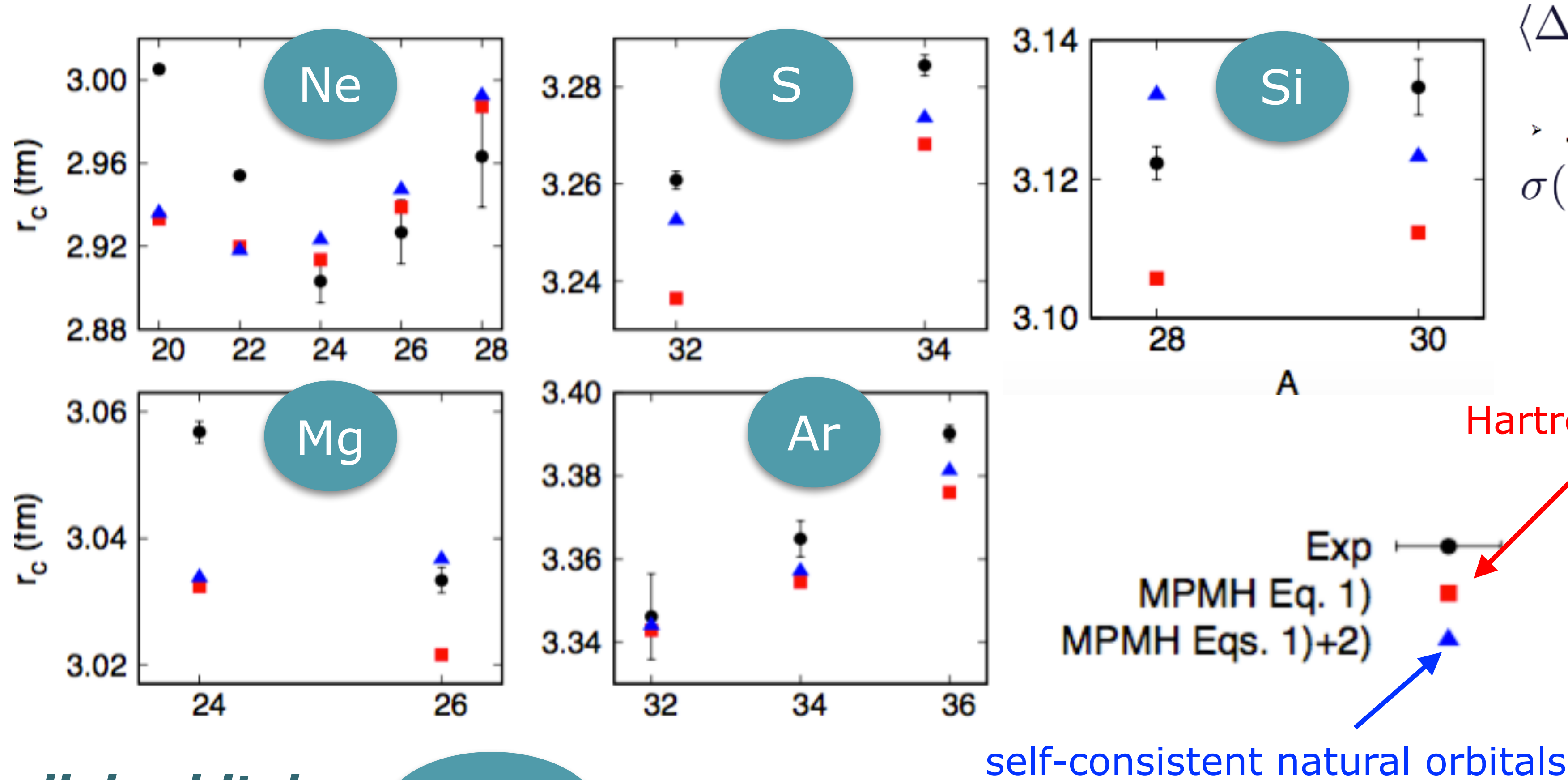
self-consistent natural orbitals

Radial orbitals:



Application to sd-shell nuclei with the Gogny force

✦ ***Charge radii:***



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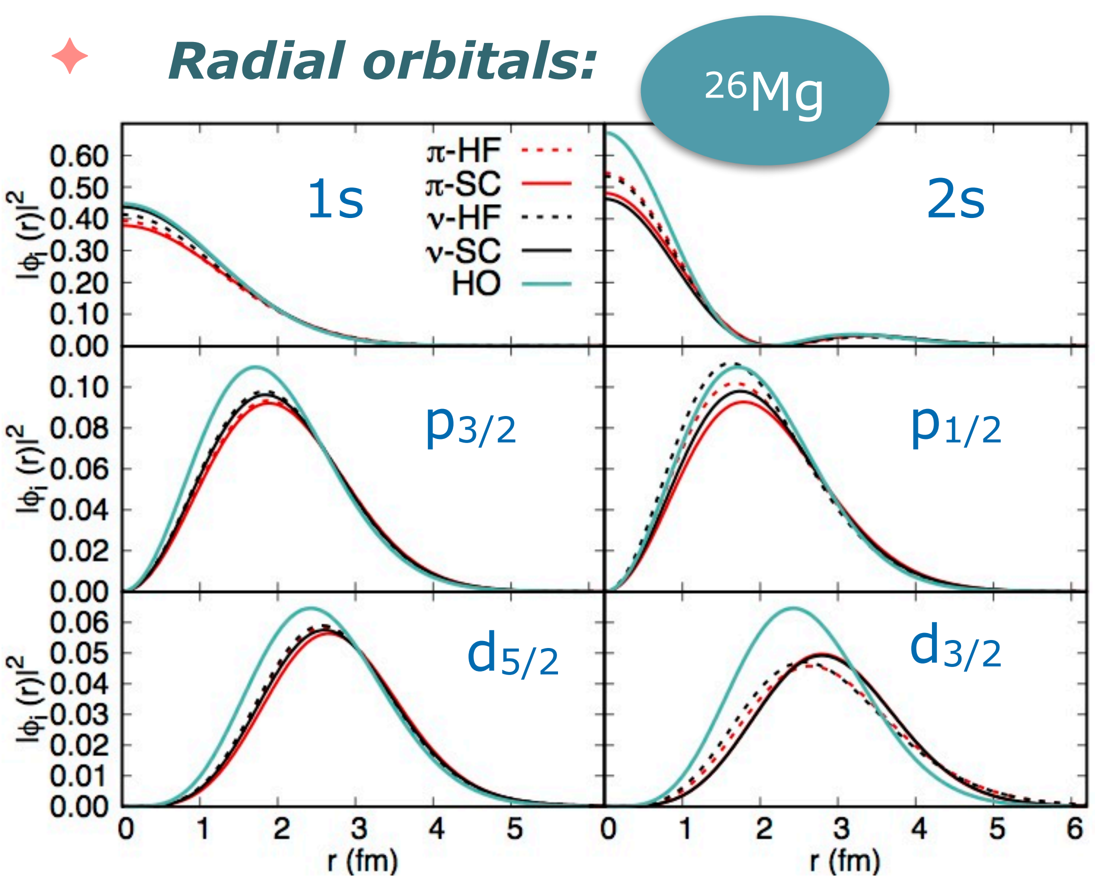
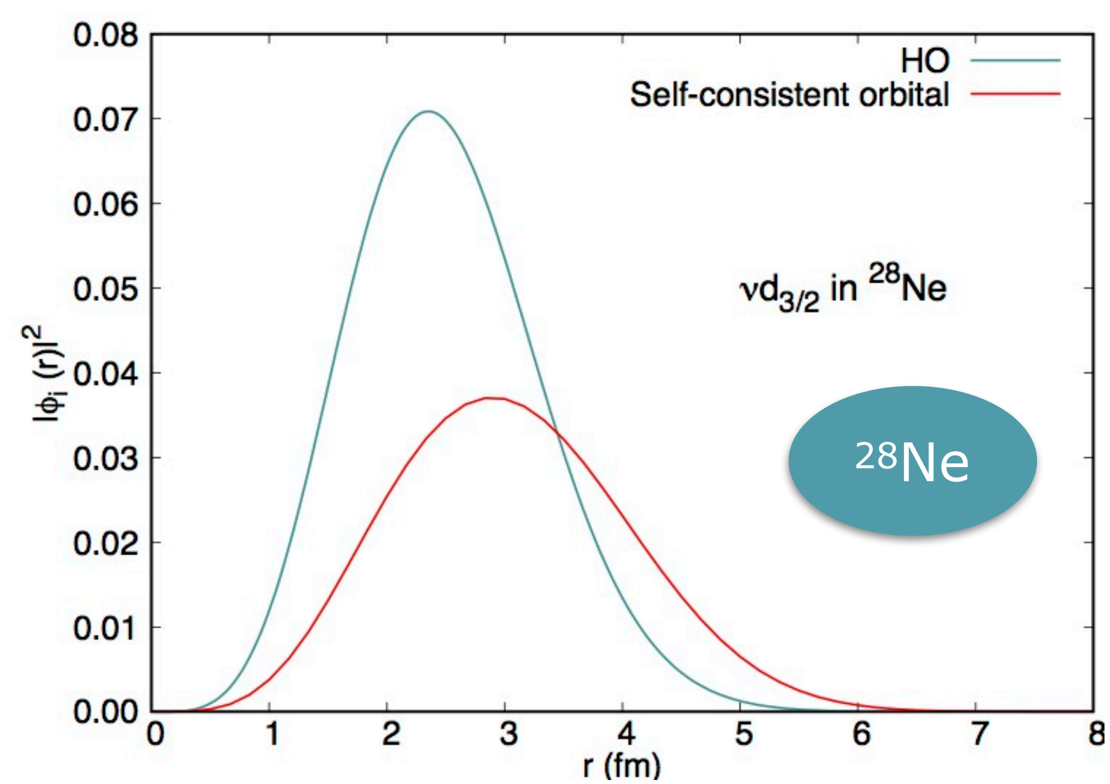
✦ ***Radial orbitals:***

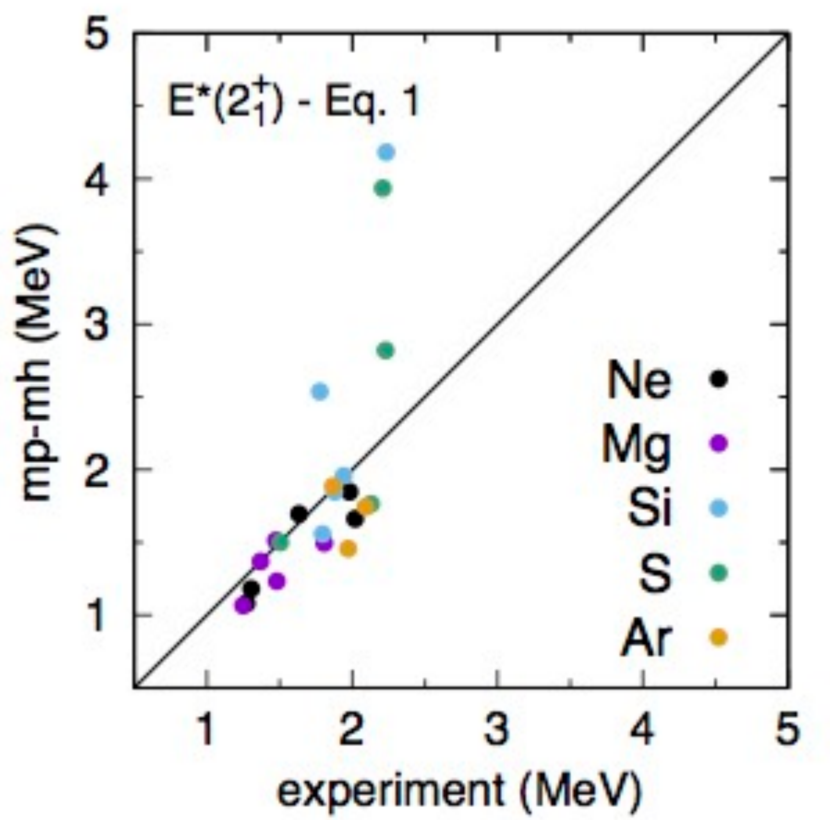




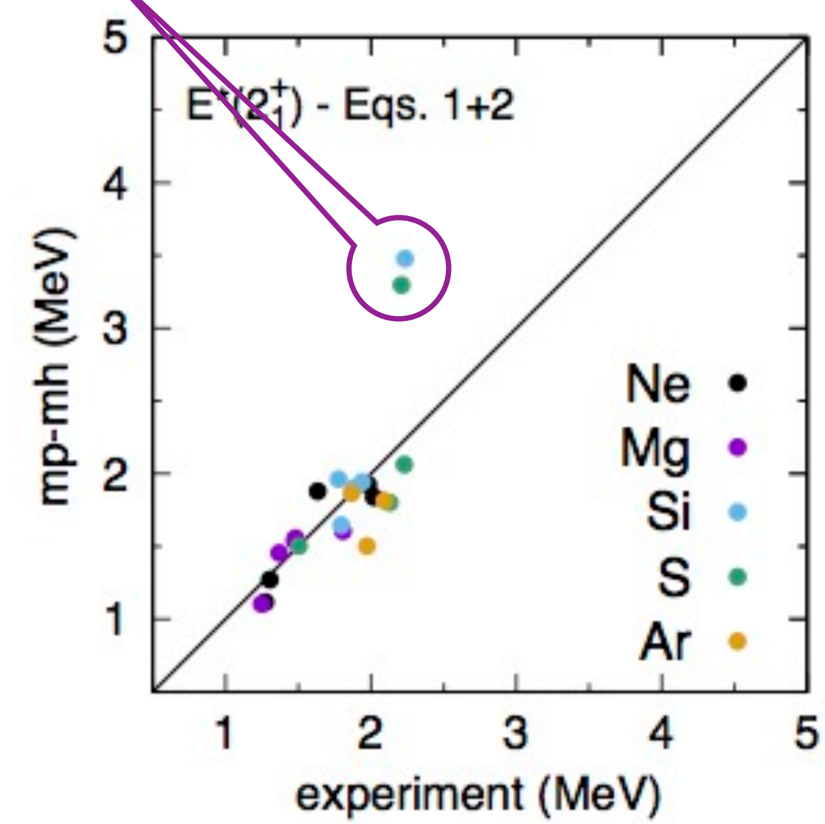
Application to sd-shell nuclei with the Gogny force

✦ ***Excitation energies:***

^{30}S and ^{30}Si:
T=0 component of the Gogny force
(lack of tensor term, *Pillet et al. PRC 85, 044315 (2012)*)



Orbital optimization



All
$$\begin{cases} \langle \Delta E^* \rangle = 373 \text{ keV} \\ \sigma(\Delta E^*) = 517 \text{ keV} \end{cases}$$

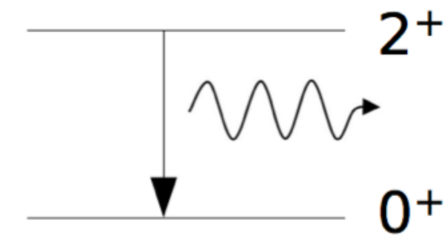
^{30}S & ^{30}Si excluded
$$\begin{cases} \langle \Delta E^* \rangle = 226 \text{keV} \\ \sigma(\Delta E^*) = 214 \text{ keV} \end{cases}$$

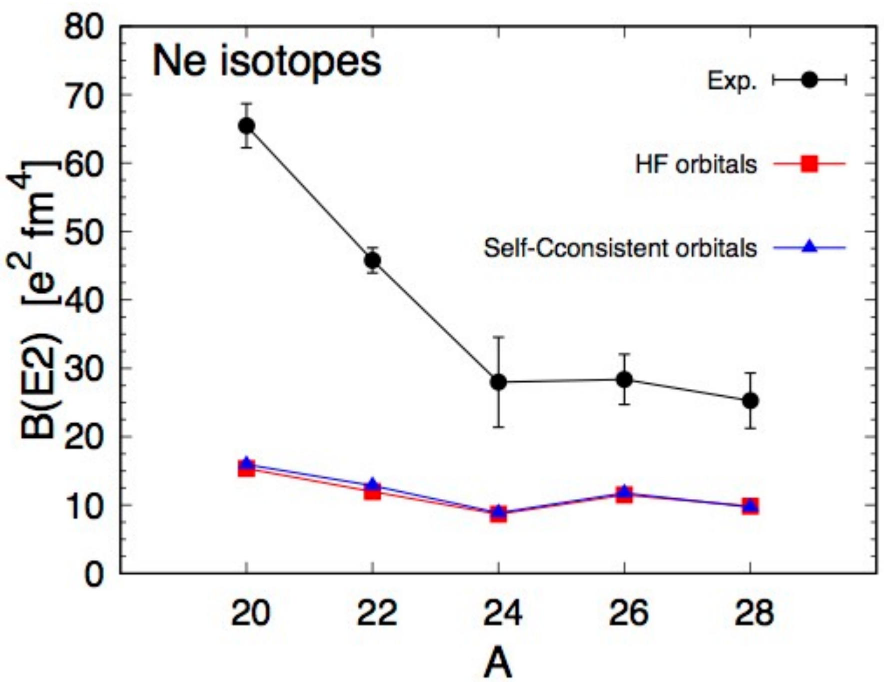
All
$$\begin{cases} \langle \Delta E^* \rangle = 235 \text{ keV} \\ \sigma(\Delta E^*) = 323 \text{ keV} \end{cases}$$

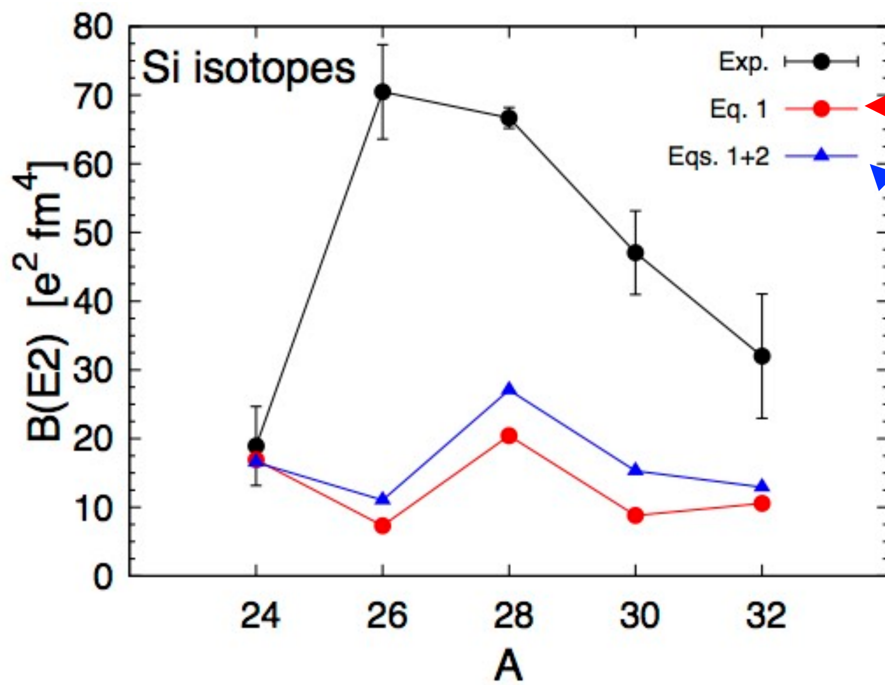
^{30}S & ^{30}Si excluded
$$\begin{cases} \langle \Delta E^* \rangle = 142 \text{ keV} \\ \sigma(\Delta E^*) = 122 \text{ keV} \end{cases}$$

Application to sd-shell nuclei with the Gogny force

✦ *Transition probabilities B(E2)*

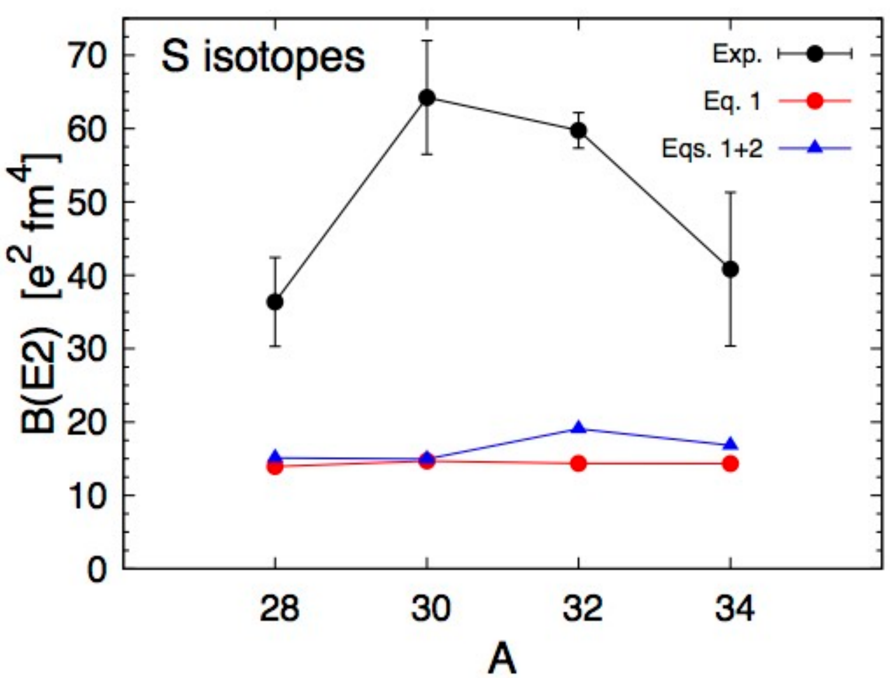






Hartree-Fock orbitals

self-consistent natural orbitals



- Trends overall well reproduced
- But clear lack of collectivity due to the restricted valence space
- Positive but small effect from the optimization of orbitals (factor 1.7 in ^{30}Si, 1.3 in ^{28}Si & ^{32}S)

No effective charges

Conclusion from the study with Gogny

* First implementation of the fully self-consistent multiparticle-multihole configuration mixing method

  ✦ Construction of a general mean-field and natural orbitals consistent with the correlation of the system, complete convergence reached.

  ✦ Effect of orbital optimization always positive.
  With single valence shell: large impact on the ground-state wave function, but small effect on the transition probabilities…

  ➡ solve orbital equation for each many-body state

  ➡ try truncation schemes involving larger single-particle spaces
  (excitation order, excitation energy, symmetry-constrained combinations etc.)

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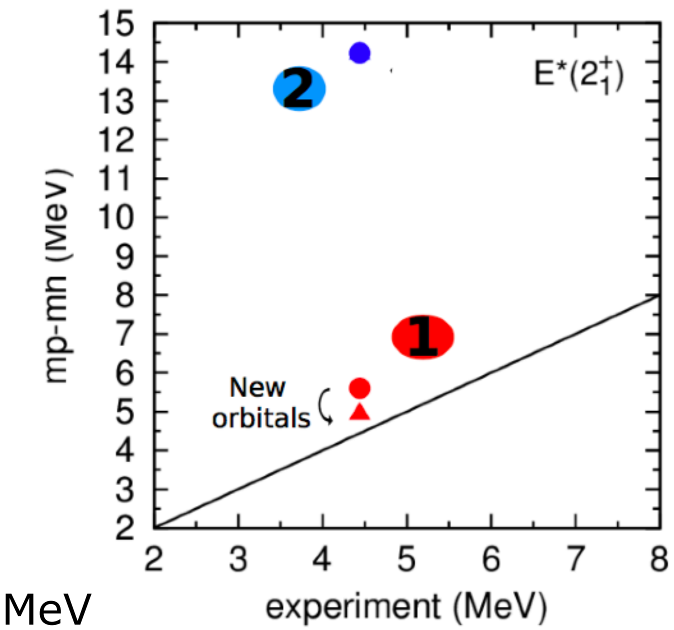
    ➡ solve orbital equation for each many-body state

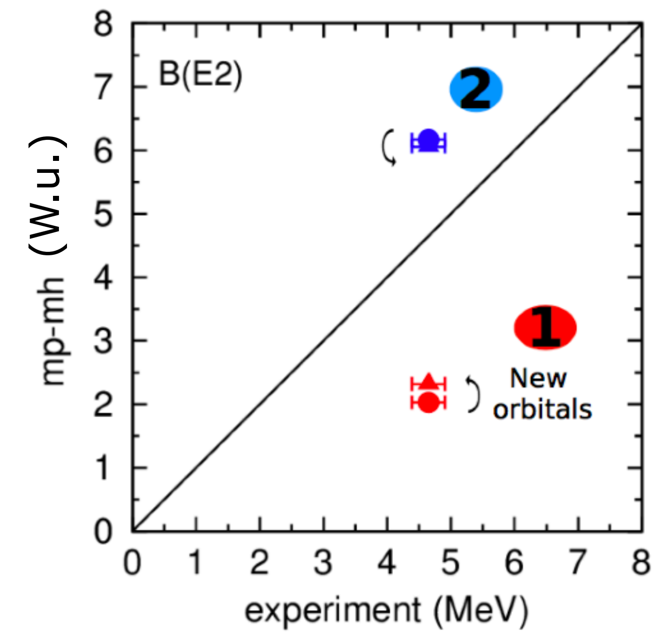
    ➡ try truncation schemes involving larger single-particle spaces (excitation order, excitation energy, symmetry-constrained combinations etc.)

- But:

  - The D1S Gogny interaction is in principle not adapted (double counting of correlations…), and

  - can lead to divergent behaviors when enlarging the valence space due to the zero-range spin-orbit and ρ-dependent terms. See e.g. study of ^{12}C:





1 $0\hbar\omega$ space

collectivity ✗, excitation energies ✓, overbinding ~ 6 MeV

2 $N\hbar\omega$ space

collectivity ✓, excitation energies ✗, overbinding ~ 60 MeV!

Conclusion from the study with Gogny

* First implementation of the fully self-consistent multiparticle-multihole configuration mixing method

  - Construction of a general mean-field and orbitals consistent with the correlation of the system, complete convergence reached.

  - Effect of orbital optimization always positive.
    With single valence shell: large impact on the ground-state wave function, but small effect on the transition probabilities…

    ➡ solve or

    ➡ try trun
    (excitat

* But:

  - The D1S Gog
    adapted (dou

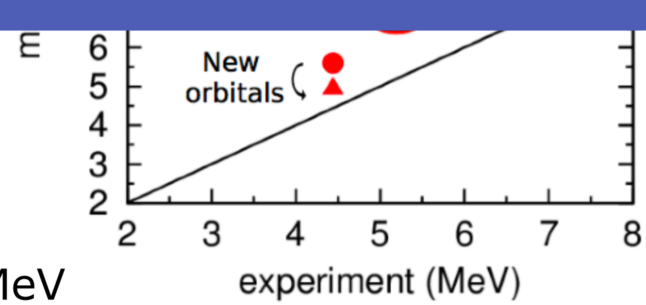
  - can lead to d
    the valence sp
    and ρ-dependent terms. See e.g. study of ^{12}C:

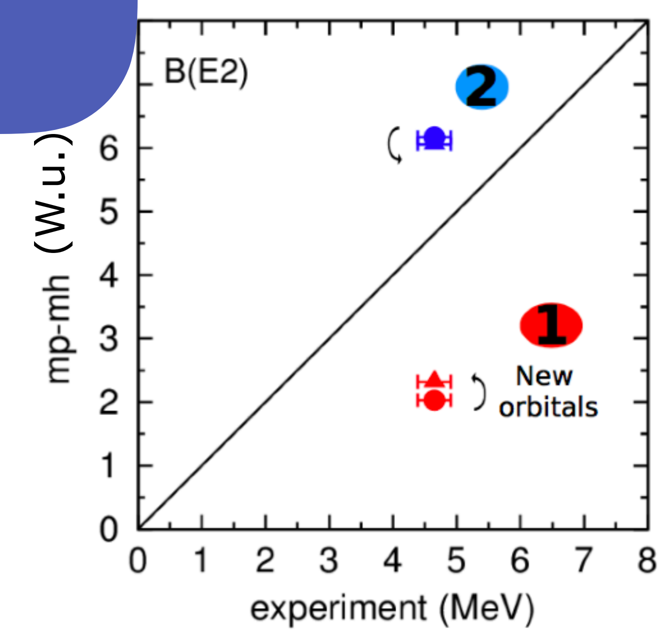
➡ *Need a better suited interaction*

- fully finite-range, better constrained Gogny interaction with tensor

or

- interaction derived from chiral EFT (here)





1 0ℏω space

collectivity ✗, excitation energies ✓, overbinding ~ 6 MeV

2 Nℏω space

collectivity ✓, excitation energies ✗, overbinding ~ 60 MeV!

Outline

- Formalism of the MPMH method

  → *role and interpretation of the orbital optimization*

- Applications with the Gogny D1S interaction

  - Numerical algorithm
    → *doubly iterative convergence process*

  - Description of even-even sd-shell nuclei
    → *Effect of the orbital optimization on ground and excited states properties: Charge radii, excitation energies, transition probabilities, inelastic electron and proton scattering…*

- *Towards an "ab-initio" theory*

  → *implementation of a chiral interaction: preliminaries*

— in collaboration with I. Tews (LANL), R. Bernard (ENS Cachan) and G. Hupin (IPN Orsay)

Application of the MPMH method with a chiral interaction

✦ In MPMH, we have to do the CI diagonalization and calculation of the mean field/source term at each iteration

↠ use matrix elements (e.g. in HO basis) as only input would be very inefficient

↠ need potential in coordinate space and ideally Gaussians

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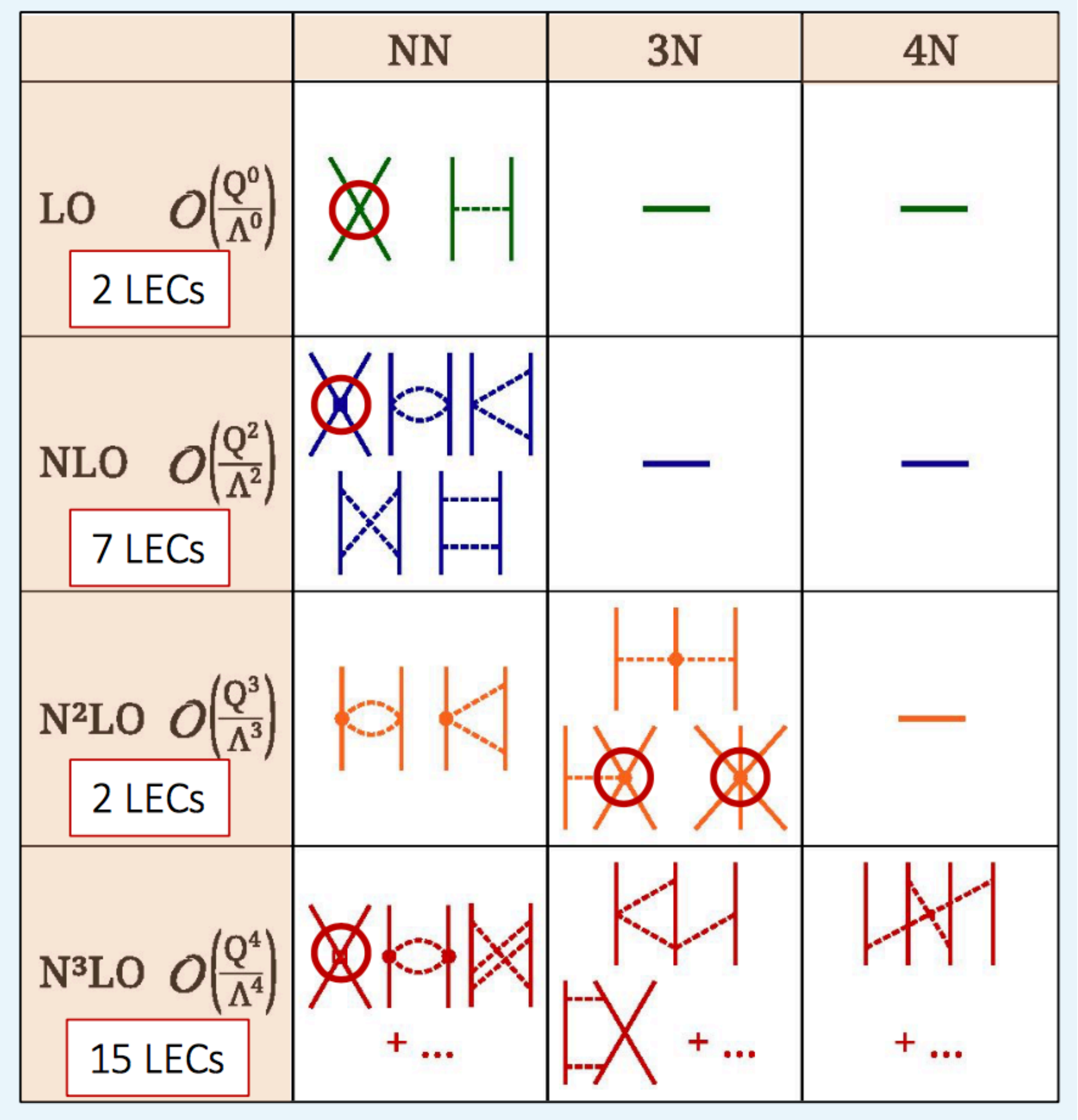
At each order:

contact terms
+
long-range pion-exchange terms

Chiral expansion:



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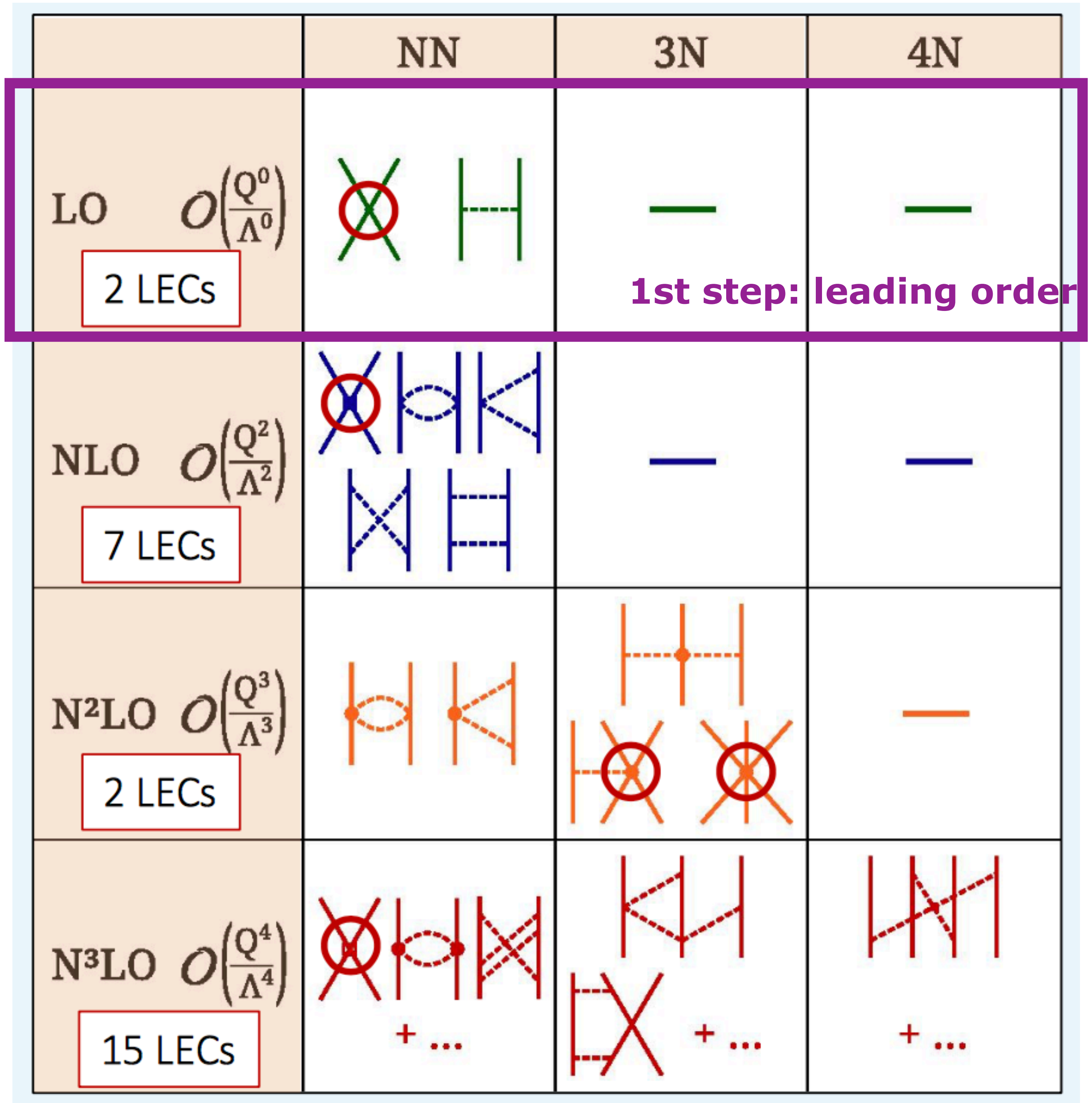
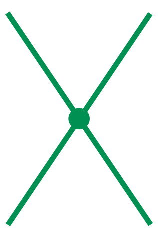


Application of the MPMH method with a chiral interaction

★ Chiral interaction at leading order with Gaussian regulators:

cut-off R_0= 1 fm

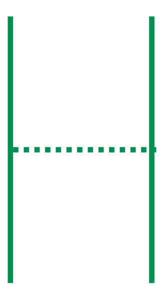
✦ contact term:



$$V^{LO}_{contact}(r) = (C_S + C_T \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \times \underbrace{\left(\alpha\, e^{-(r/R_0)^2}\right)}_{\text{regulator}}$$

↠ purely gaussian

✦ long-range one-pion exchange:



$$V^{LO}_{OPE}(r) = \left(W_S^{(0)}(r)\, \vec{\tau}_1 \cdot \vec{\tau}_2\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + W_T^{(0)}(r)\, \vec{\tau}_1 \cdot \vec{\tau}_2\, S_{12}\right) \times \underbrace{\left(1 - e^{-(r/R_0)^2}\right)^2}_{\text{regulator}}$$

central spin-isospin term:

$$W_S^{(0)}(r) = \frac{M_\pi^3}{12\pi} \left(\frac{g_A}{2F_\pi}\right)^2 \frac{e^{-M_\pi r}}{M_\pi r}$$

tensor isospin term:

$$W_T^{(0)}(r) = \frac{M_\pi^3}{12\pi} \left(\frac{g_A}{2F_\pi}\right)^2 \frac{e^{-M_\pi r}}{M_\pi r} \left(1 + \frac{3}{M_\pi r} + \frac{3}{(M_\pi r)^2}\right)$$

↠ Yukawa or Yukawa-like x Gaussians

Application of the MPMH method with a chiral interaction

★ Strategy: fit the regularized Yukawa or Yukawa-like functions to a sum of Gaussians

$$W^{(0)}_{S,reg}(r) \propto \frac{e^{-M_\pi r}}{r} \times (1 - e^{-(r/R_0)^2})^2 \simeq \sum_i a_i^S e^{-(r/b_i^S)^2}$$

$$W^{(0)}_{T,reg}(r) \propto \frac{e^{-M_\pi r}}{r} \left(1 + \frac{3}{M_\pi r} + \frac{3}{(M_\pi r)^2}\right) \times (1 - e^{-(r/R_0)^2})^2 \simeq \sum_i a_i^T e^{-(r/b_i^T)^2}$$

to use the machinery already developed in the original code for the Gogny interaction

Note:

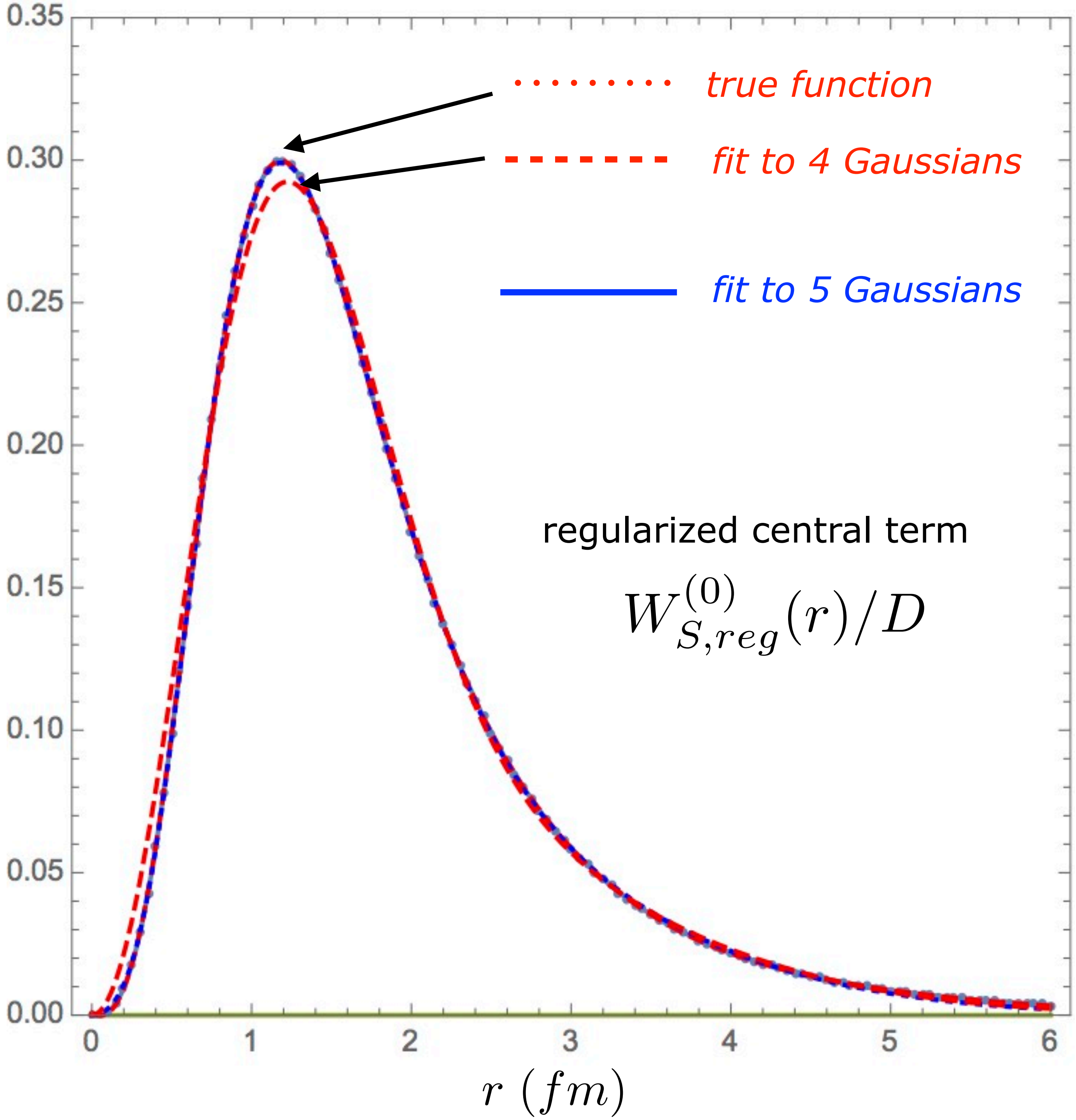
such fits of Yukawa to Gaussians already applied in *J. Dobaczewski & J. Engel, Phys. Rev. Lett. 94, 232502 (2005), or more recently in e.g. R. Navarro Perez et al. PRC 97, 054304 (2018).*

Application of the MPMH method with a chiral interaction

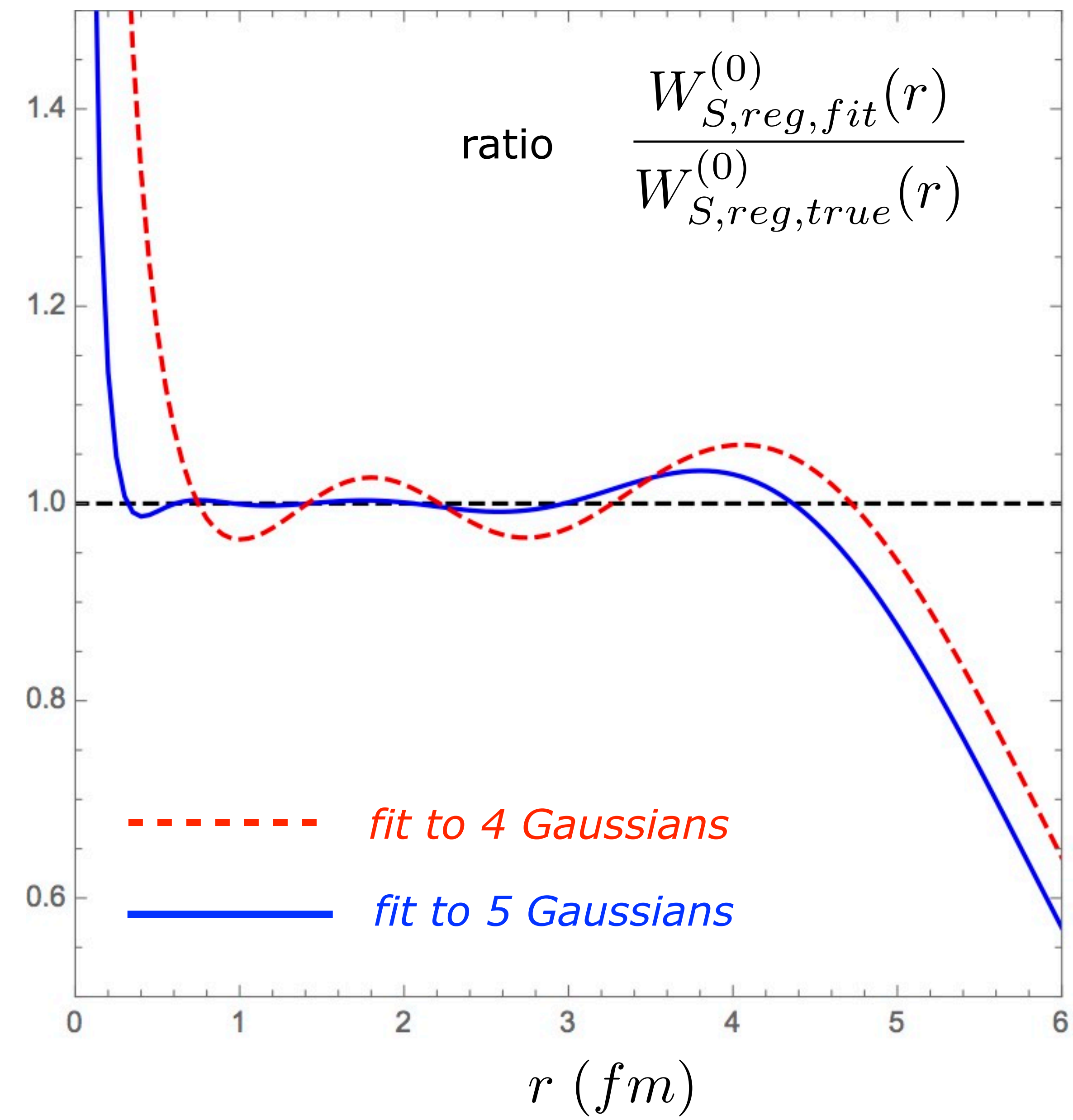
↠ ***Central term:***

Very preliminary!

$$D = \frac{M_\pi^3}{12\pi}\left(\frac{g_A}{2F_\pi}\right)^2$$



Choose 5 Gaussians



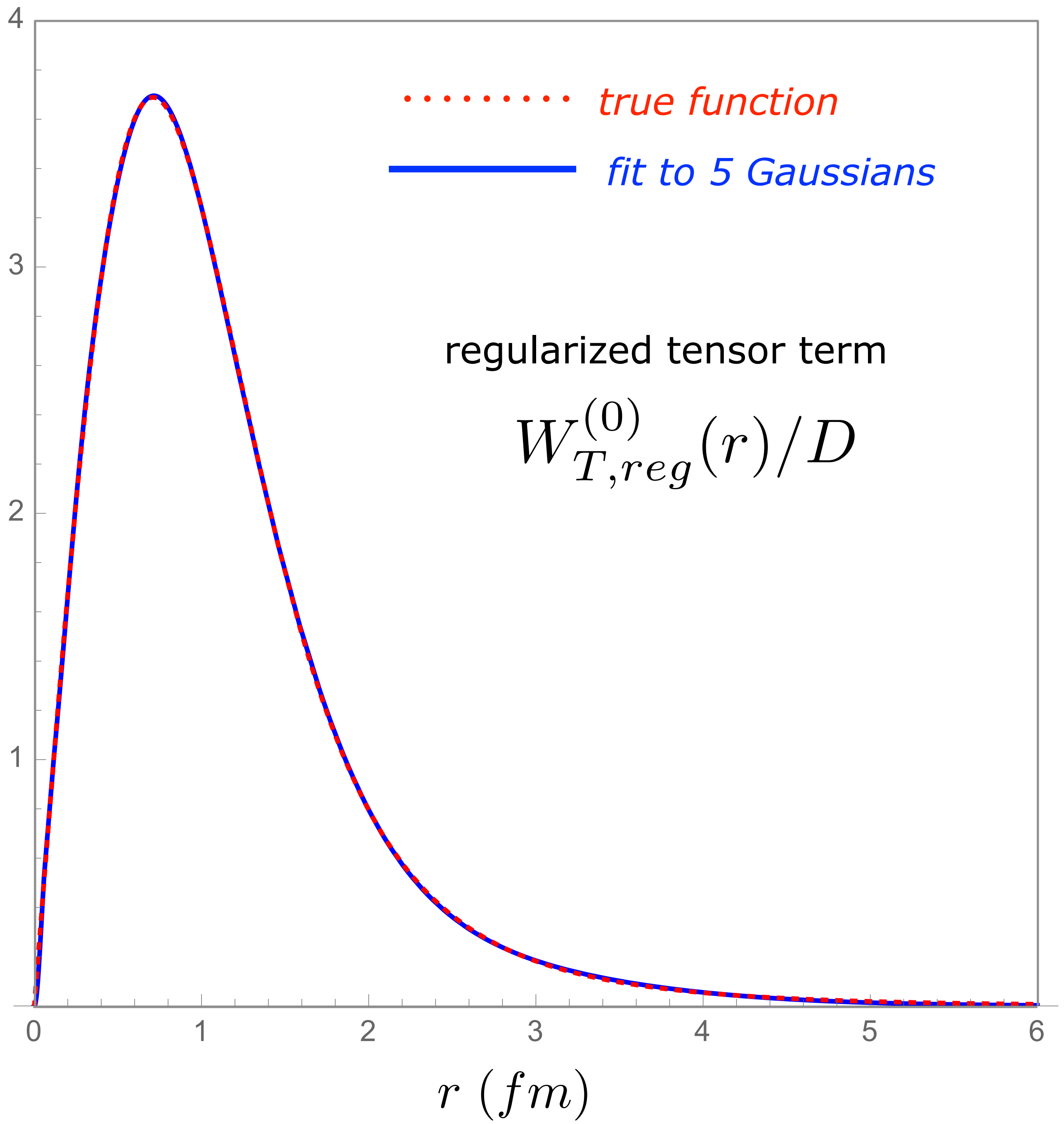
Courtesy of I. Tews

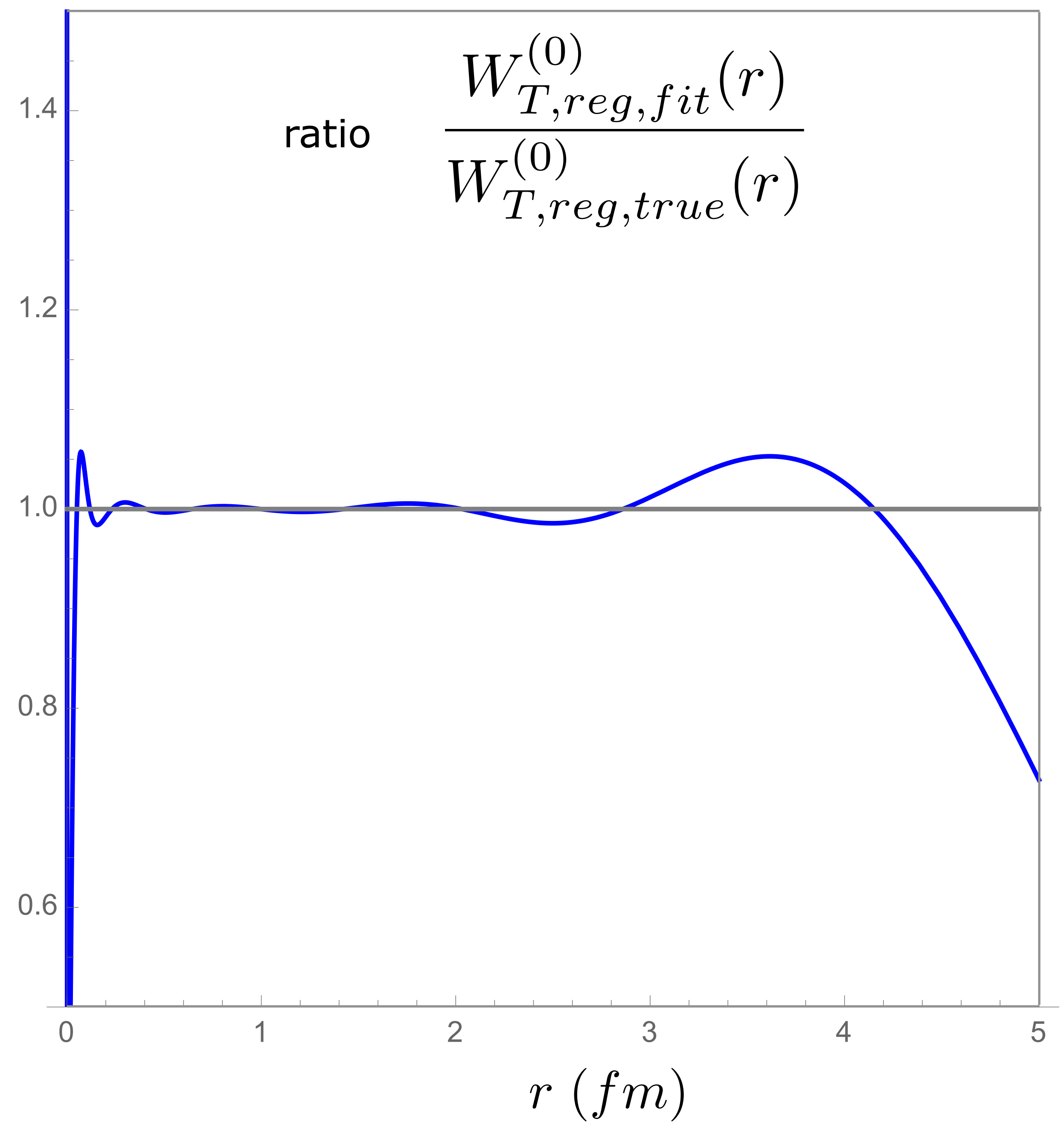
Application of the MPMH method with a chiral interaction

↠ **Tensor term:**

Very preliminary!

$$D = \frac{M_\pi^3}{12\pi}\left(\frac{g_A}{2F_\pi}\right)^2$$





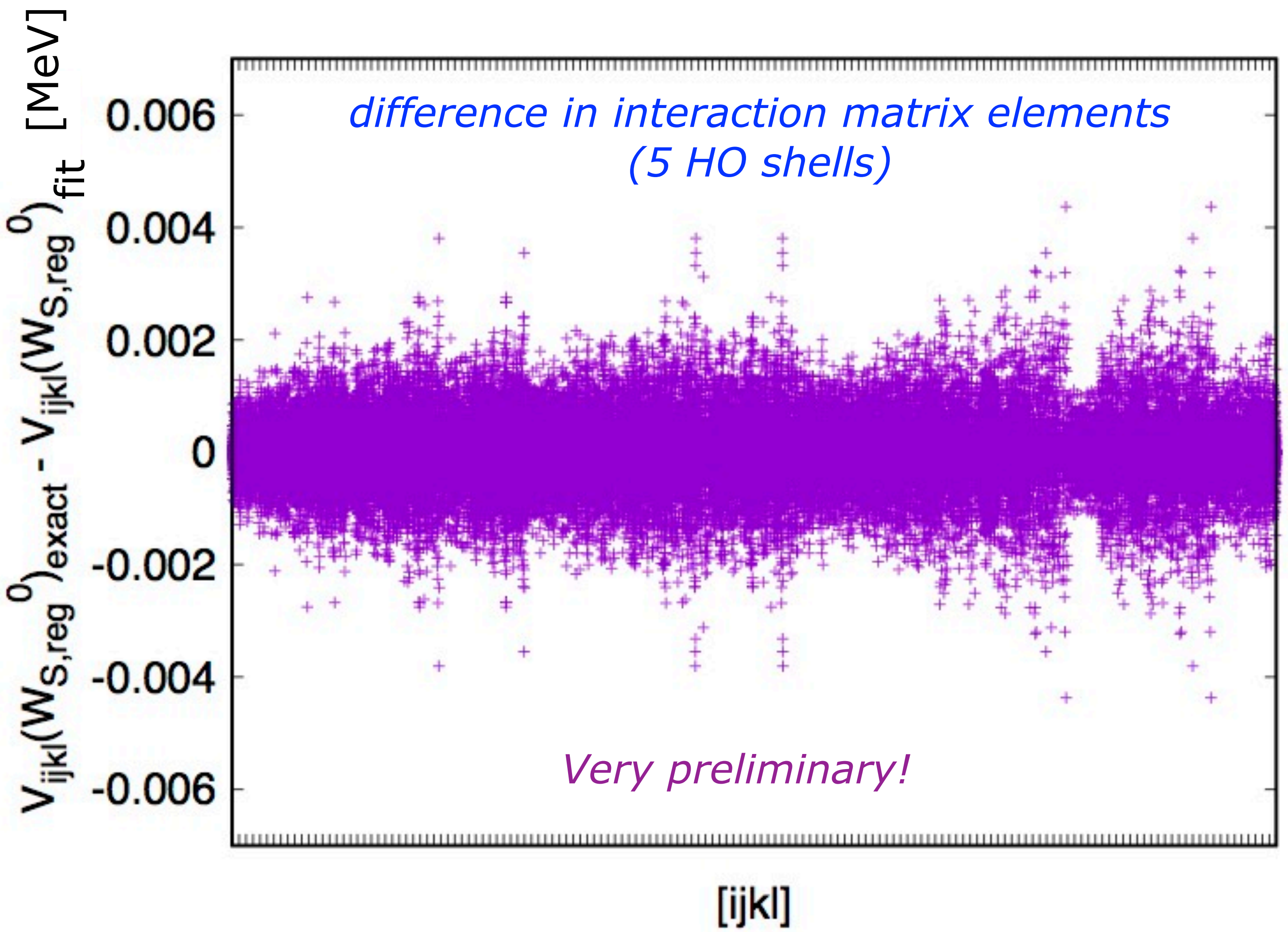
Courtesy of I. Tews

Application of the MPMH method with a chiral interaction

↠ ***Test for the central term:***

Use the relation $$\frac{e^{-M_\pi r}}{r} = \frac{2}{\sqrt{\pi}} \int_0^\infty dX e^{-r^2 X^2 - M_\pi^2/4X^2}$$ (exact)

to do the exact integration of the central term and check the accuracy of the Gaussian fit



✳ Average difference:

$$\langle \Delta\widetilde{V} \rangle = \frac{1}{N} \sum_{\{ijkl\}=1}^{N} |\widetilde{V}_{ijkl}^{exact} - \widetilde{V}_{ijkl}^{fit}|$$

$$= 2.10 \times 10^{-5} \text{ MeV}$$

✳ standard deviation:

$$s = \sqrt{\langle \Delta\widetilde{V}^2 \rangle - \langle \Delta\widetilde{V} \rangle^2}$$

$$= 1.20 \times 10^{-4} \text{ MeV}$$

↠ impact on observables to be investigated...

Application of the MPMH method with a chiral interaction

To do next:

- Finish the implementation of the tensor term
- Implement the next orders: NLO, N^2LO
  - ↠ finite range spin-orbit
  - ↠ three-body interaction
- Check convergence of the results with respect to the cut-off and the size of the single-particle basis …

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Thank you!

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