ESNT workshop "Symmetry-breaking versus symmetry-preserving many-body schemes"
May 13-17th, CEA Saclay

INSTITUTE for NUCLEAR THEORY

Single-particle relaxation effects from the multi-particle-multi-hole configuration mixing approach

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Guillaume Hupin, *IPN Orsay, France*
Marc Dupuis, *CEA, DAM, DIF, France*

Introduction

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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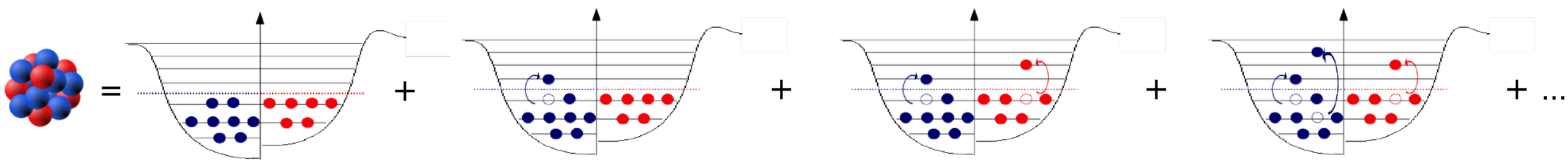
MPMH method: Formalism

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

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



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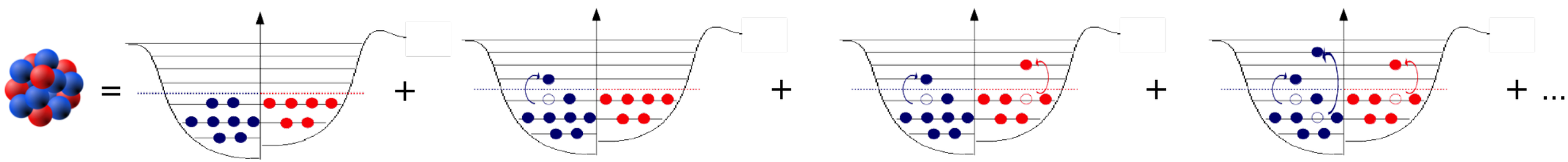

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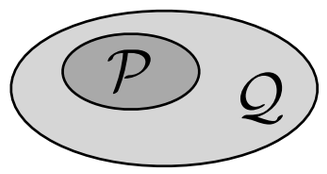
Combinatorial growth of the number of configurations $\Longrightarrow$ select the most relevant ones

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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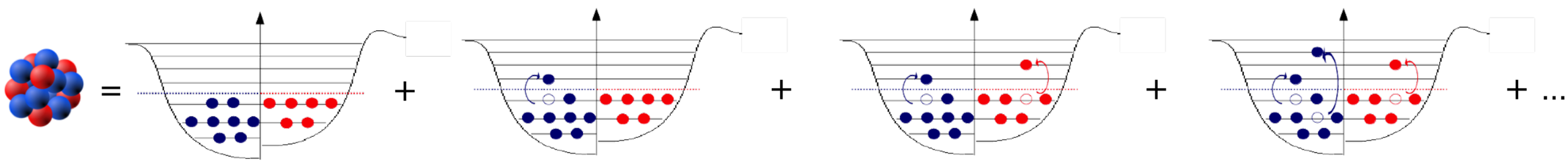

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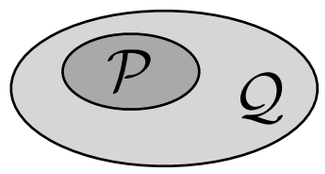
$\mathcal{H} =$ 

Unknowns?

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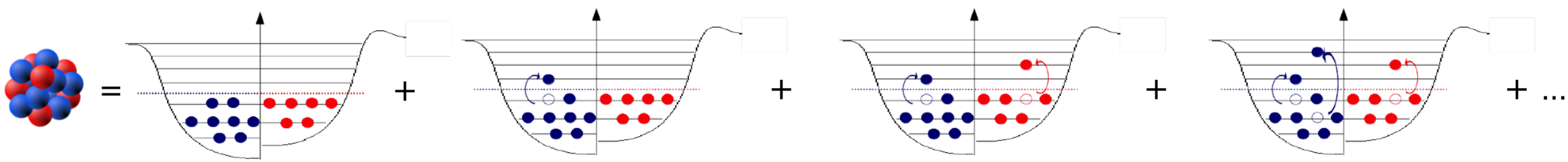

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Unknowns? { The mixing coefficients $\{A_\alpha\}$

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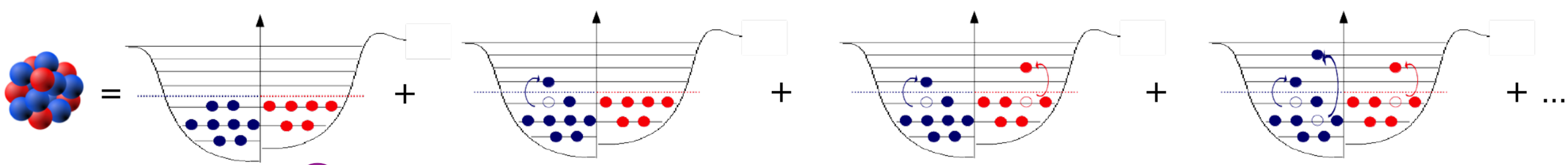

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$$\mathcal{H} = \mathcal{P} \quad \mathcal{Q}$$

Unknowns? $\begin{cases} \text{The mixing coefficients } \{A_\alpha\} \\ \text{The single-particle states } \{\varphi_i\} \end{cases}$

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).*

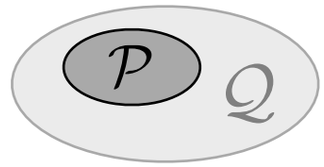
MPMH method: Formalism

Usual CI diagonalization

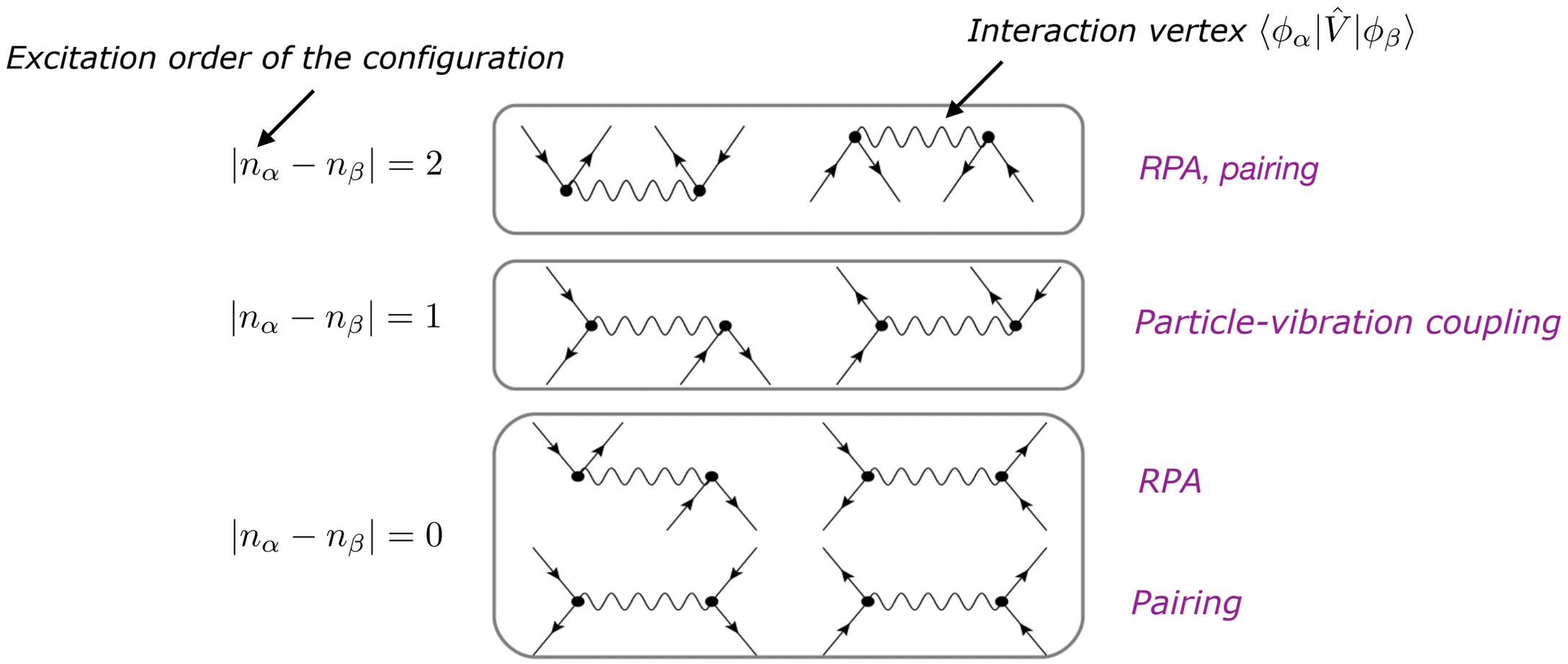
$$\begin{pmatrix} & H & \end{pmatrix} \begin{pmatrix} A \end{pmatrix} = E \begin{pmatrix} A \end{pmatrix}$$

★ 1st variational equation: The mixing coefficients

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



➡ introduces explicit correlations in restricted configuration space $\mathcal{P}$
All types of long-range correlations are treated at the same time:



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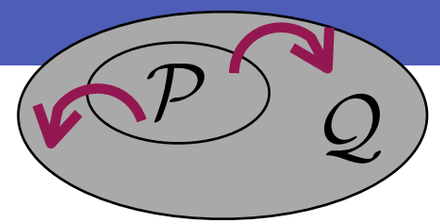

★ 2nd variational equation: The single-particle states

✦ 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:

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

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

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

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

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

"Generalized Brillouin condition"

Generalized mean-field equation

MPMH method: Formalism

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Generalized mean-field equation

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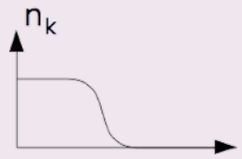
correlated one-body density

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

➡ "natural" basis

➡ occupation numbers



MPMH method: Formalism

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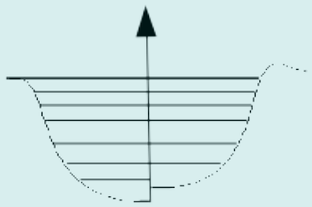
general mean field

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

contribution from particles & holes

➡ "canonical basis"

➡ single-particle energies



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

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

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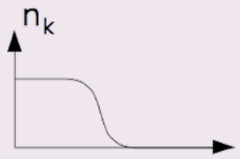

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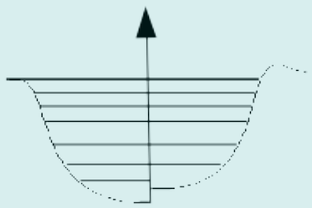

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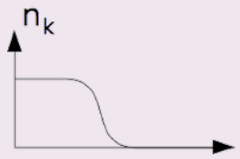

source term

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

σ = two-body correlation matrix

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

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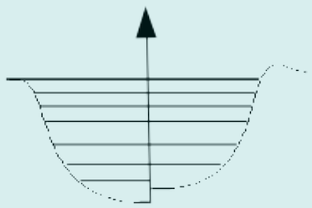

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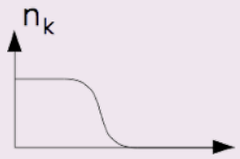

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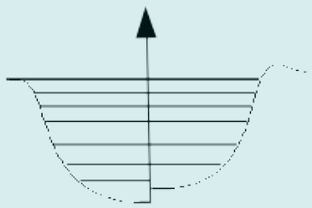

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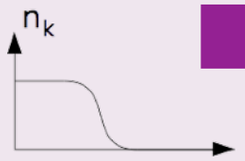

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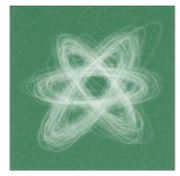
single-particle orbitals



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the mean field h(ρ) is related to the energy while the density ρ contains information on the wave function

➡ single-particle states= natural orbitals= eigenfunctions of the density that satisfies the general mean field equation

MPMH method: Formalism

★ ***Role of the orbital equation:***

I) Consistency between correlations and single-particle picture

General equation in physics:

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

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

1-body GF $\mathcal{G}^{(1)}$ — Connected 2-body GF $\mathcal{G}^{(2)}_C$

Renormalization of the one-body propagator

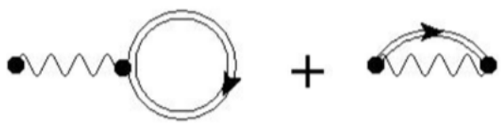
—

equivalent to solving a Dyson equation

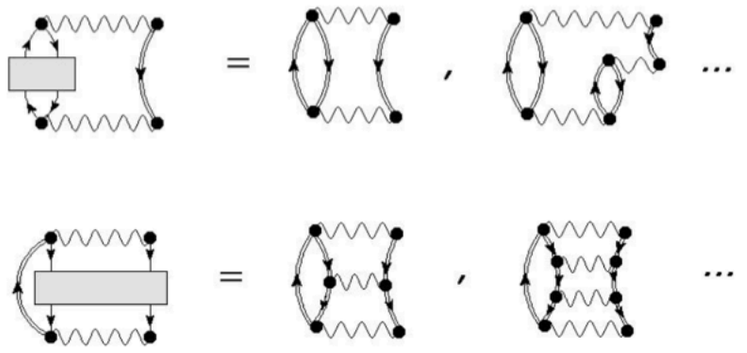
Self-energy: $\Sigma(t_1 - t_2) = \Sigma^{(0)}\delta(t_1 - t_2) + \Sigma^{(dyn)}(t_1 - t_2)$

Static part — Dynamical part

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



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



➡ full consistency between mean-field and correlations, which is important to have a fully variational theory

(see e.g. "*Quantum Theory of Finite systems*" by Blaizot and Ripka)

MPMH method: Formalism

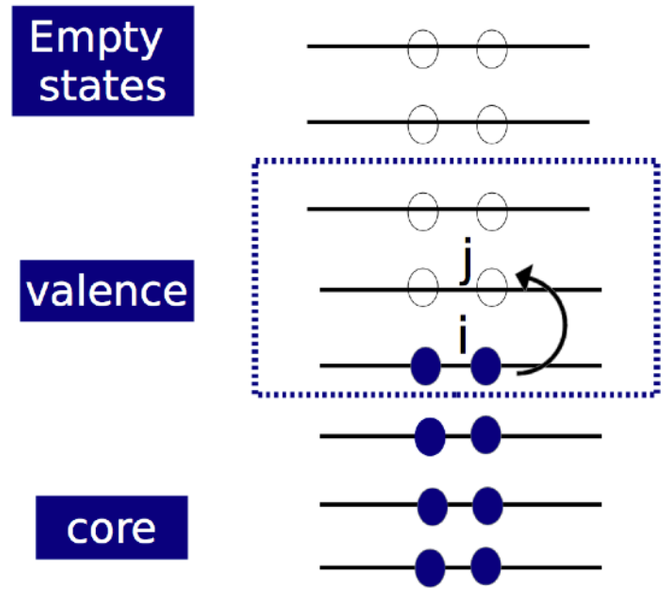
★ ***Role of the orbital equation:***

II) Partial compensation of the truncation P/Q

- Ex: truncation core/valence space

→ Without orbital equation:

$$\rho_{ij} \begin{cases} = \delta_{ij} \text{ if } i,j \in \text{core} \\ \in [0,1] \text{ if } i,j \in \text{valence} \\ = 0 \text{ otherwise} \end{cases}$$



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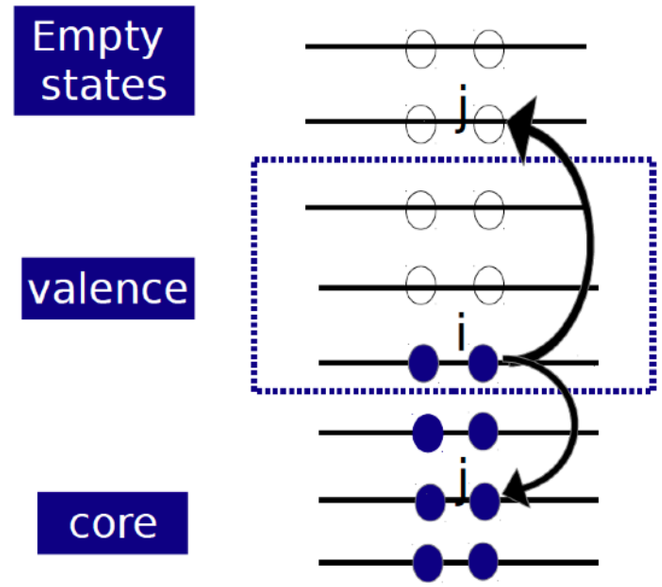
→ Without orbital equation:

$$\rho_{ij} \begin{cases} = \delta_{ij} \text{ if } i,j \in \text{core} \\ \in [0,1] \text{ if } i,j \in \text{valence} \\ = 0 \text{ otherwise} \end{cases}$$



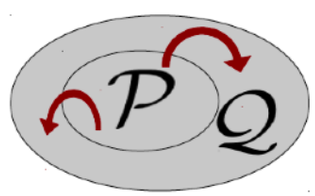
→ With orbital equation:

$$\left[h[\rho], \rho\right] = G[\sigma] \Rightarrow \rho_{ij} = \frac{G_{ij}[\sigma]}{\varepsilon_i - \varepsilon_j}$$

Single-particle energies

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

∈ whole basis ∈ valence

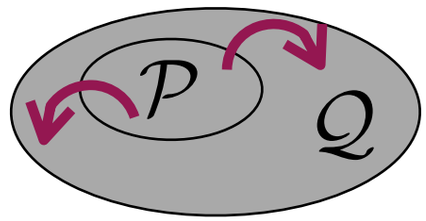


⇒ coupling between valence space and rest of the basis.

MPMH method: Formalism

★ ***Role of the orbital equation:***

II) Partial compensation of the truncation P/Q

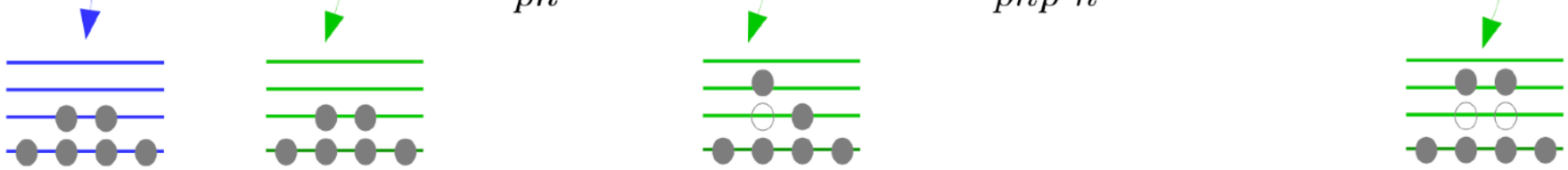


- Ex: truncation in term of the excitation order NpNh

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

➡ $|\phi^{(f)}\rangle = e^{iT}|\phi^{(i)}\rangle$

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



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

➡ should have a higher weight in the correlated wave function than the initial one

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*

Application to sd-shell nuclei with the Gogny force

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

$$V[\rho] = \sum_{j=1,2} (W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau)\, e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{\mu_j^2}}$$

$$+ t_3(1 + x_0 P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)\rho^\alpha\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)$$

$$+ iW_{LS}\vec{\nabla}_{12}\delta(\vec{r}_1 - \vec{r}_2) \times \overleftarrow{\nabla}_{12}(\sigma_1 + \sigma_2)$$

$$+ (1 + 2\tau_{1z})(1 + 2\tau_{2z})\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

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

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

Spin-Orbit
(zero-range)

Coulomb

ρ-dependency ↔ resummation of short range correlations, many-body effects ...

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

correlated density

Application to sd-shell nuclei with the Gogny force

➡ **modified coupled equations to solve:**

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

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

rearrangement terms

- ρ and σ-dependency ➡ non-linear equation

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

- 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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MPMH 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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The full solution requires a doubly-iterative algorithm:

Solve the 2nd equation:

$$\left[\hat{h}(\rho,\sigma),\hat{\rho}\right] = \hat{G}(\sigma) \Leftrightarrow \left[\hat{h}(\rho,\sigma) - \hat{Q}(\rho,\sigma),\hat{\rho}\right] = 0$$

New "correlation field"

In the natural basis $\hat{\rho}|\mu\rangle = n_\mu|\mu\rangle$

$$\begin{cases} Q_{\mu\nu}(\rho,\sigma) = \dfrac{G_{\mu\nu}(\sigma)}{n_\mu - n_\nu} \text{ , if } n_\mu \neq n_\nu \\ Q_{\mu\nu}(\rho,\sigma) = 0 \text{ , otherwise.} \end{cases}$$

⇒ self-consistent single-particle states $\{\varphi_i\}$ = eigenfunctions of h-Q and ρ

⇒ *non-linear problem ⇒ iterative solution:*

orbitals $\{\varphi^{(0)}\}$ density $\rho^{(0)}$ *(from 1st eq.)* → $h(\rho^{(0)},\sigma) - Q(\rho^{(0)},\sigma)$ → orbitals $\{\varphi^{(1)}\}$ density $\rho^{(1)}$ → $h(\rho^{(1)},\sigma) - Q(\rho^{(1)},\sigma)$ → ...

→ *until convergence* → *Back to the 1st equation…*

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

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Solve 2nd equation

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

$h(\rho,\sigma) - Q(\rho,\sigma)$ $\quad\leftrightarrow\quad$ $\rho, \{\varphi_i\}$

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

Calculation of the densities and source term

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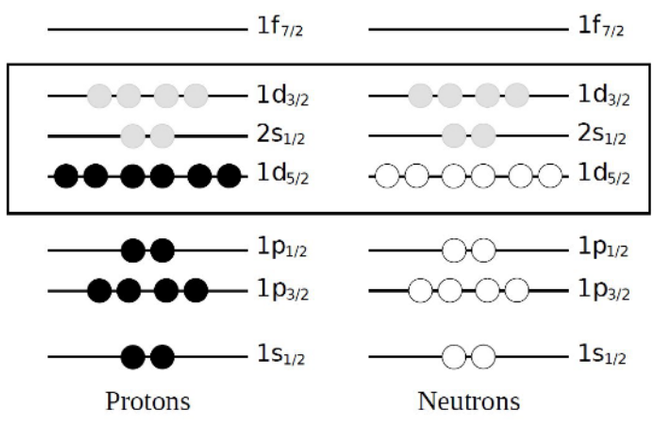
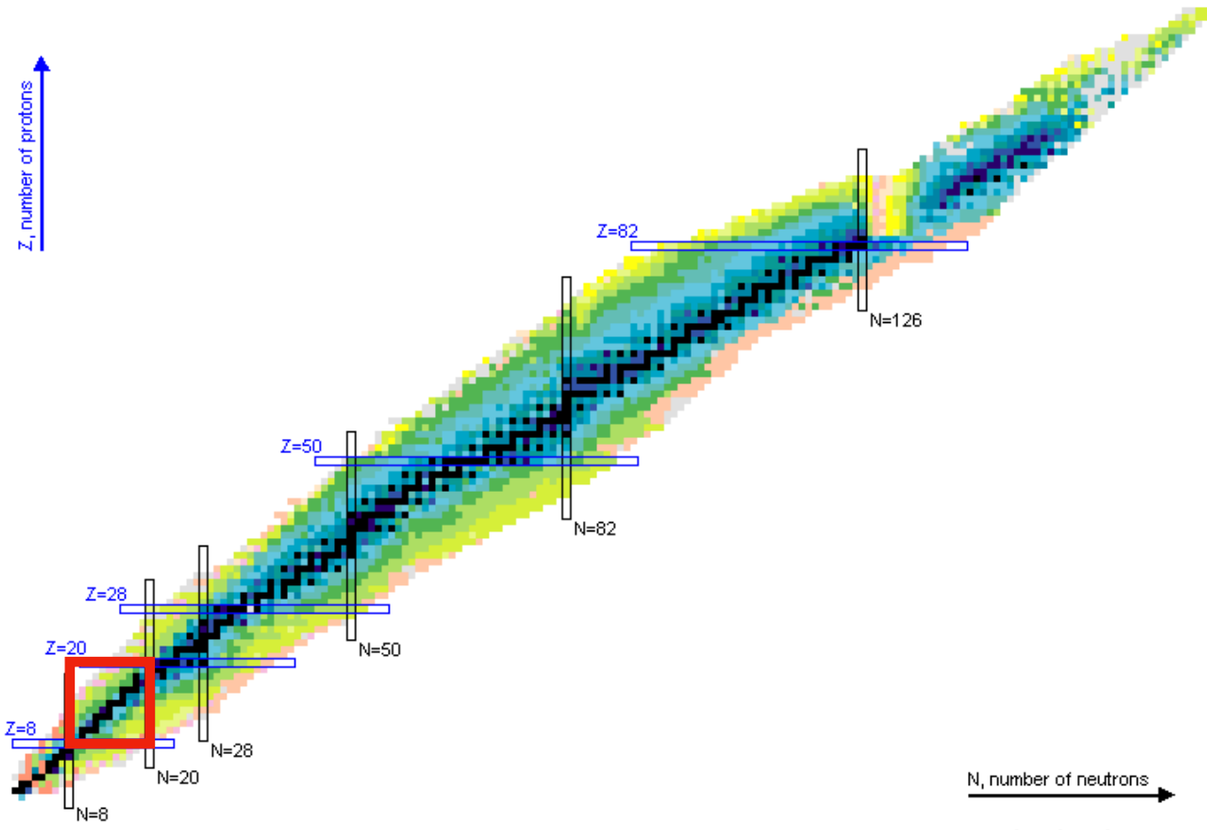
Application to sd-shell nuclei with the Gogny force

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)…

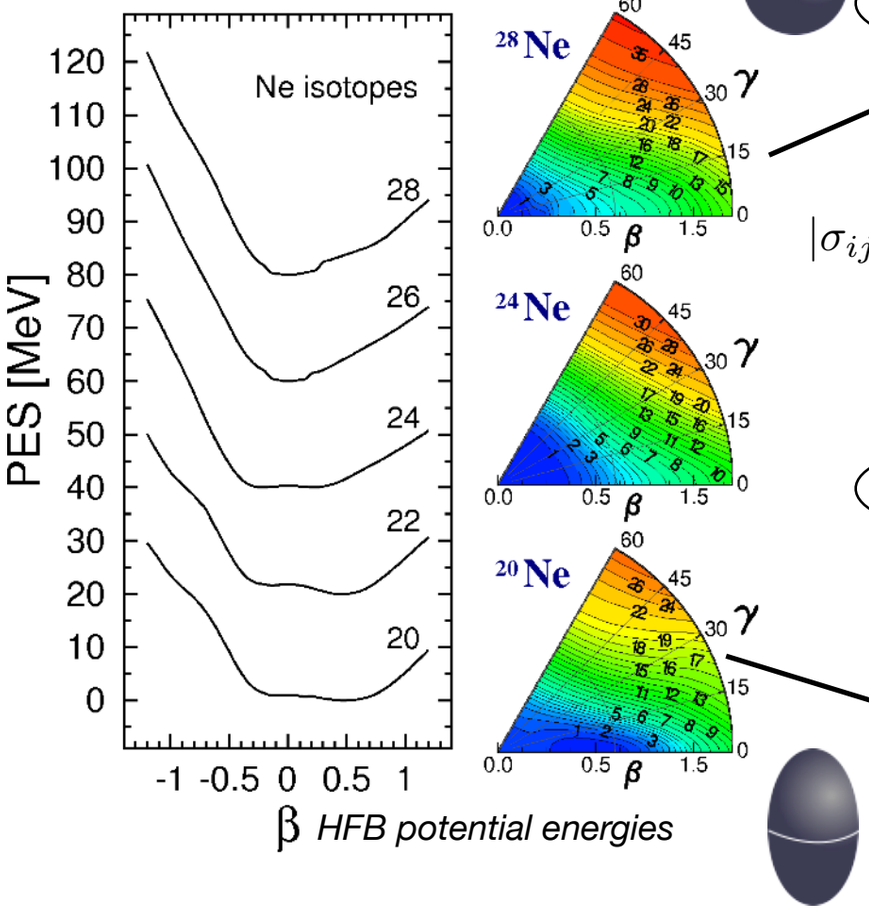
➡ How are these observables impacted by the optimization of orbitals?

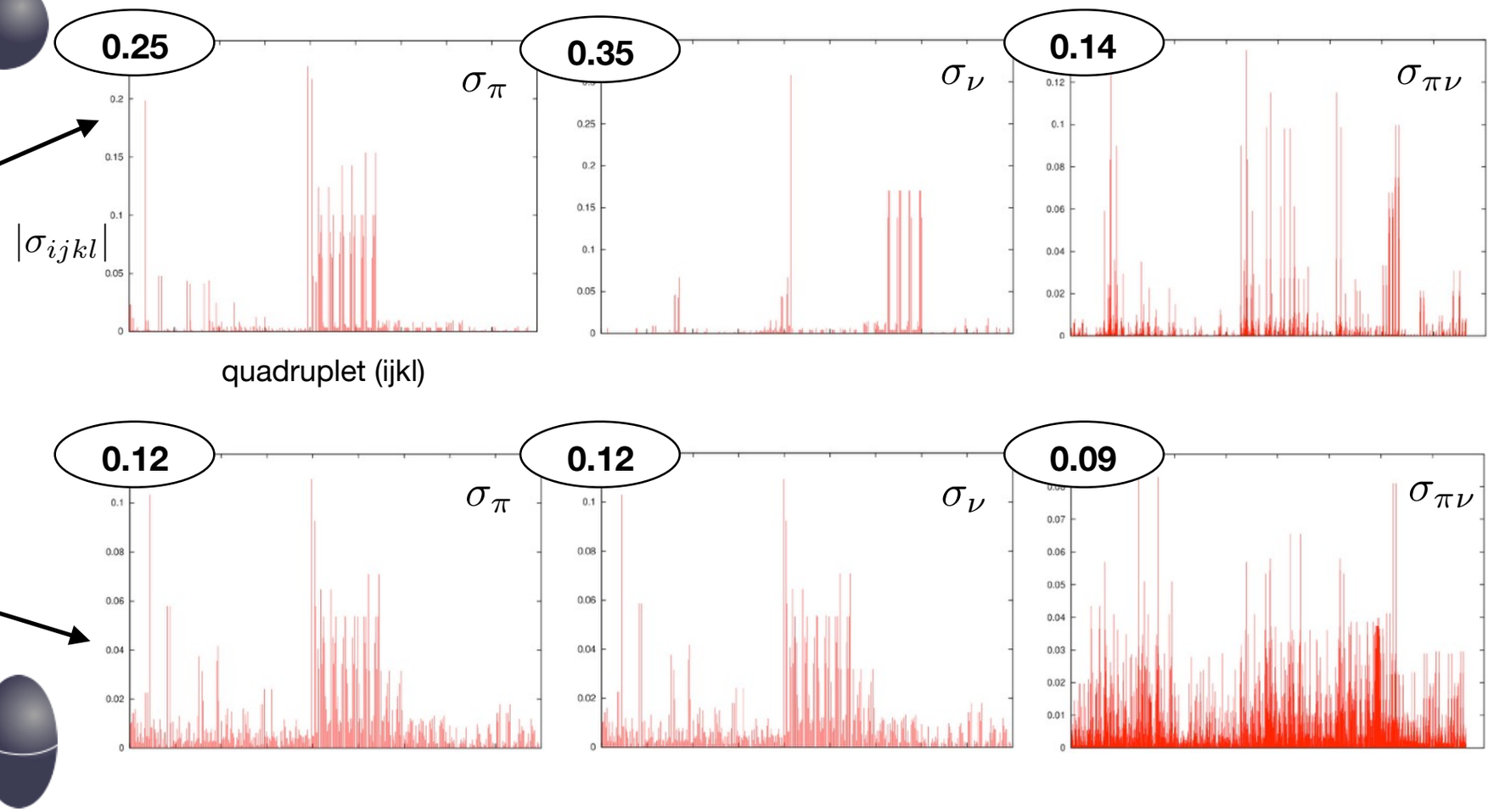
C. Robin, N. Pillet, M. Dupuis, J. Le Bloas, D. Peña Arteaga and J.F. Berger, PRC 95 044315 (2017).

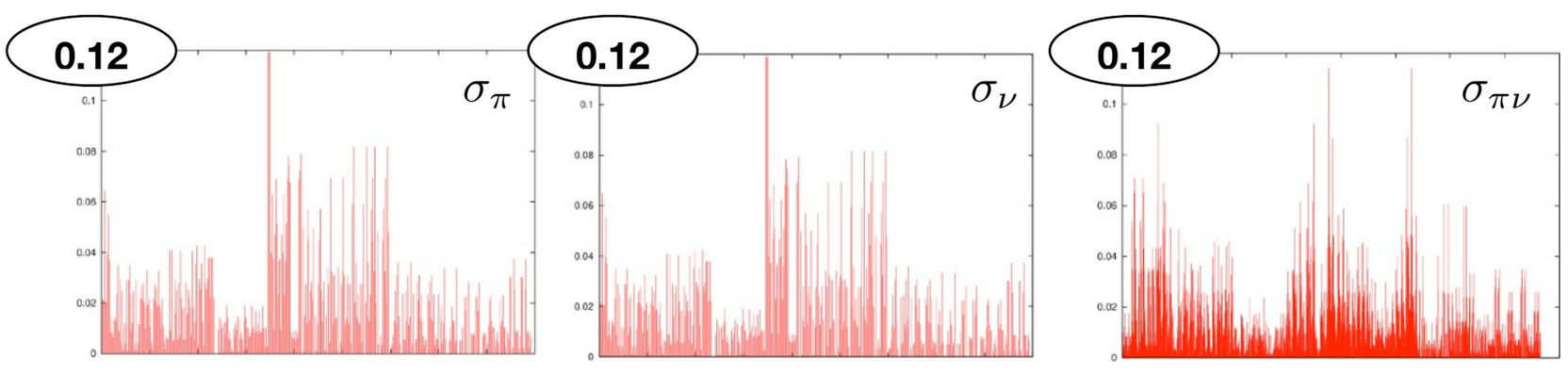
Application to sd-shell nuclei with the Gogny force

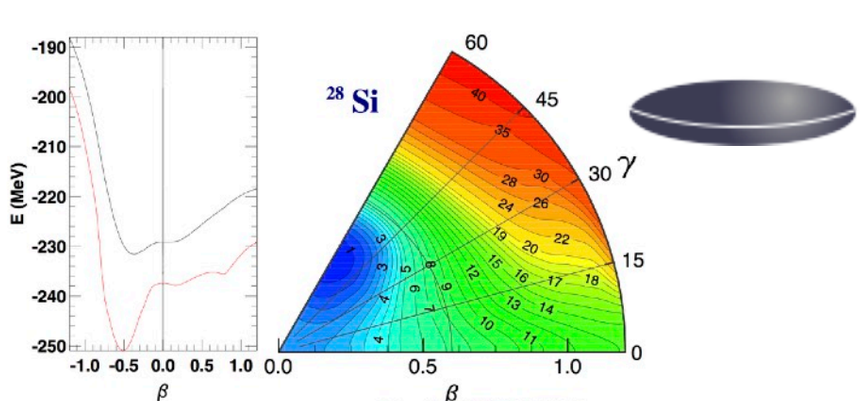
Symmetry-preserving scheme

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







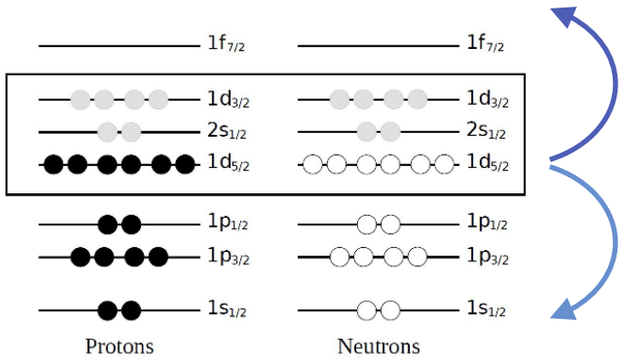


Application to sd-shell nuclei with the Gogny force

✱ **Source term of the orbital equation:**

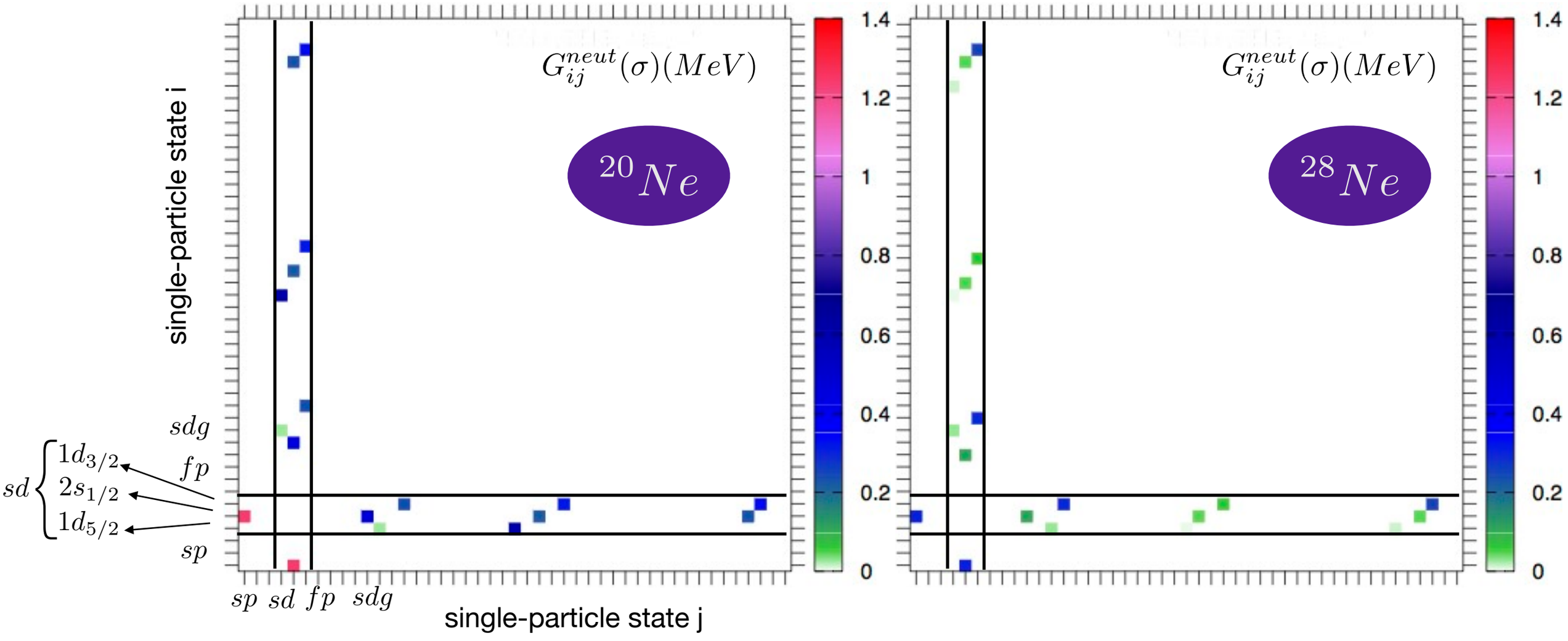
$$G_{ij}(\sigma) = \frac{1}{2}\sum_{klm}\widetilde{V}_{kmjl}\sigma_{kiml} - \frac{1}{2}\sum_{klm}\widetilde{V}_{kiml}\sigma_{jlkm}$$

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



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

At iteration #1:

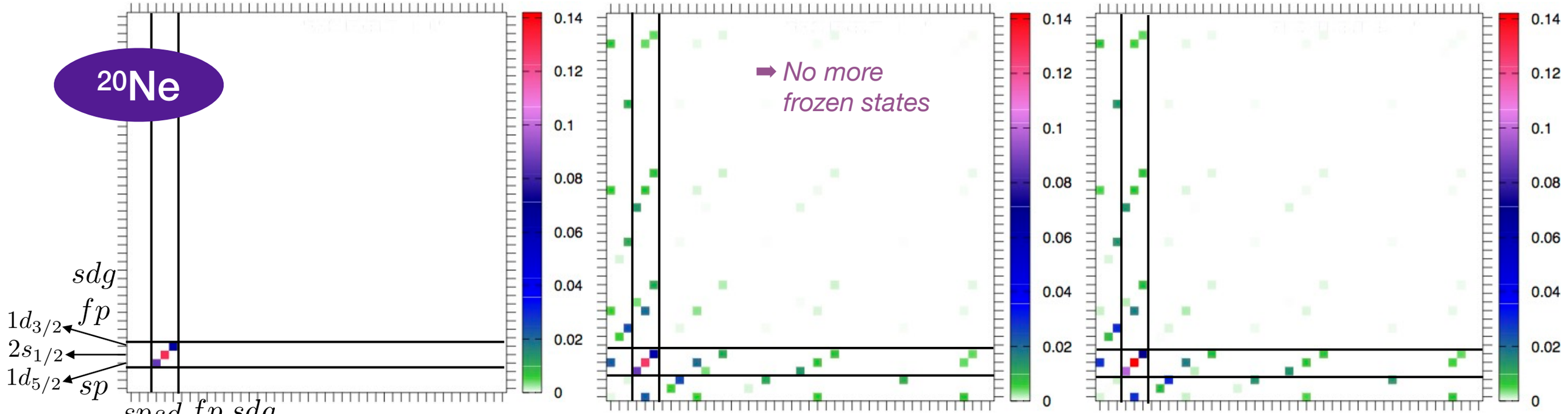


Application to sd-shell nuclei with the Gogny force

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

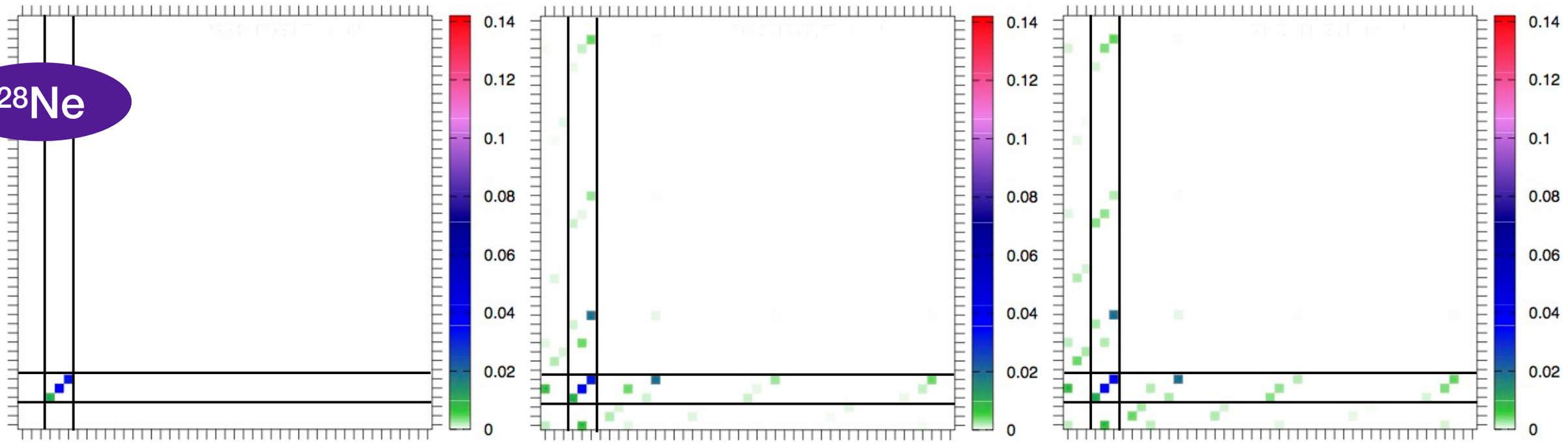
Equation 1 - iteration 1 | *Equations 1&2 - iteration 1* | *After convergence (iteration 22)*

^{20}Ne



➡ *No more frozen states*

^{28}Ne



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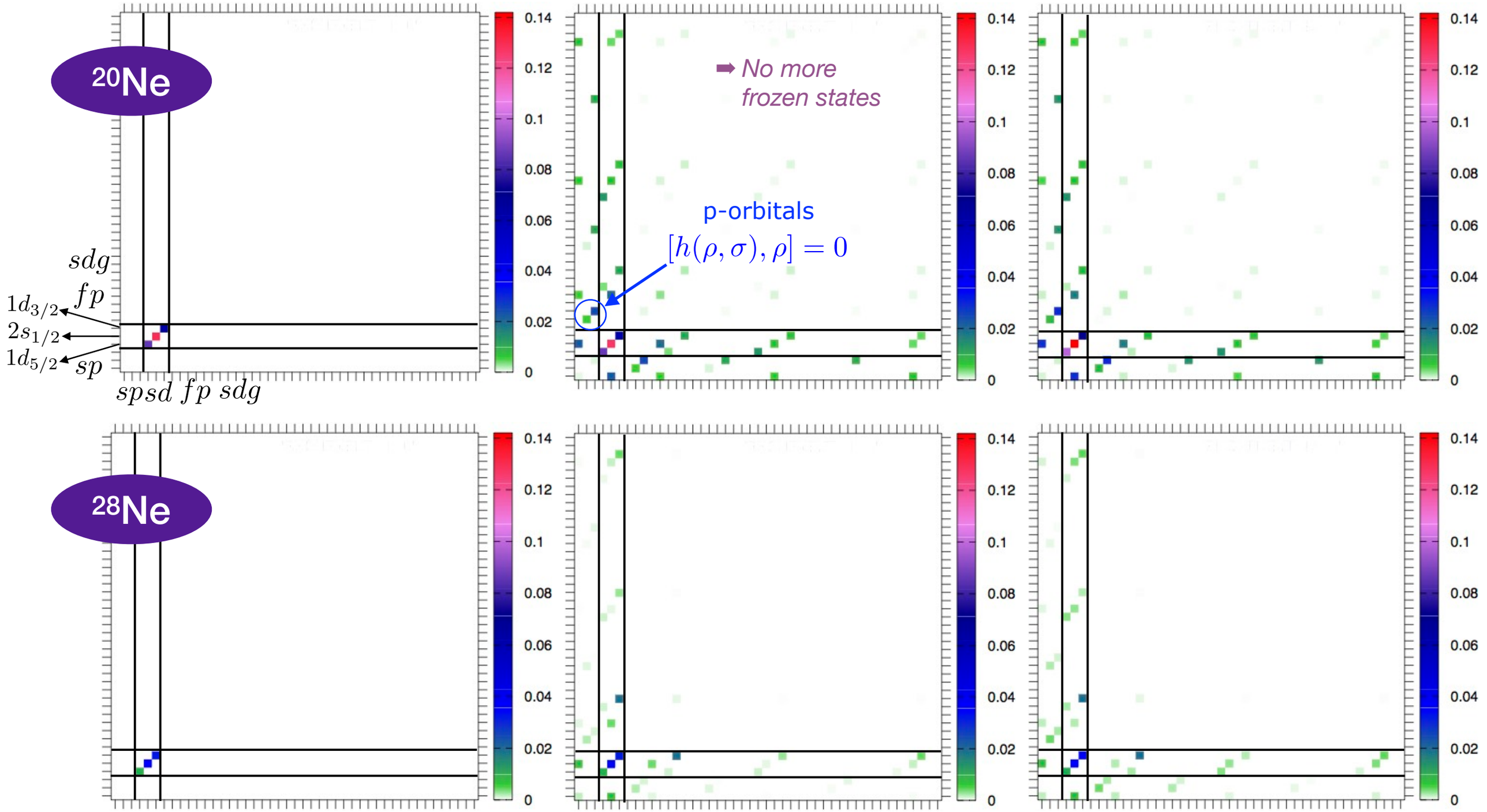
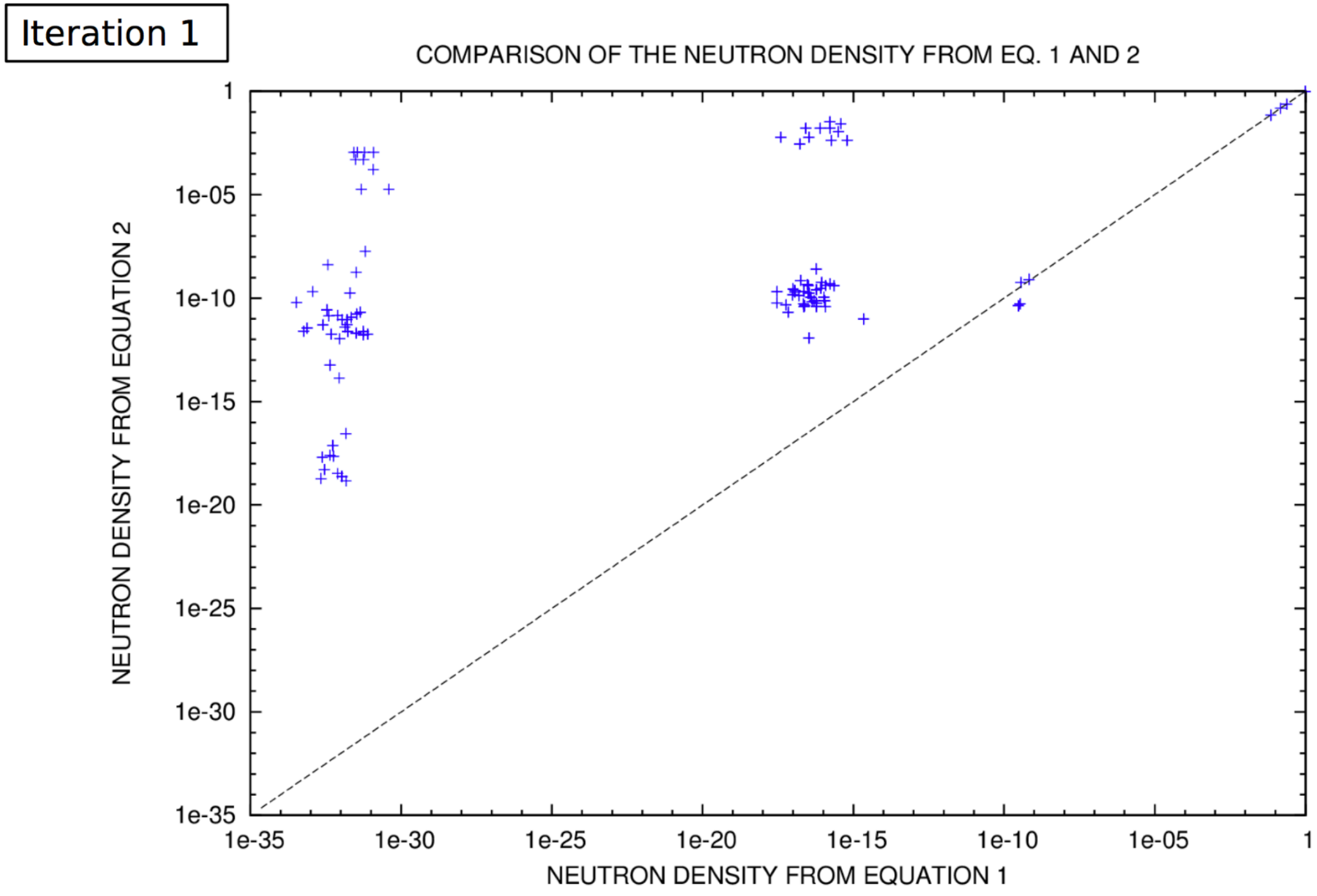


Application to sd-shell nuclei

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

^{20}Ne



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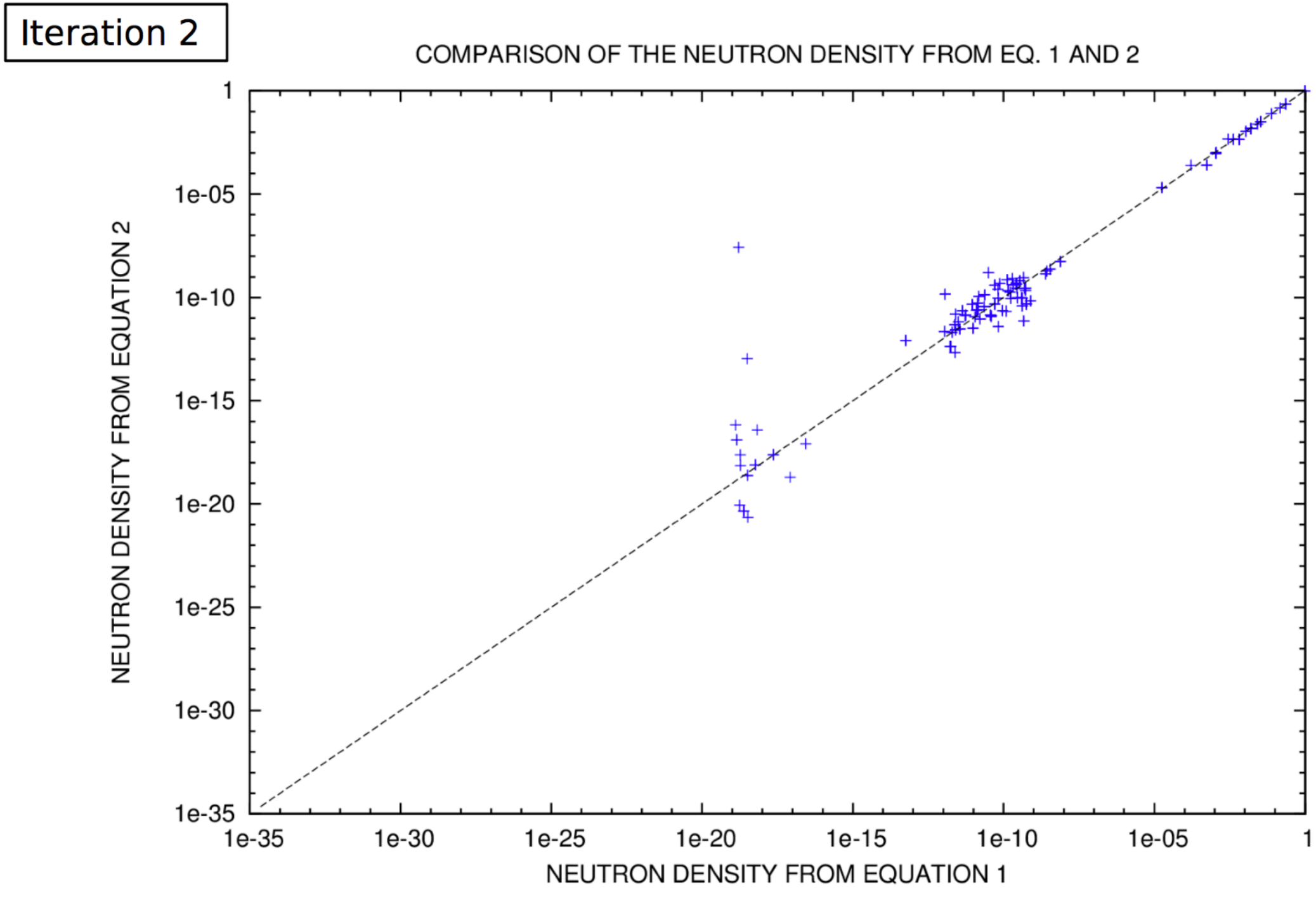

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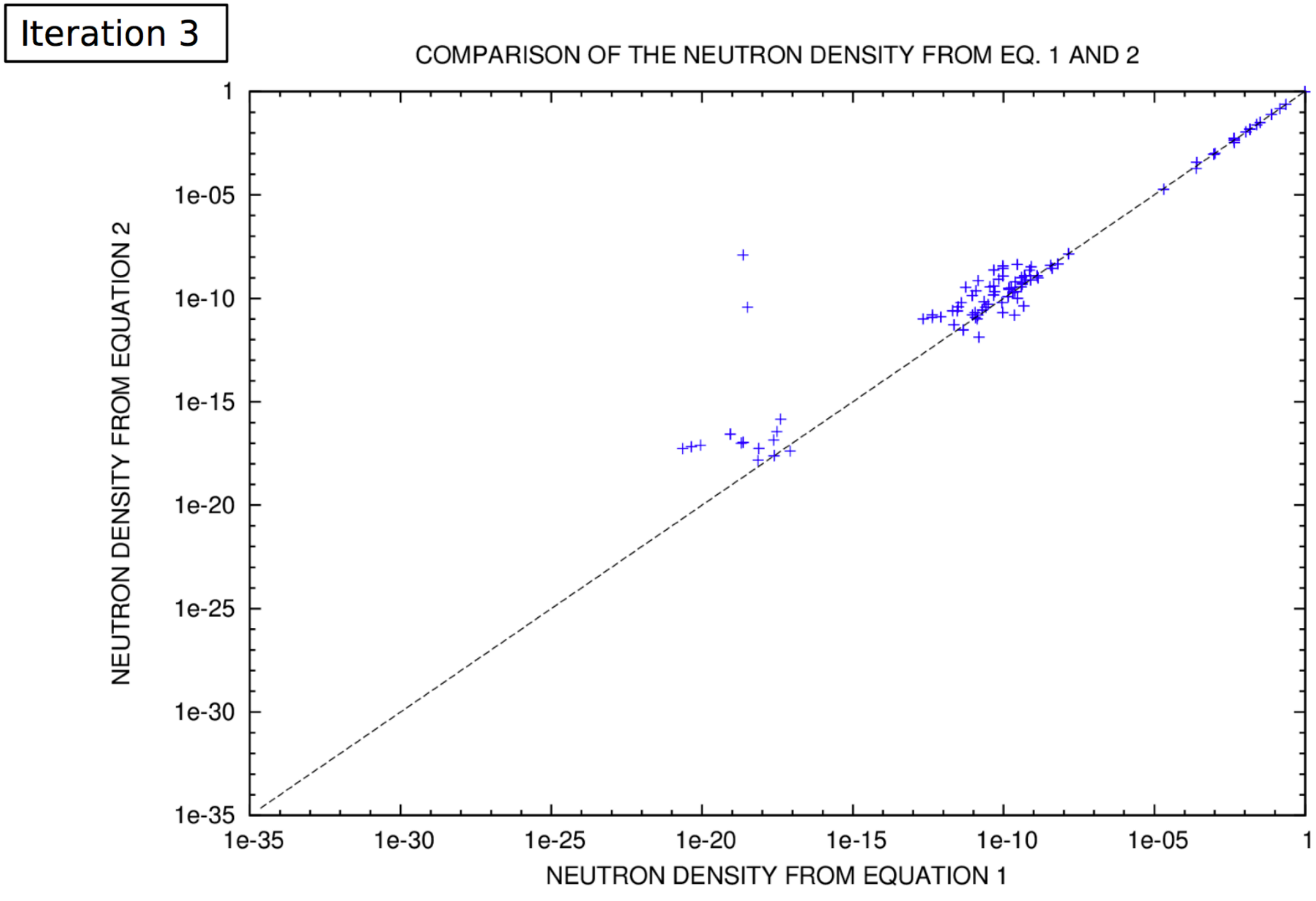

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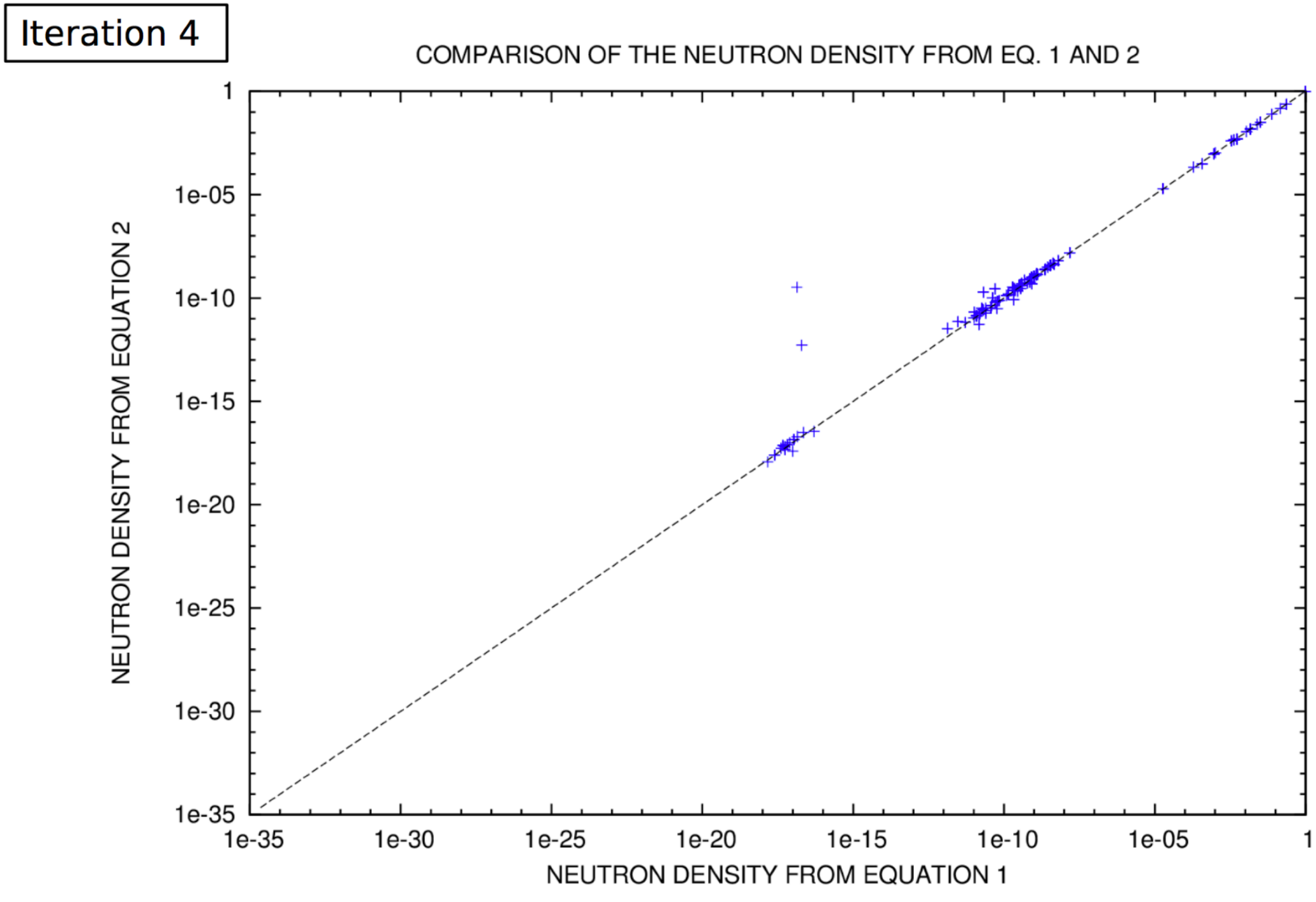

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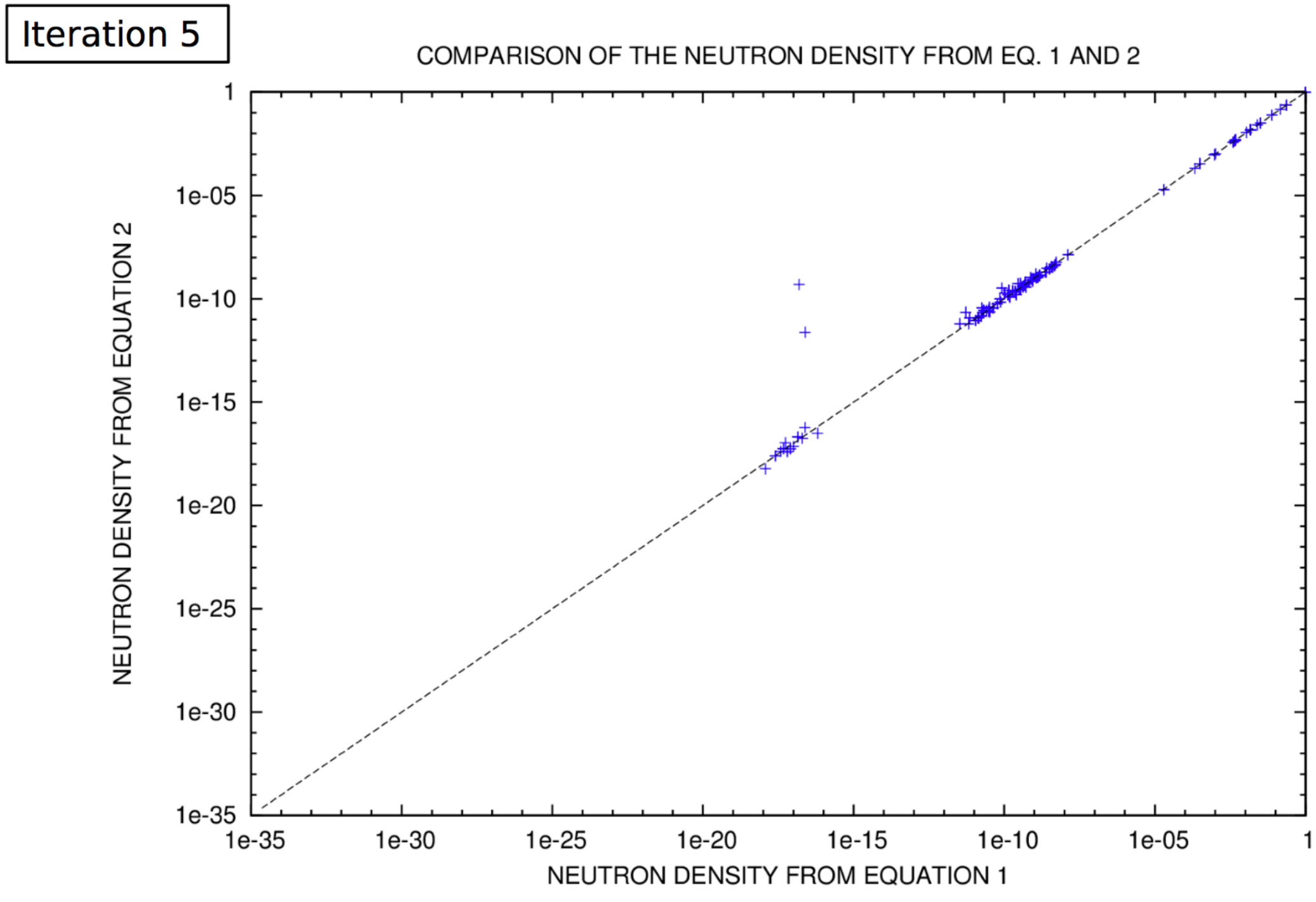

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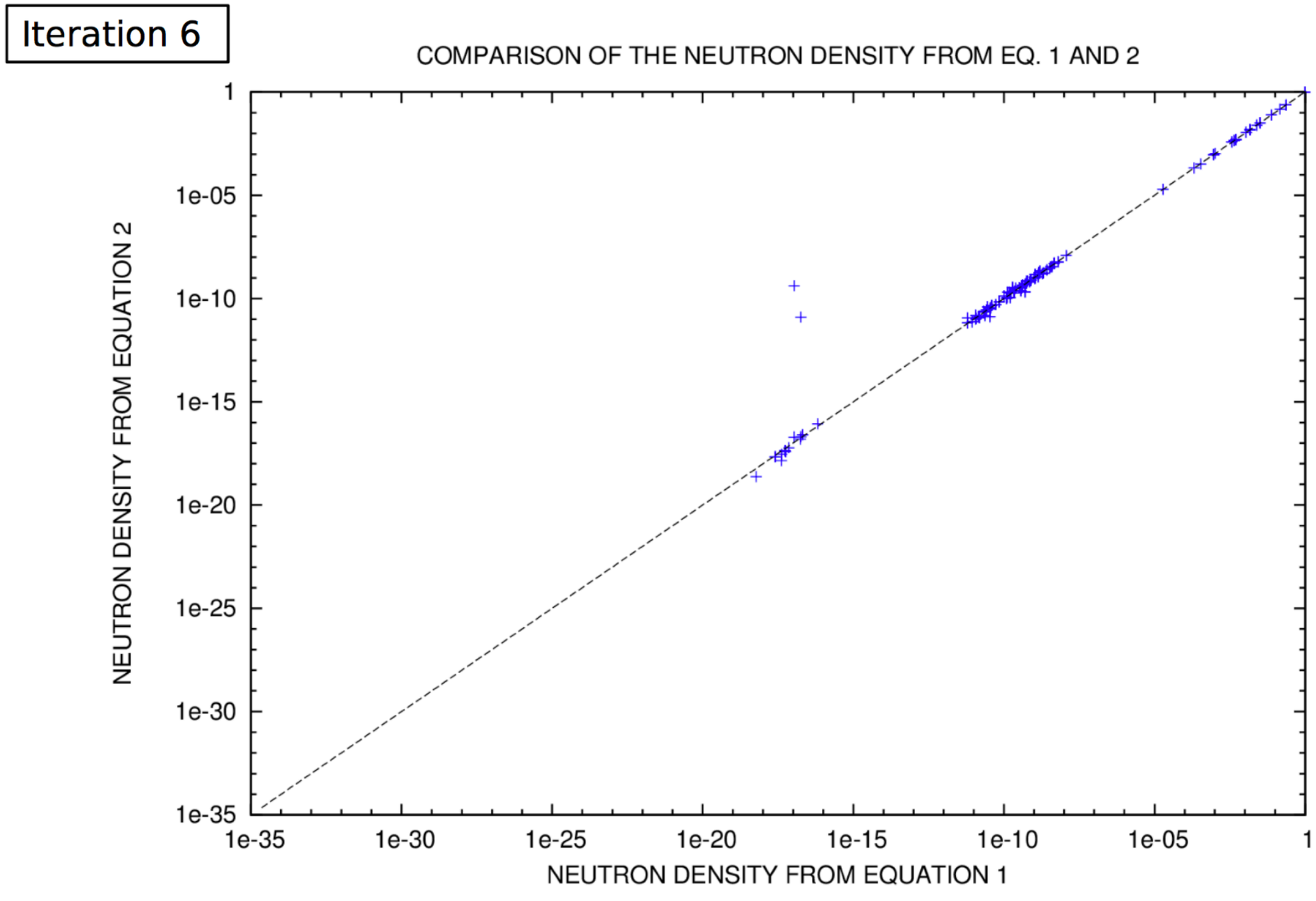

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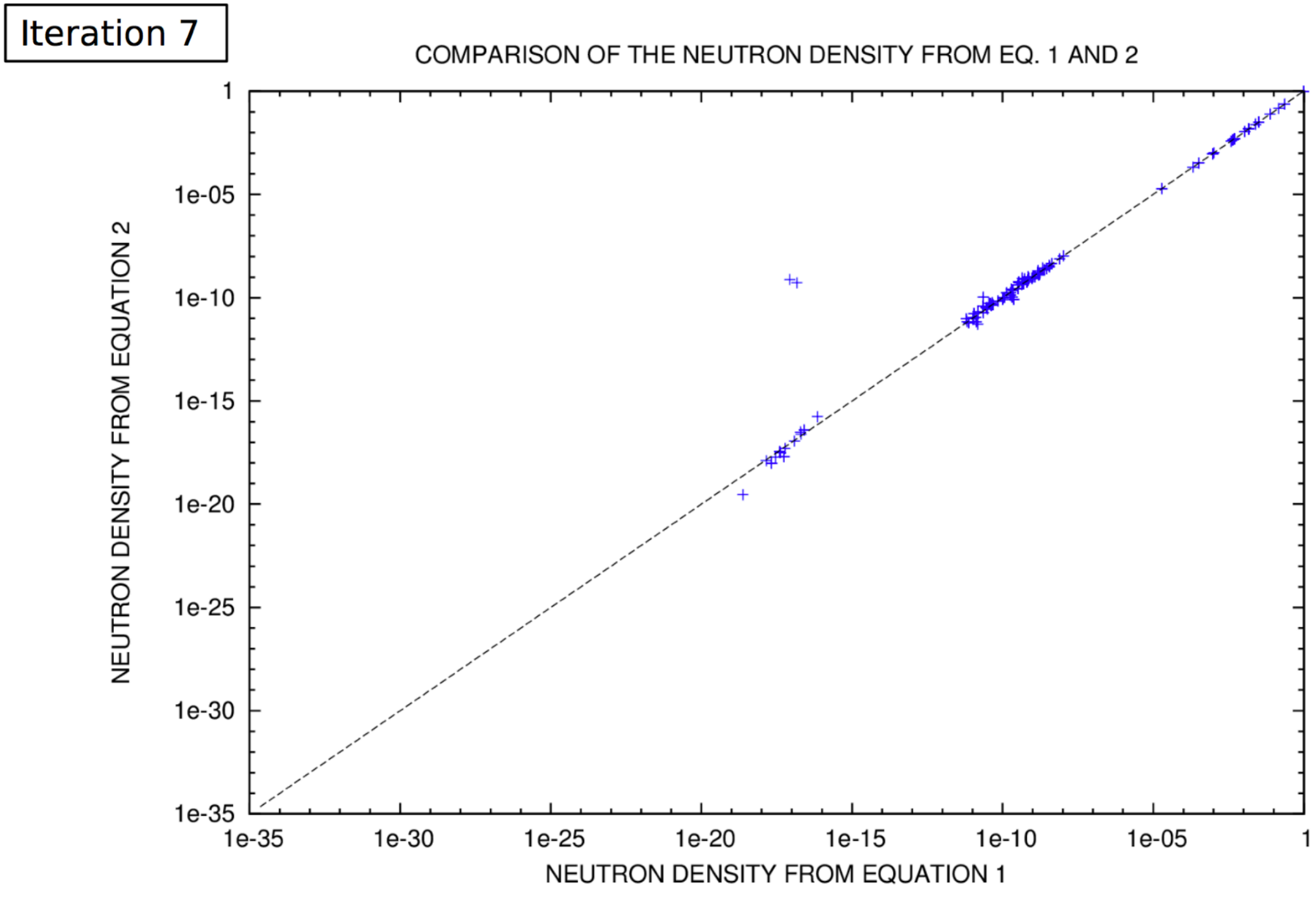

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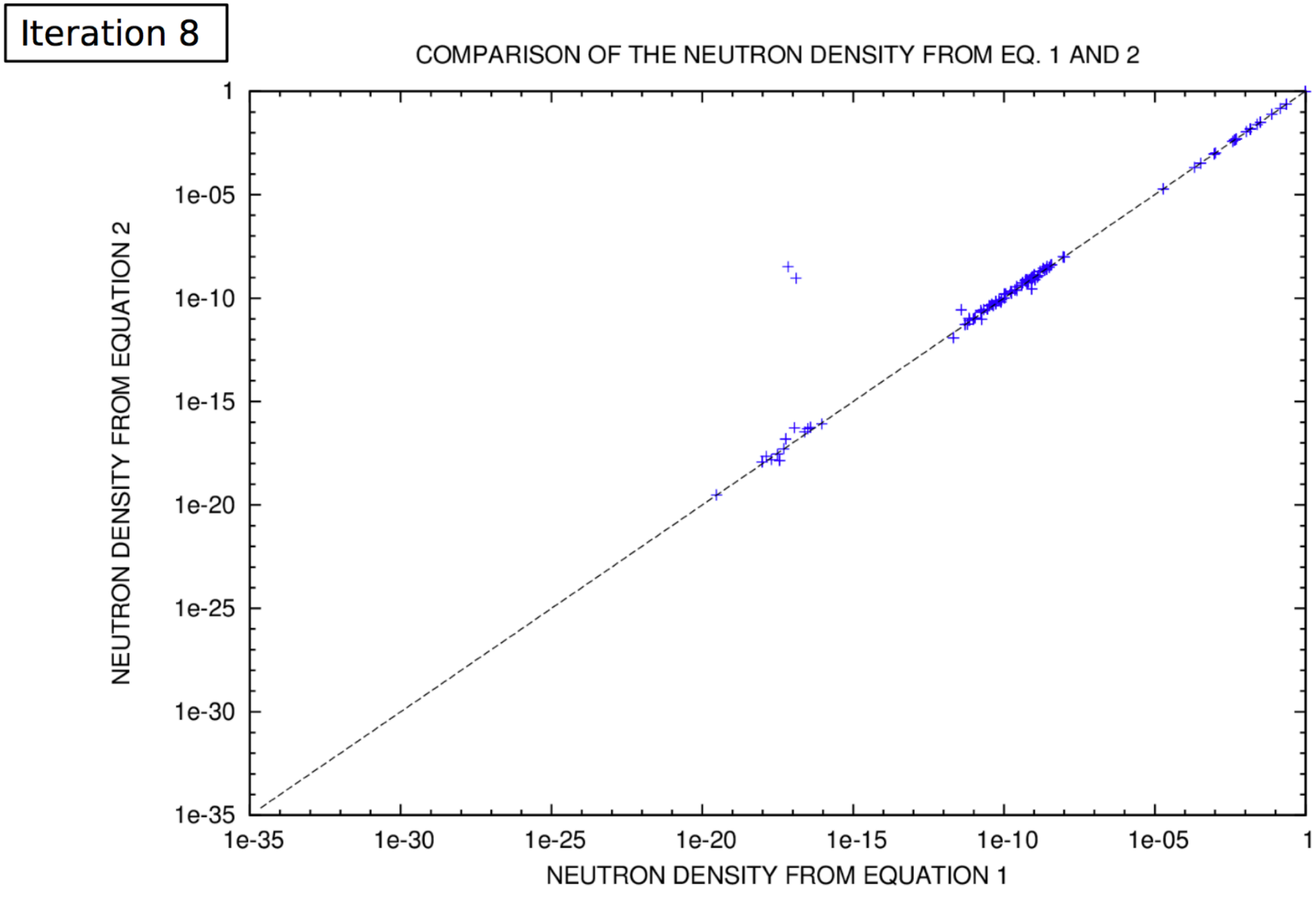

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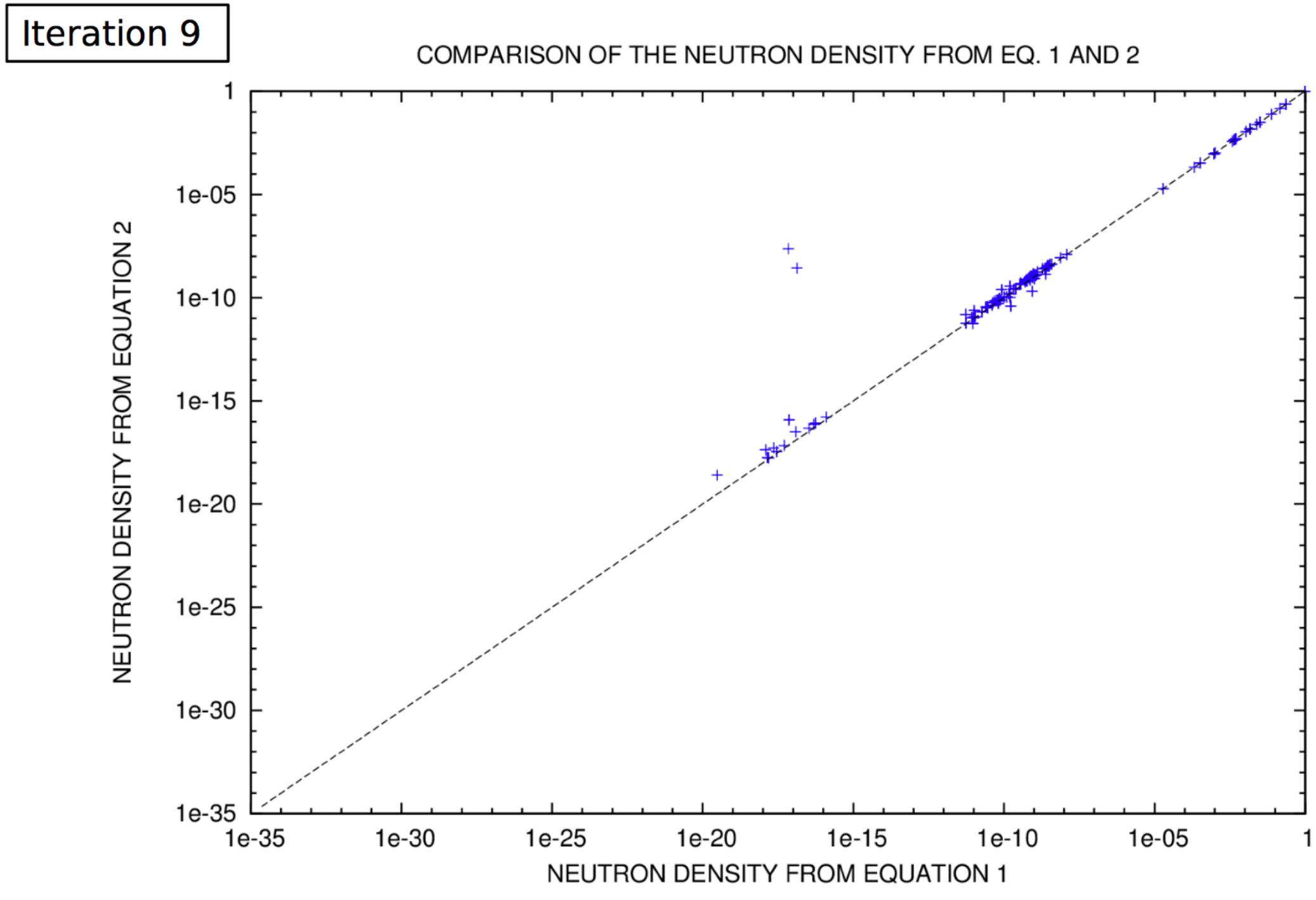

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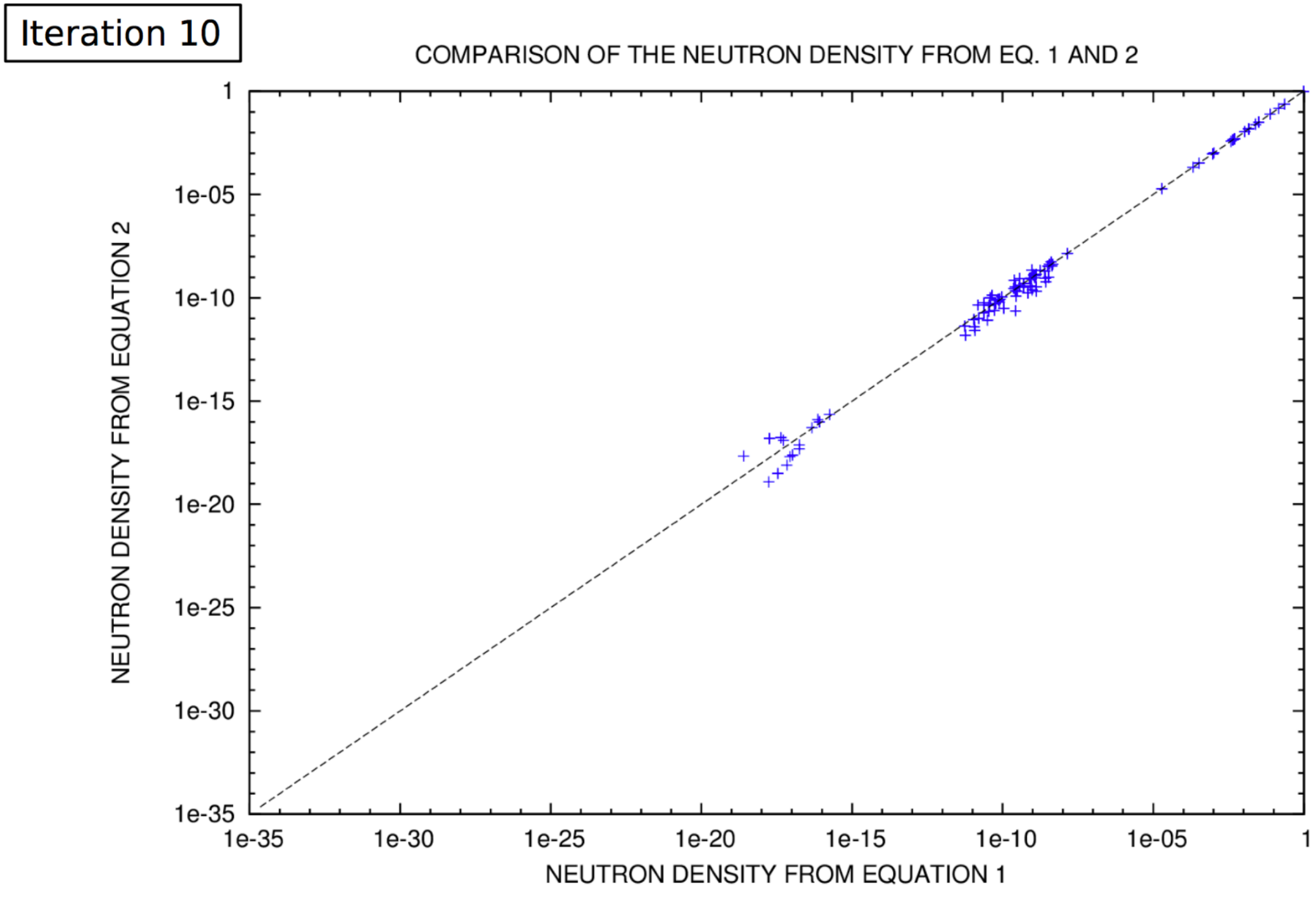

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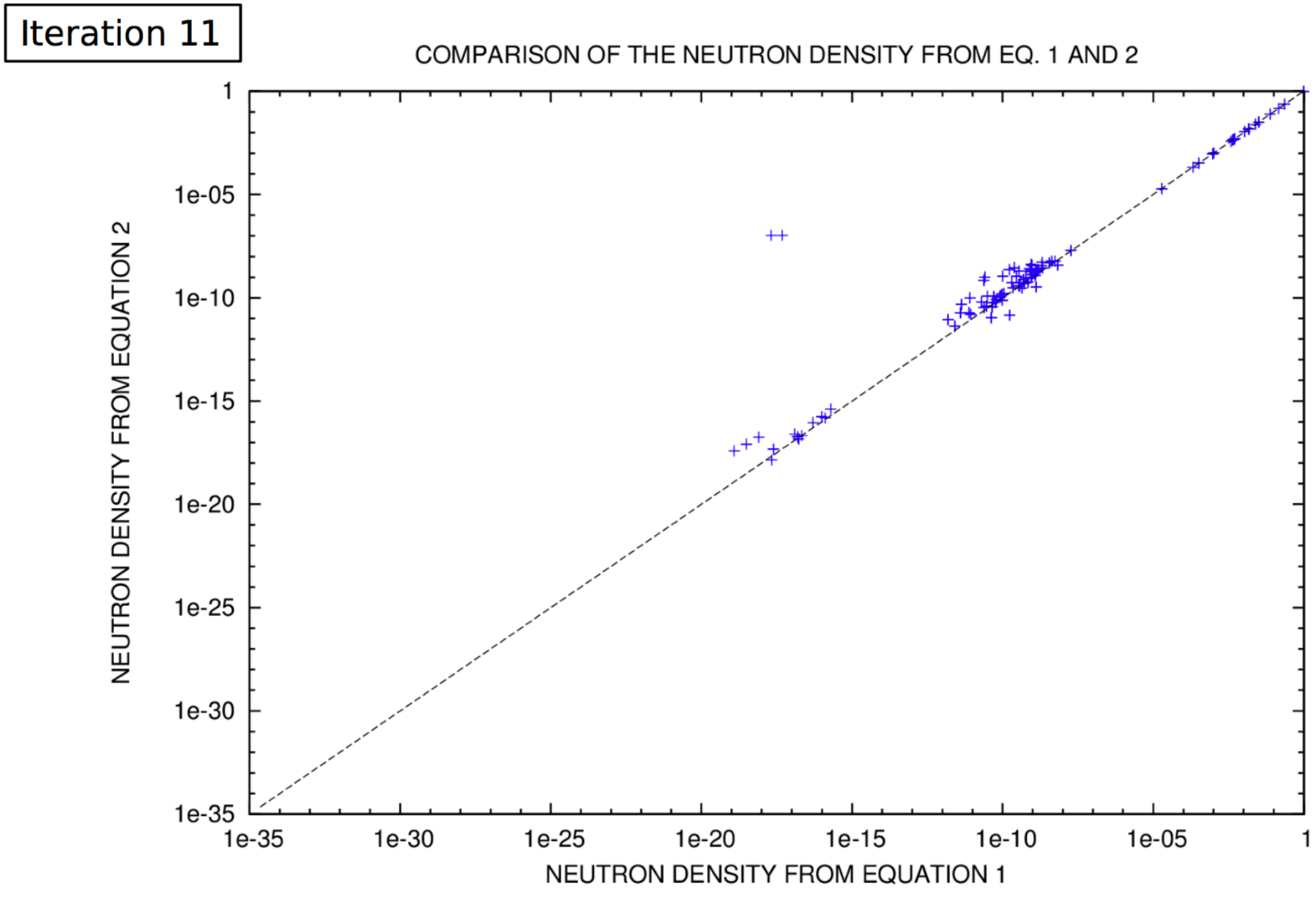

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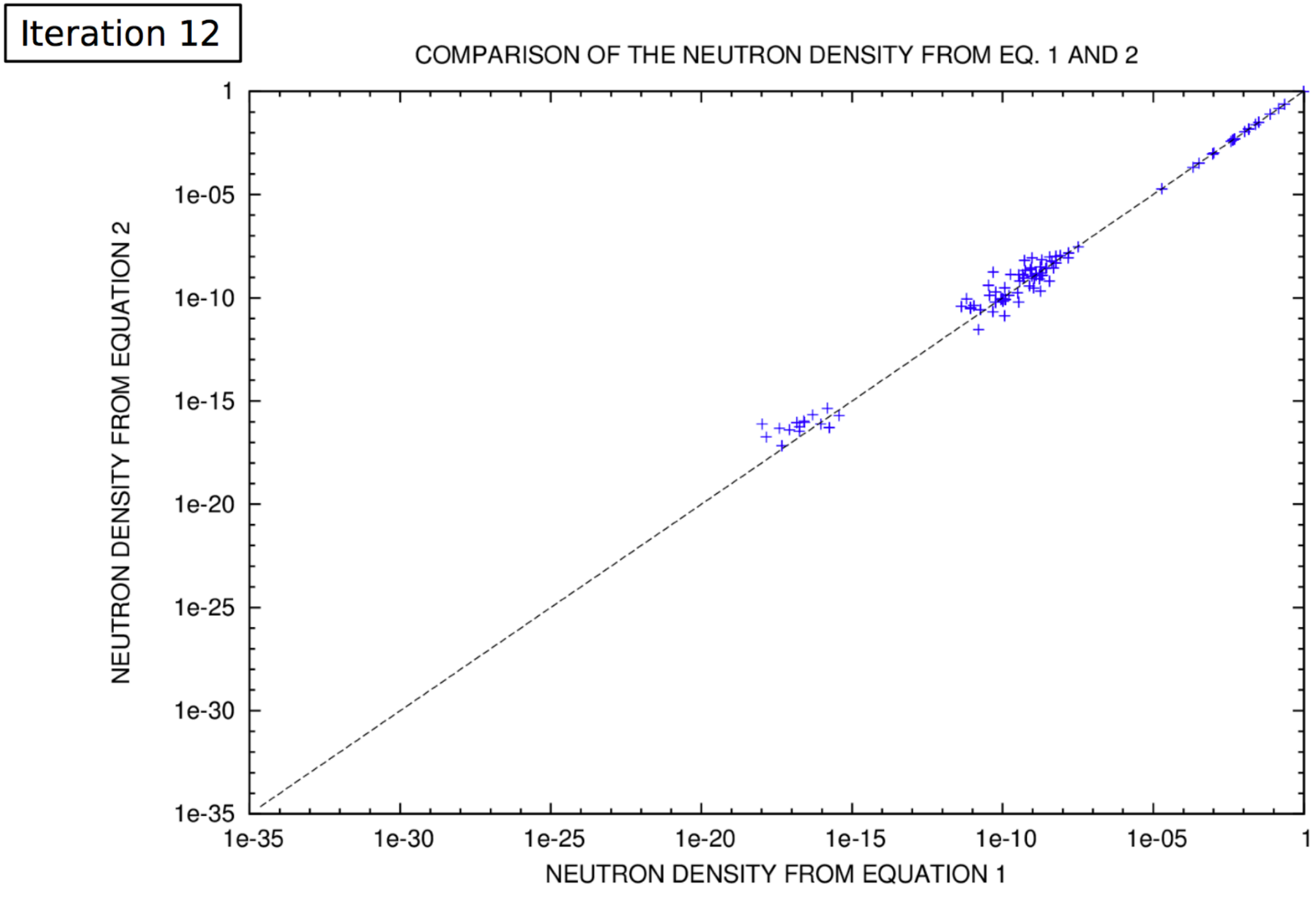

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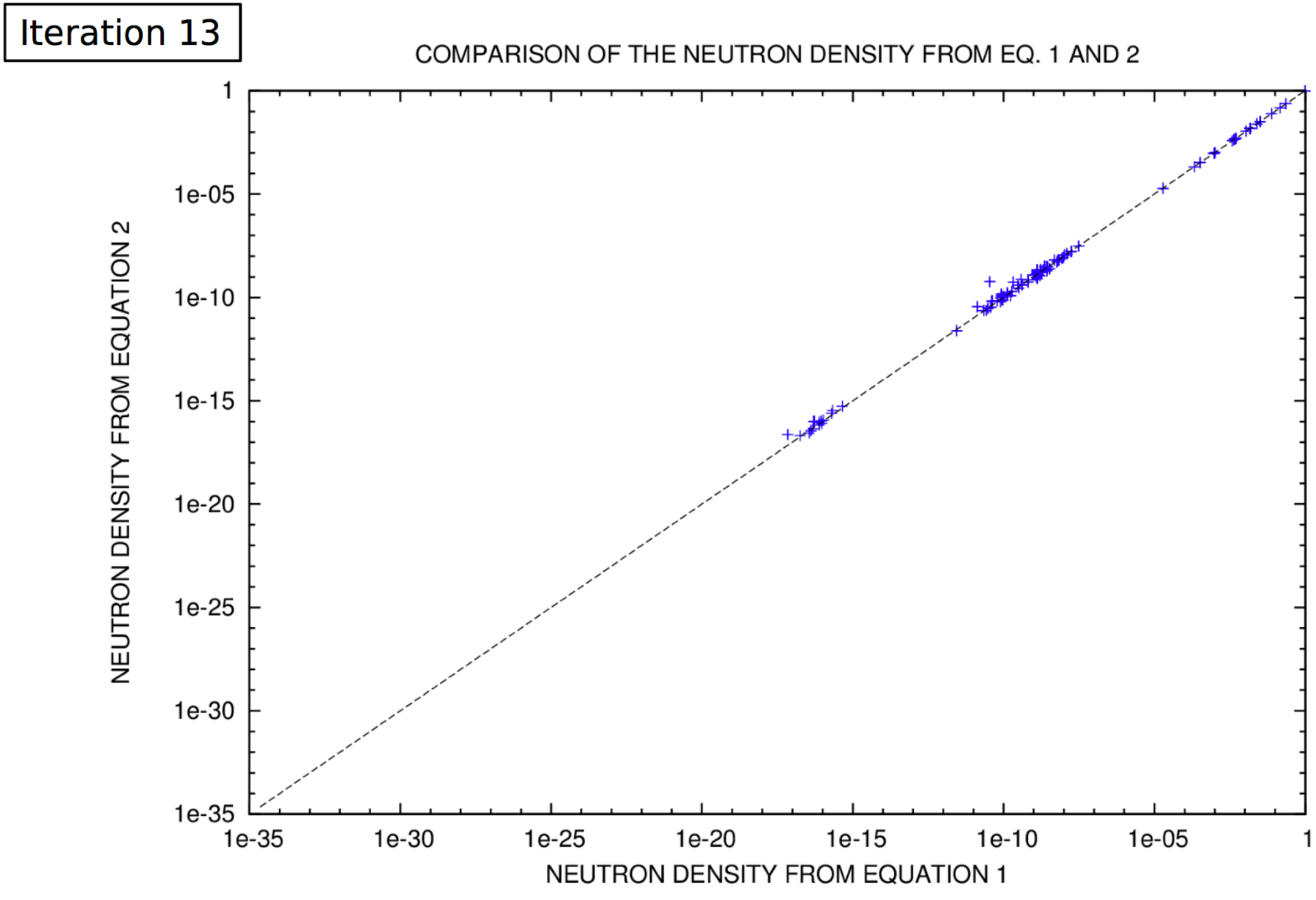

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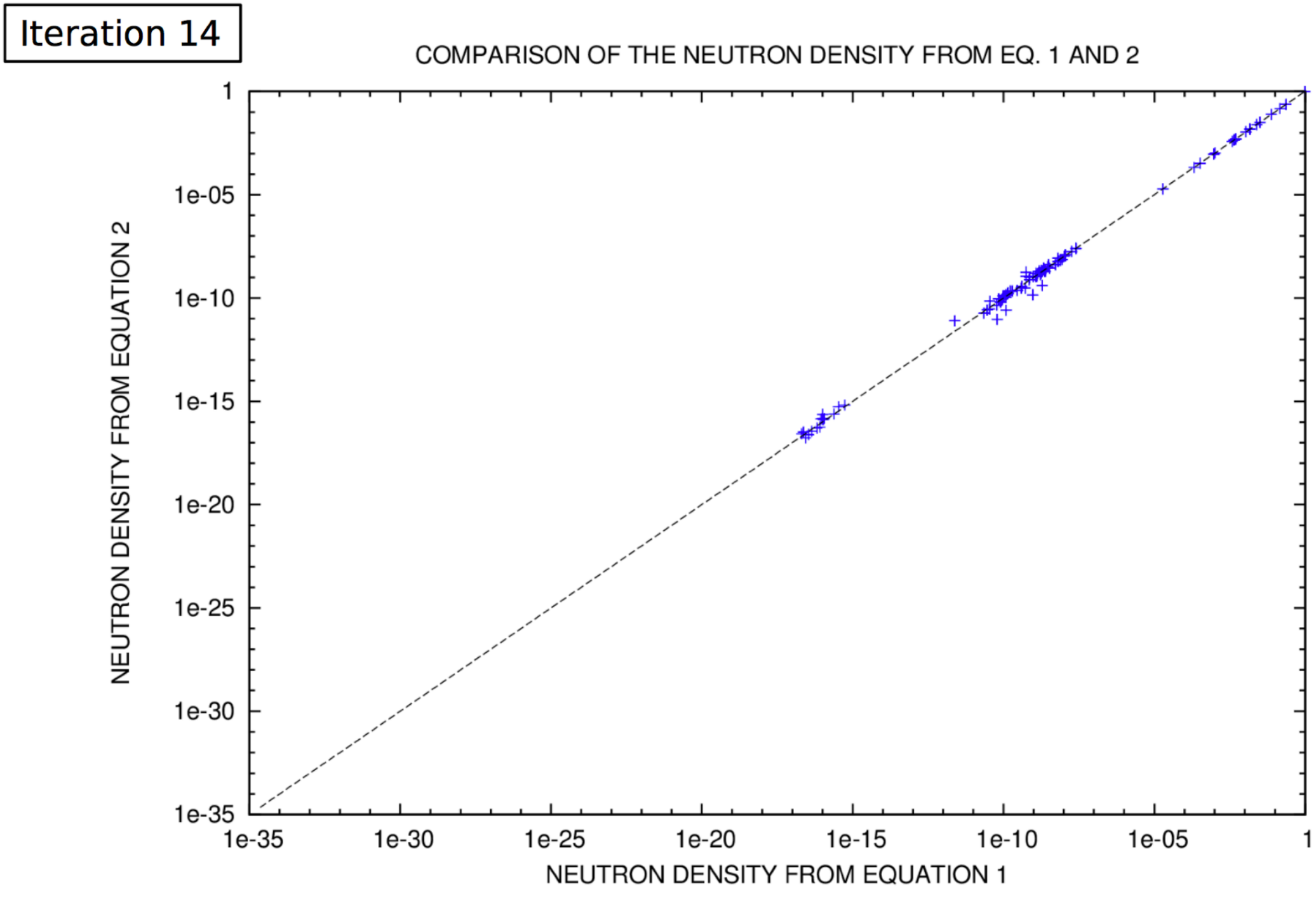

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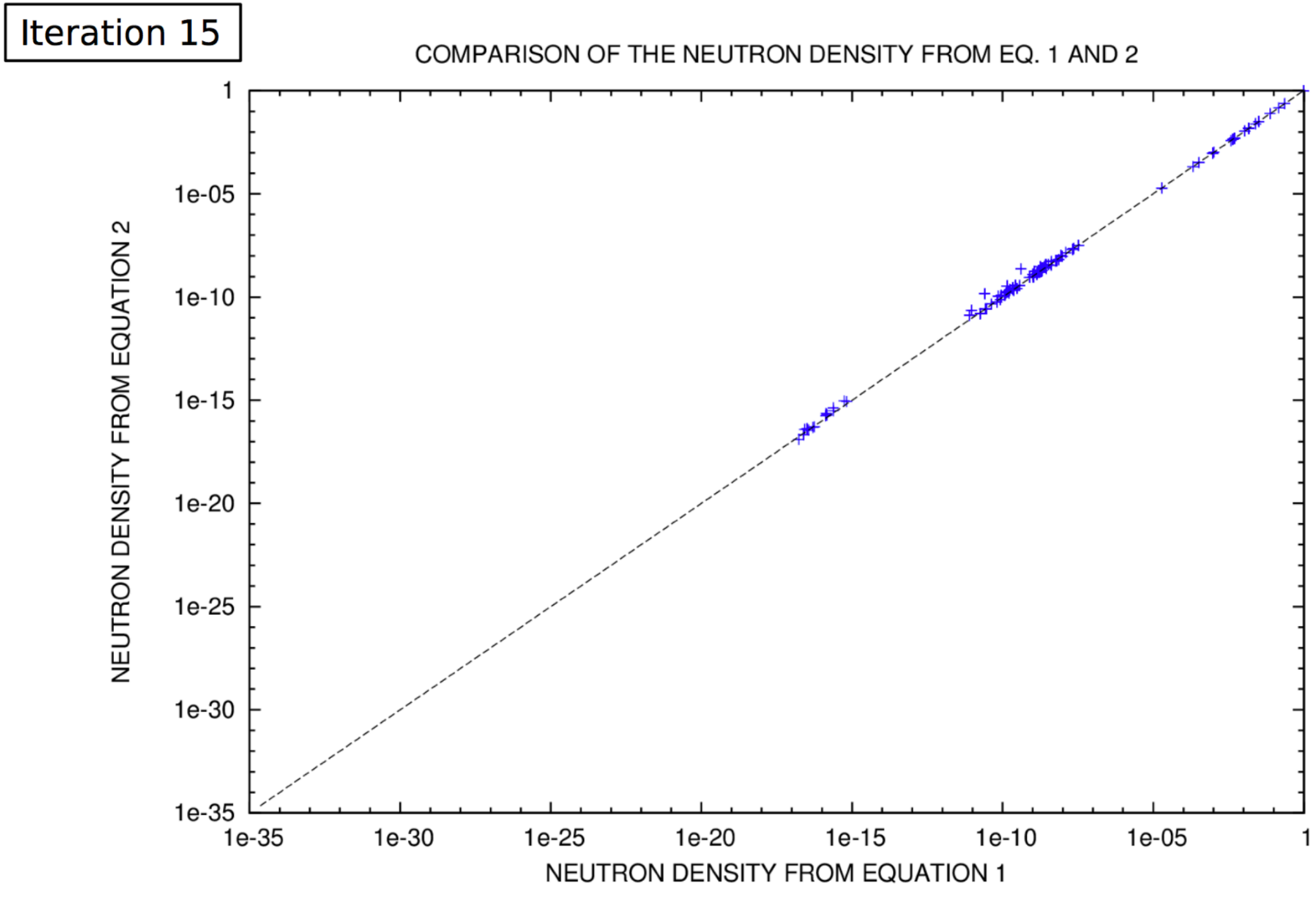
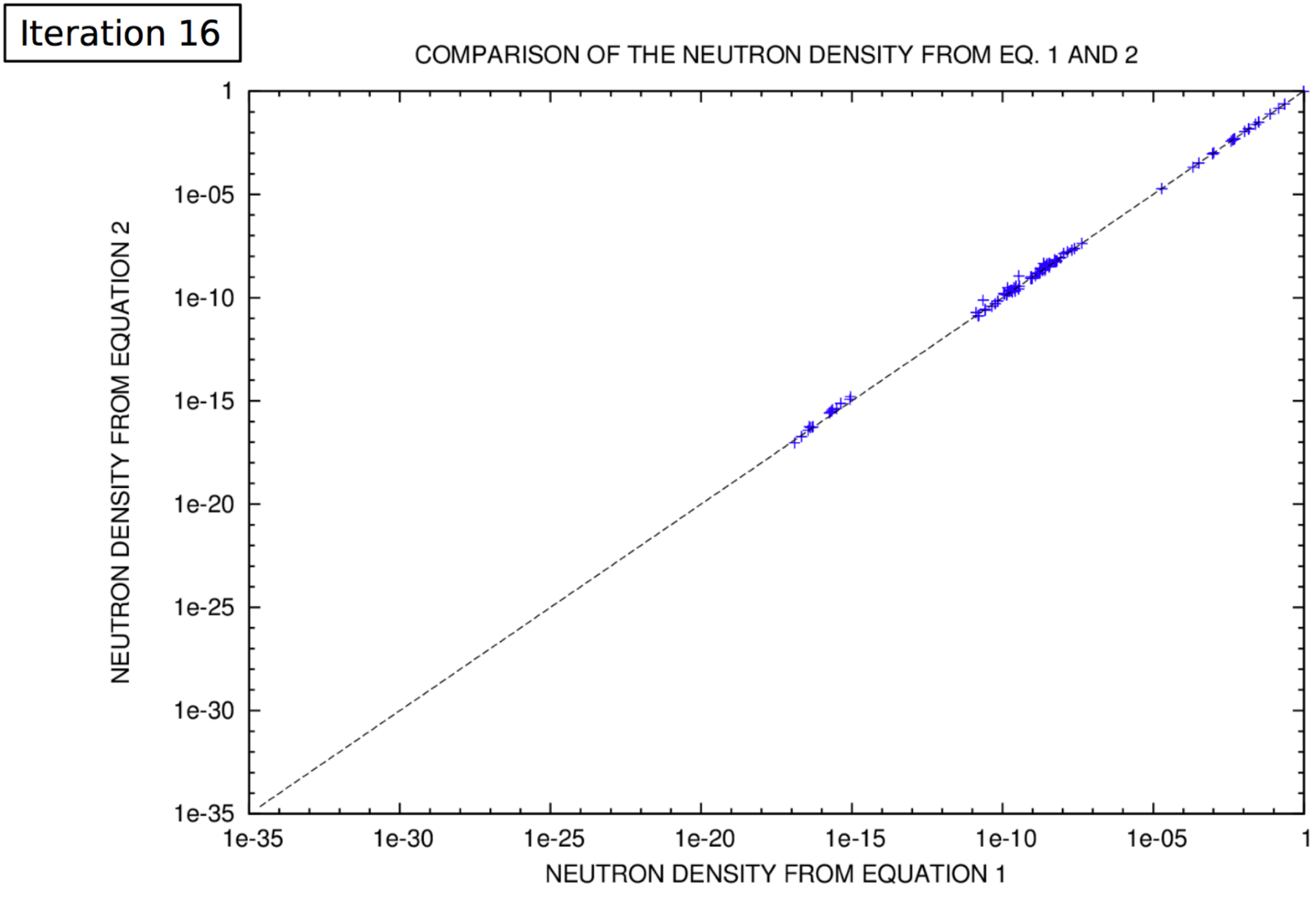


Application to sd-shell nuclei

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

^{20}Ne



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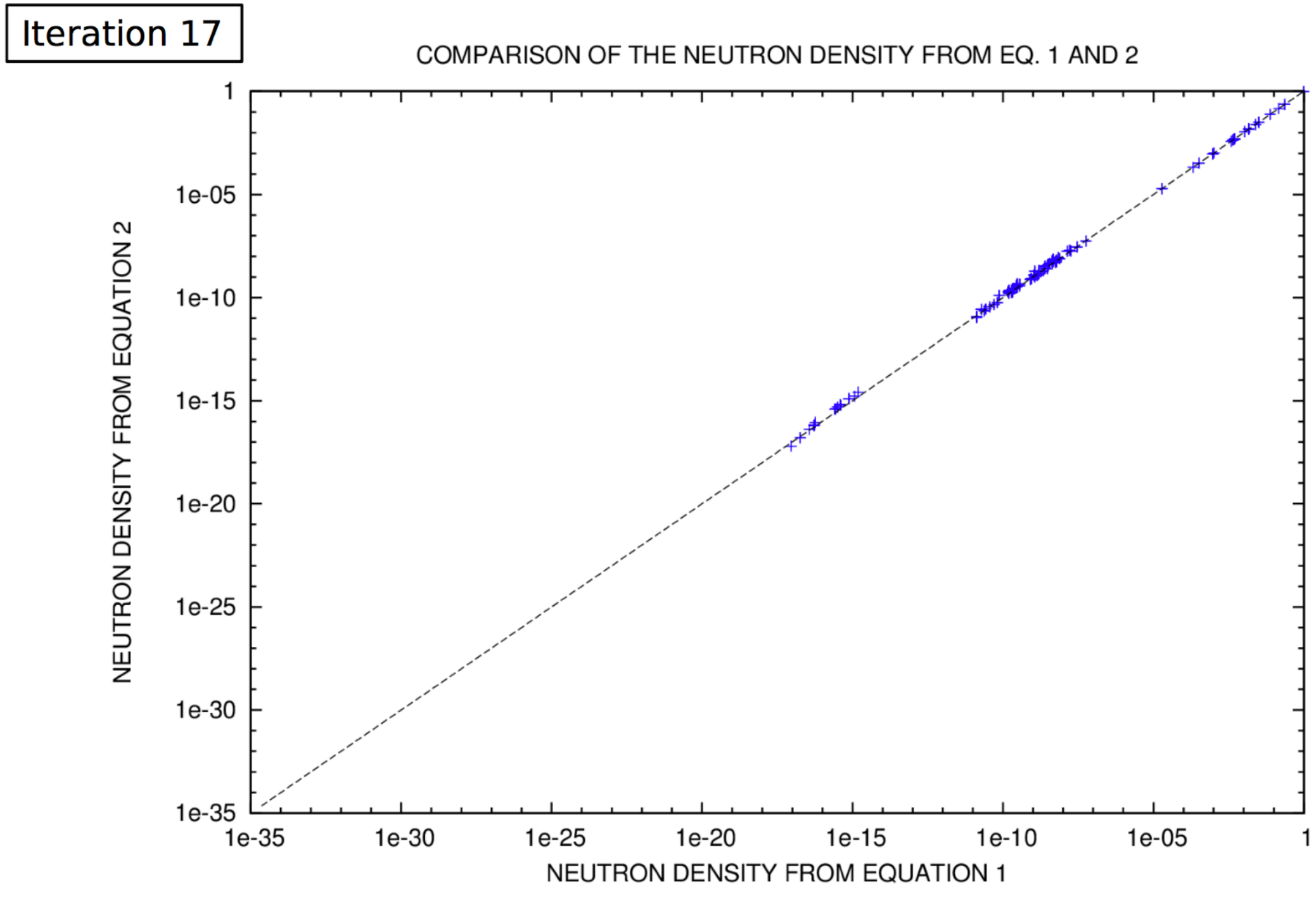

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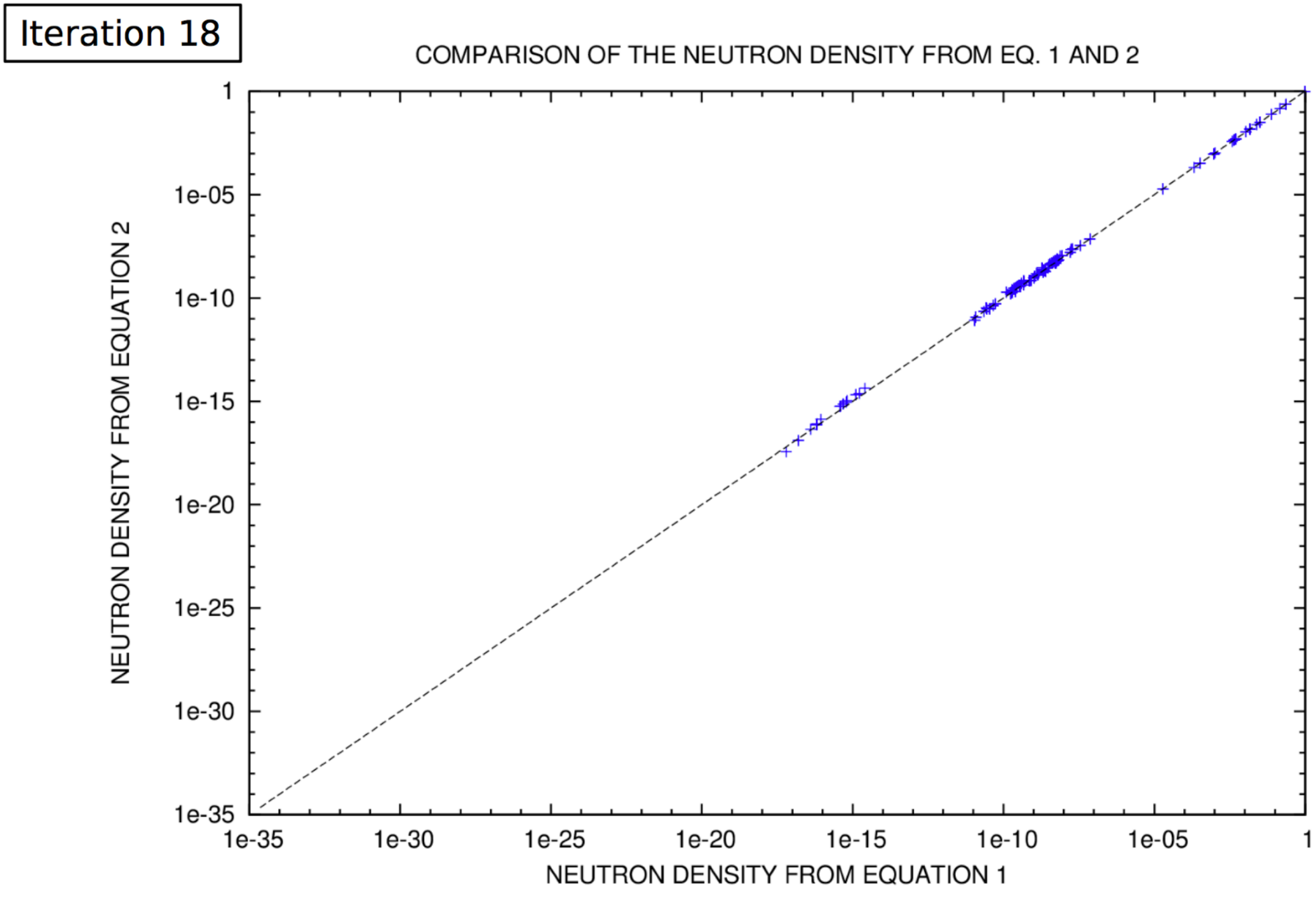

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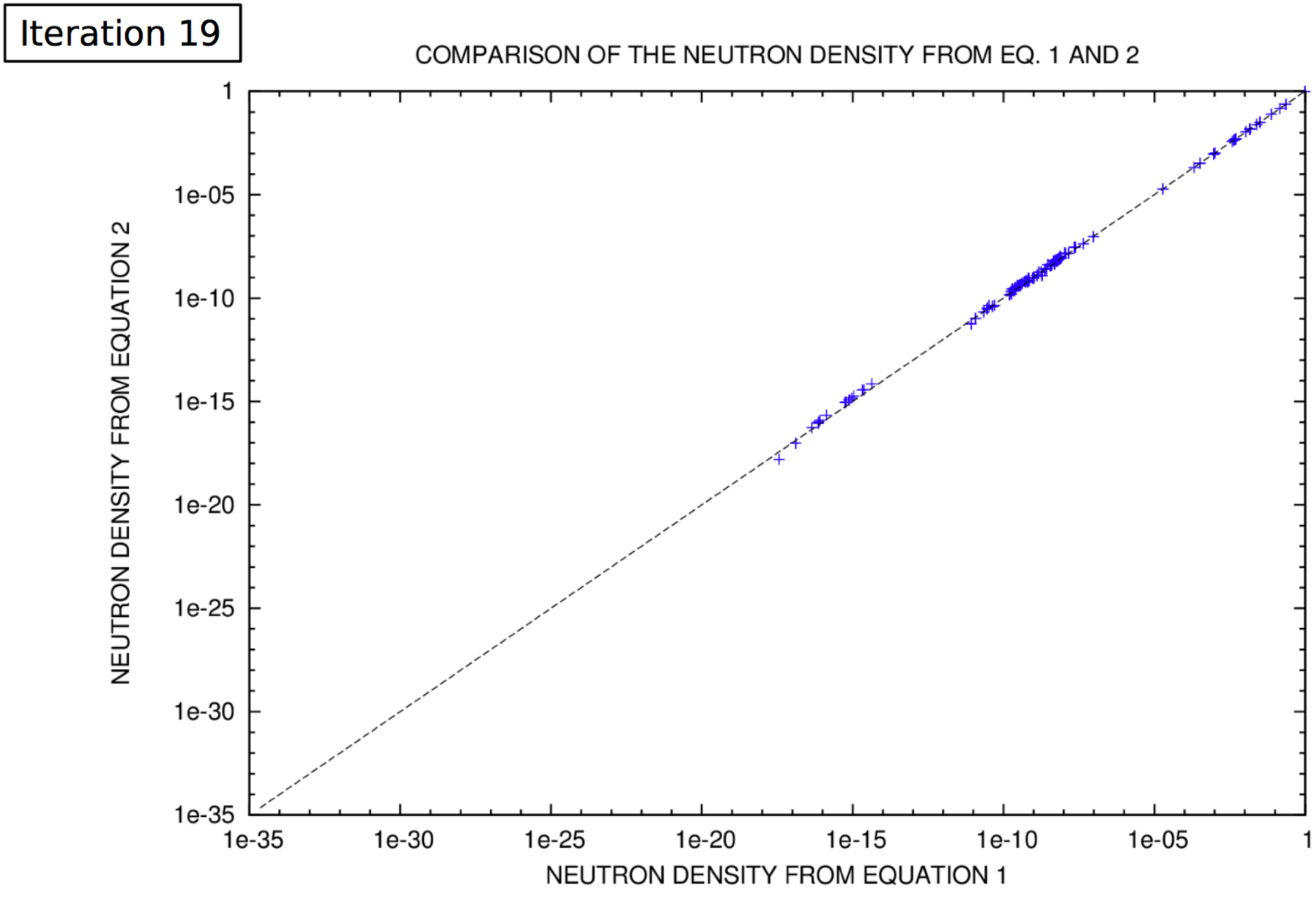

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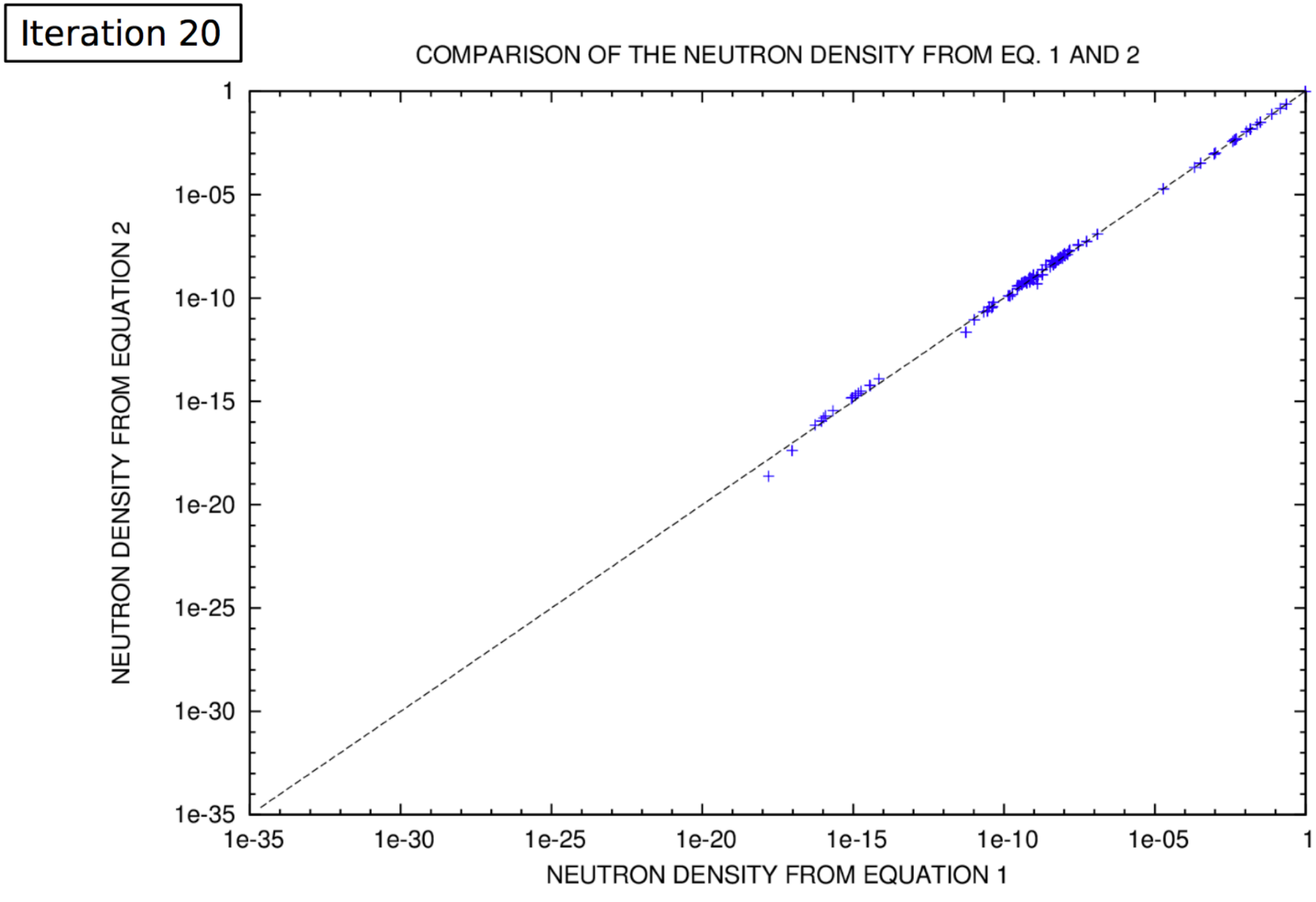

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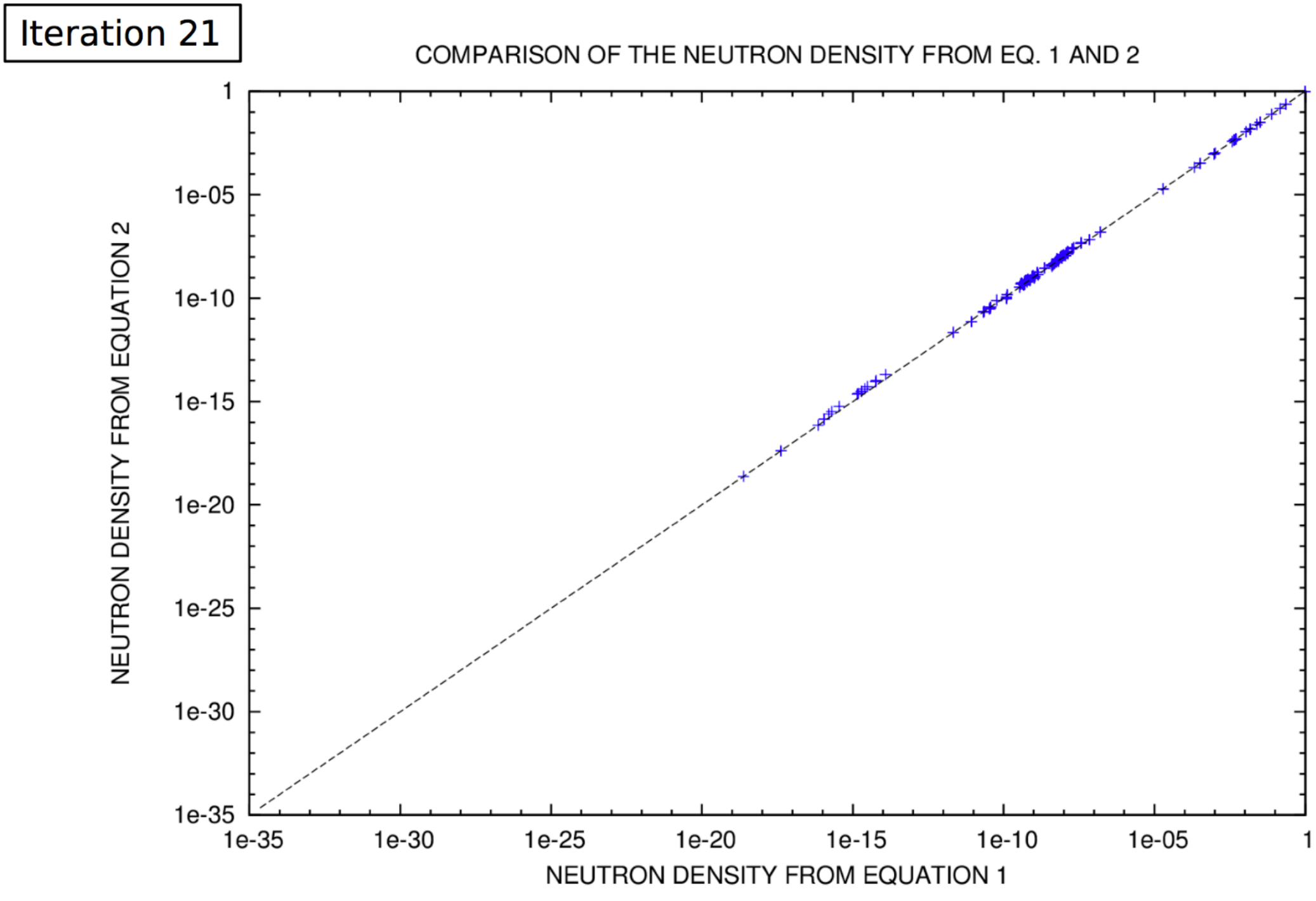

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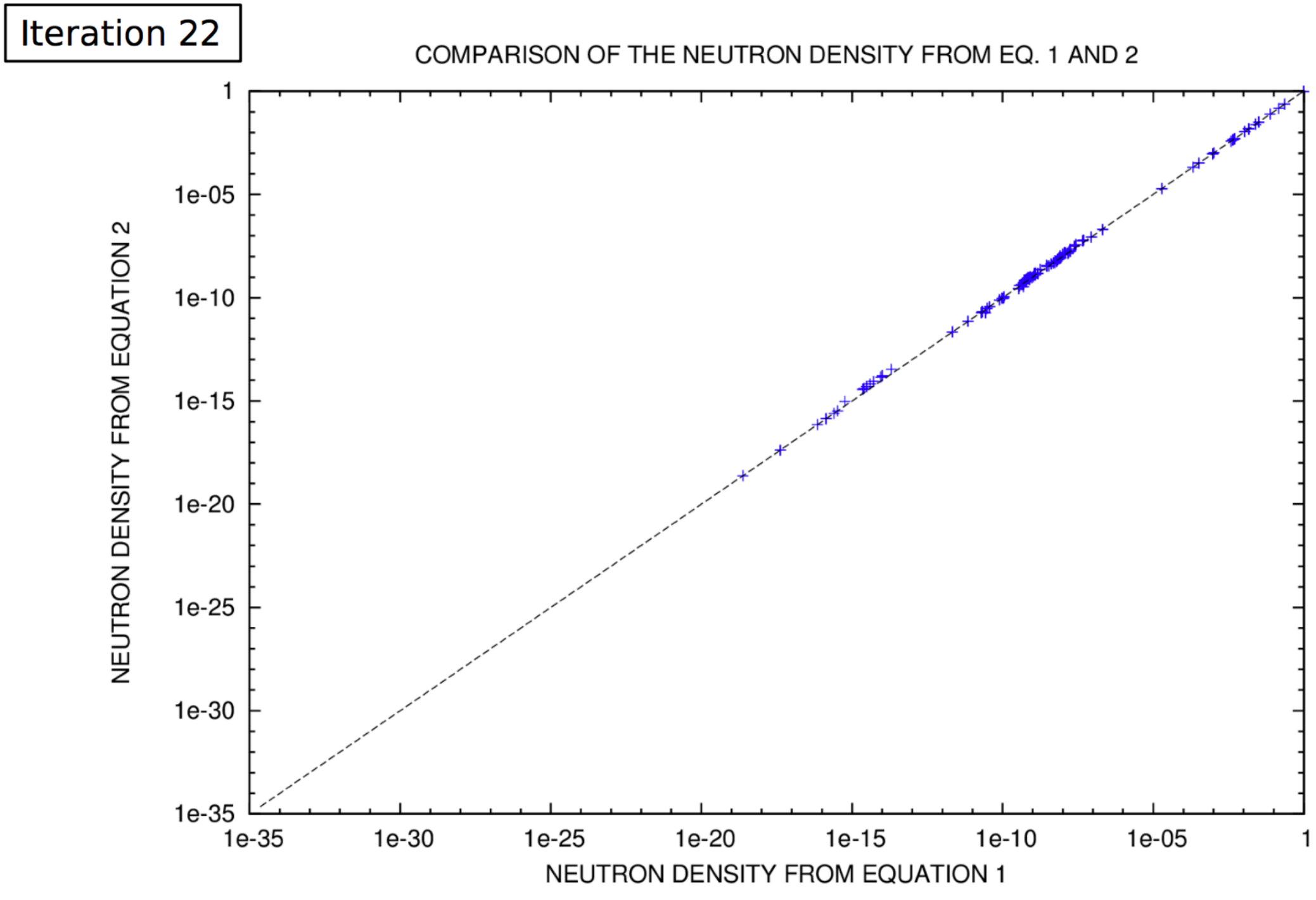
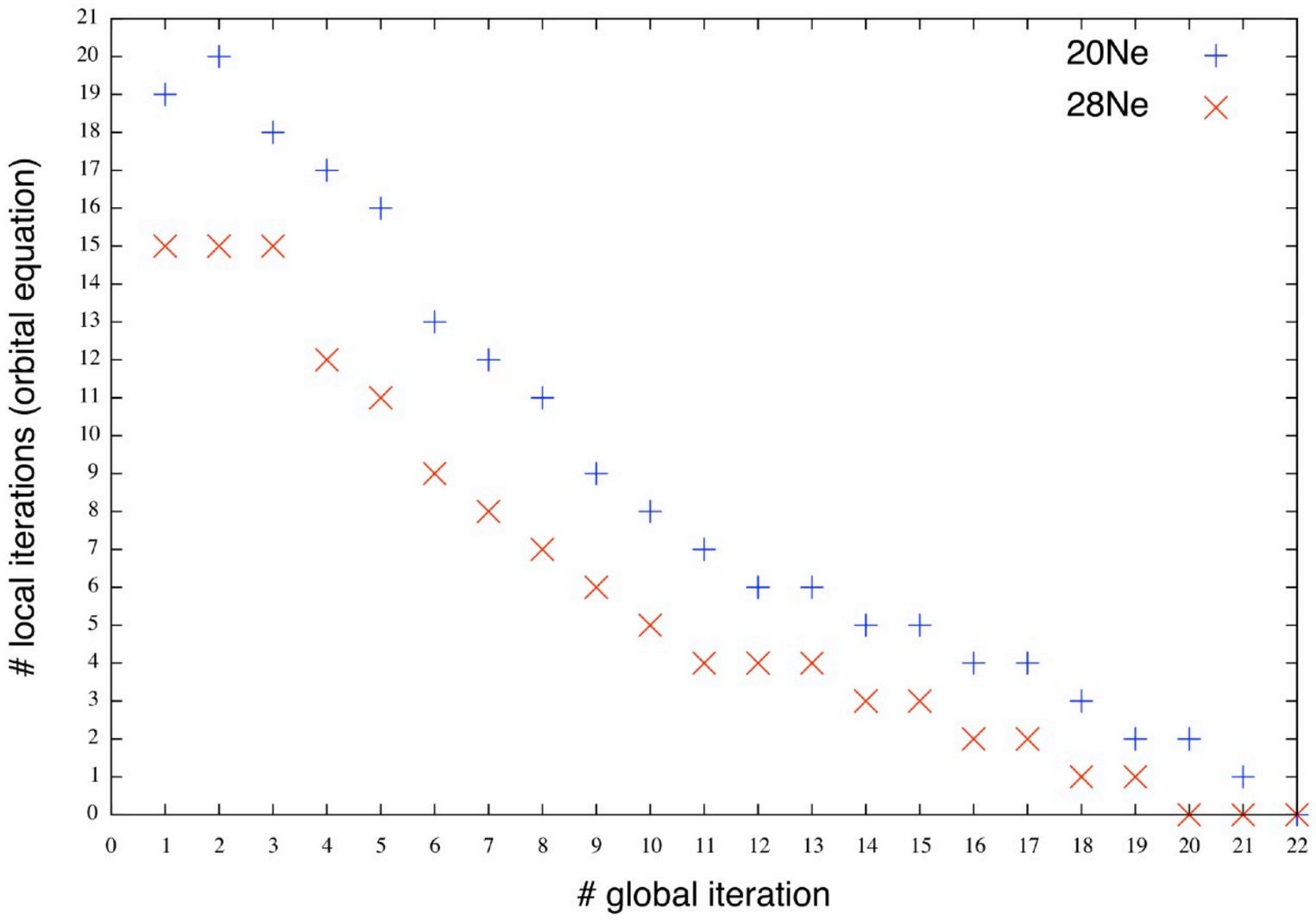


Application to sd-shell nuclei with the Gogny force

✱ ***Convergence process:***

Global vs local iterations

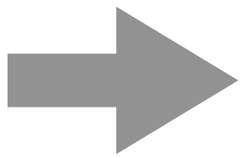


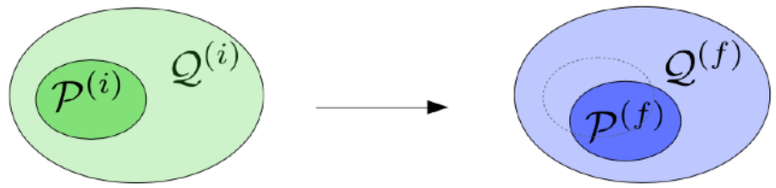
# global iteration	# of iterations of the orbital equation	
	^{20}Ne	^{28}Ne
1	19	15
2	20	15
3	18	15
4	17	12
5	16	11
6	13	9
7	12	8
8	11	7
9	9	6
10	8	5
11	7	4
12	6	4
13	6	4
14	5	3
15	5	3
16	4	2
17	4	2
18	3	1
19	2	1
20	2	1
21	1	
22	1	

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

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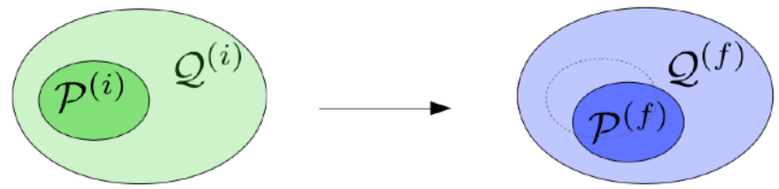

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How big?

	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%

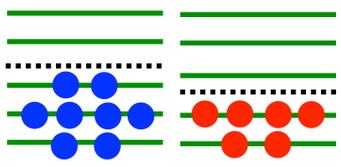
The weight of the initial Q space increases when starting further from the final solution

Application to sd-shell nuclei with the Gogny force

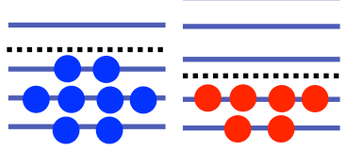
✱ ***Effect on the many-body wave function:*** Orbital transformation: $b_i^\dagger = e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}}$

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 componentd state
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

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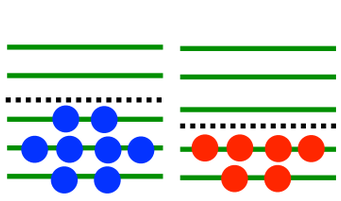

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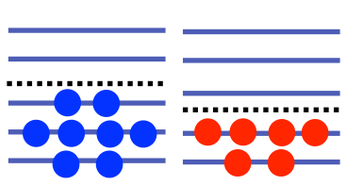

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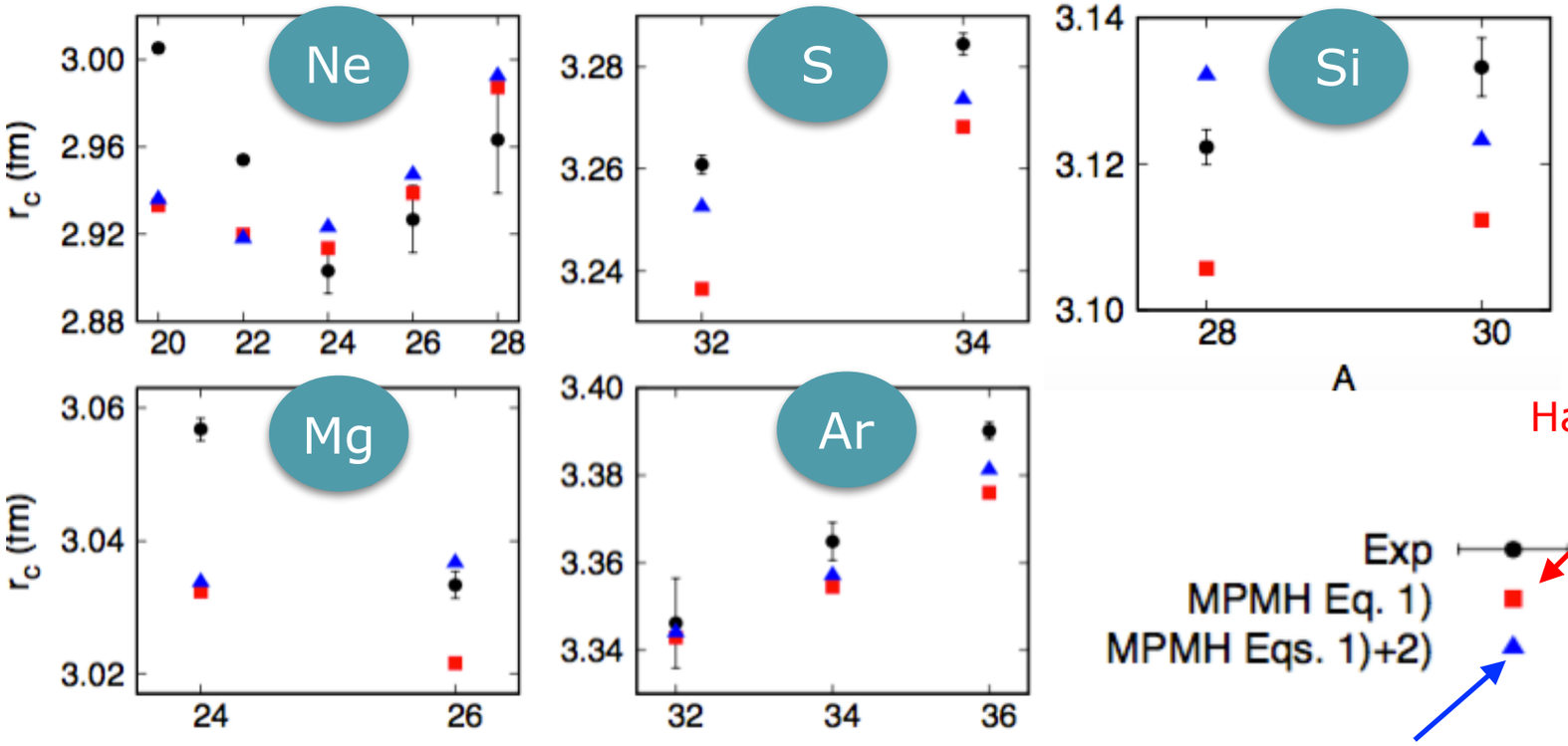
✱ ***Correlation energies:*** $E_{corr} = E(\Psi) - E(\Phi_{HF}^{(0)})$

Correlation energy E_{corr} (MeV)			
nucleus	1st equation only	1st + 2nd equations	ΔE_{corr}
^{28}Ne	1.17	1.59	**0.42**
^{26}Ne	7.32	8.46	**1.14**
^{24}Ne	5.75	6.98	**1.23**
^{22}Ne	10.48	12.12	**1.64**
^{20}Ne	10.93	13.30	**2.37**

Correlation energy E_{corr} (MeV)			
nucleus	1st equation only	1st + 2nd equations	ΔE_{corr}
^{28}S	8.05	10.05	**2.00**
^{30}S	0.59	2.06	**1.47**
^{32}S	2.82	5.22	**2.40**
^{34}S	4.27	5.62	**1.35**

Application to sd-shell nuclei with the Gogny force

✦ Charge radii:



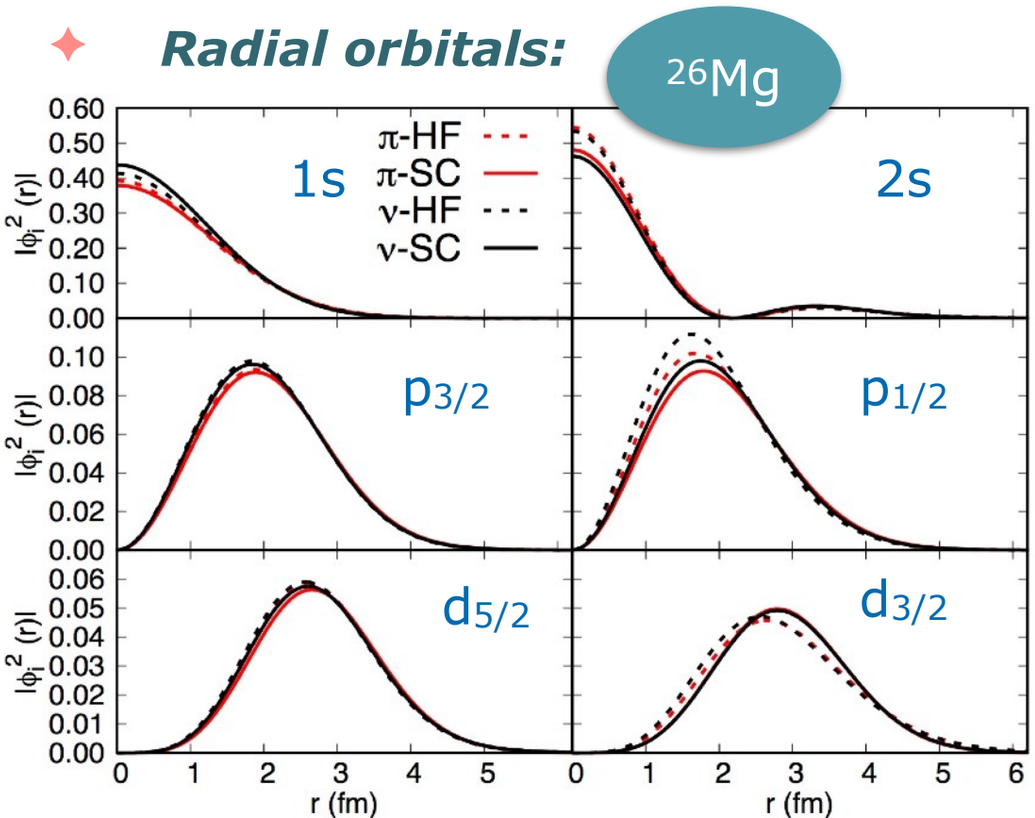
- *Average difference:*

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

- *Standard deviation*:

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

✦ Radial orbitals:



Application to sd-shell nuclei with the Gogny force

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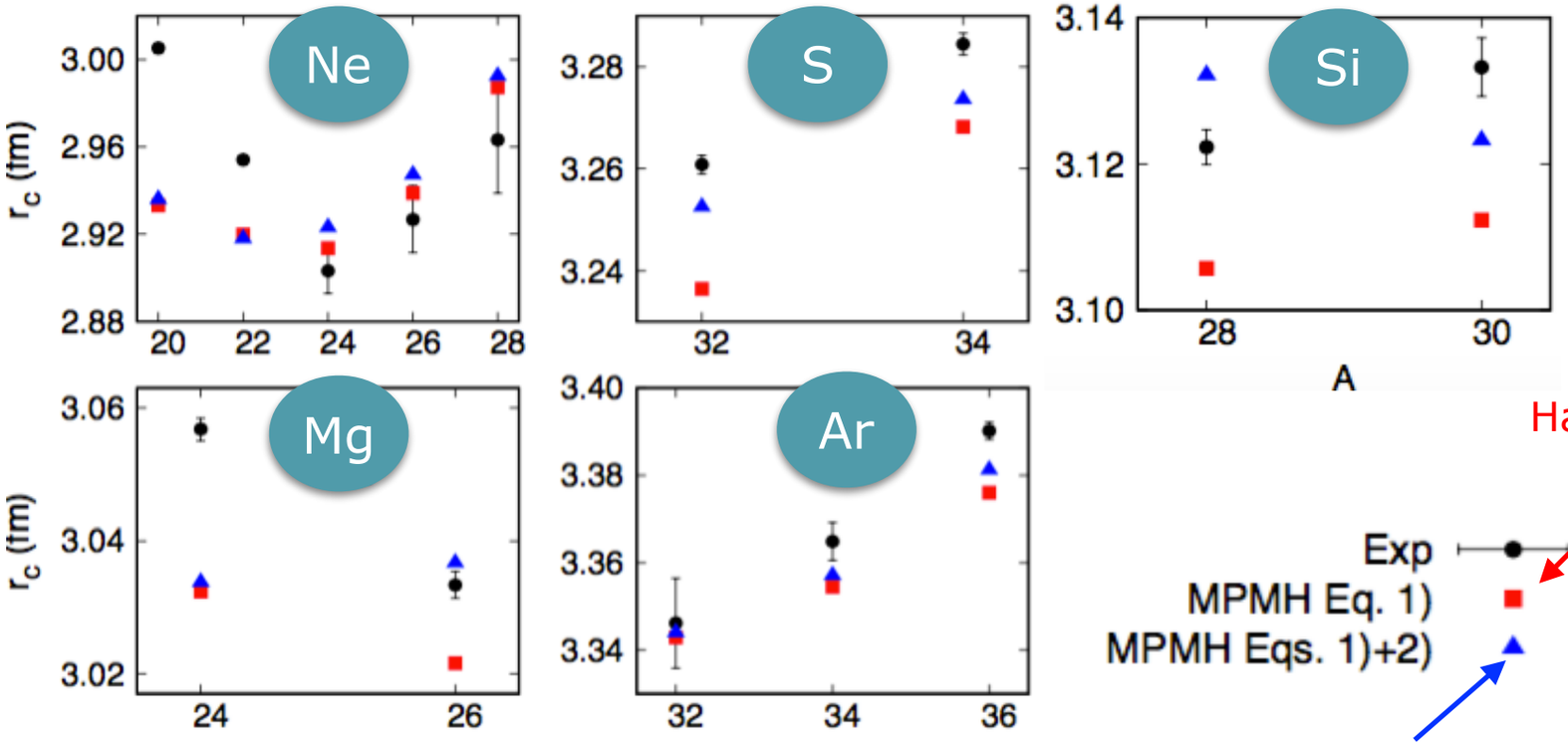

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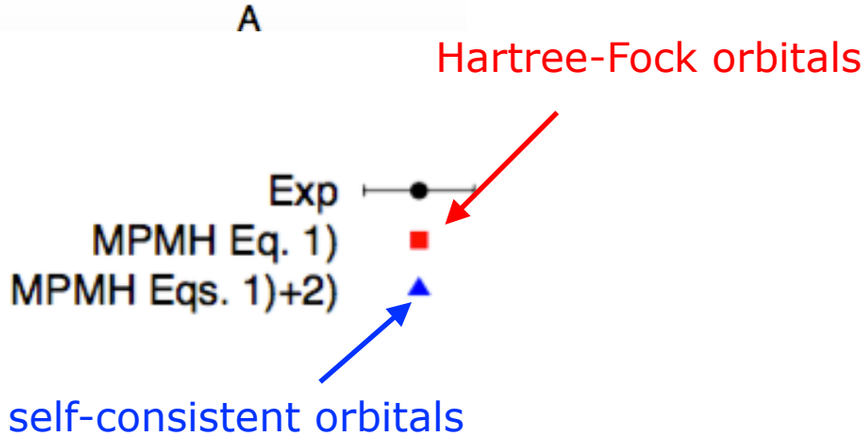

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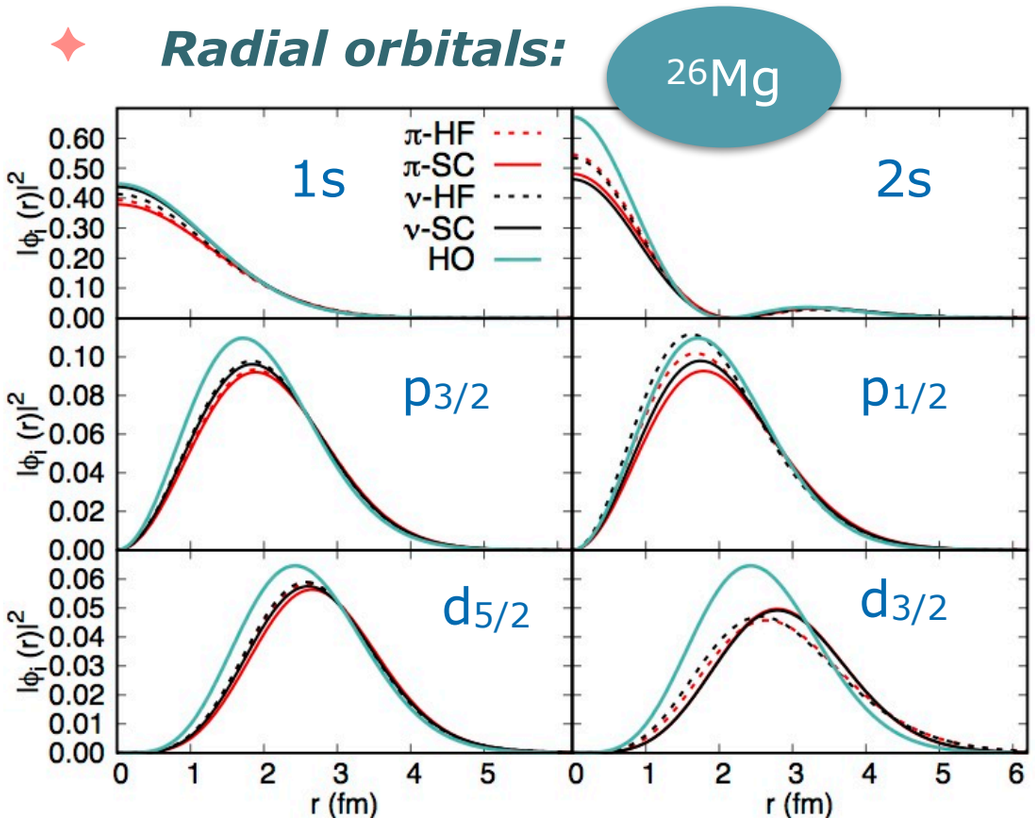
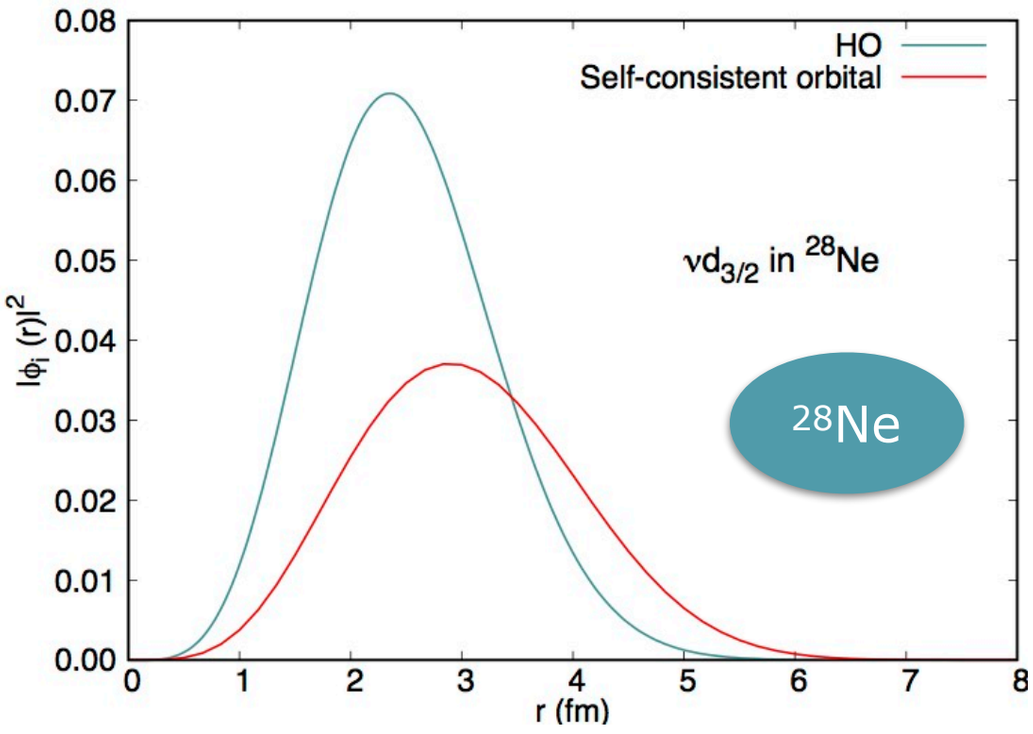
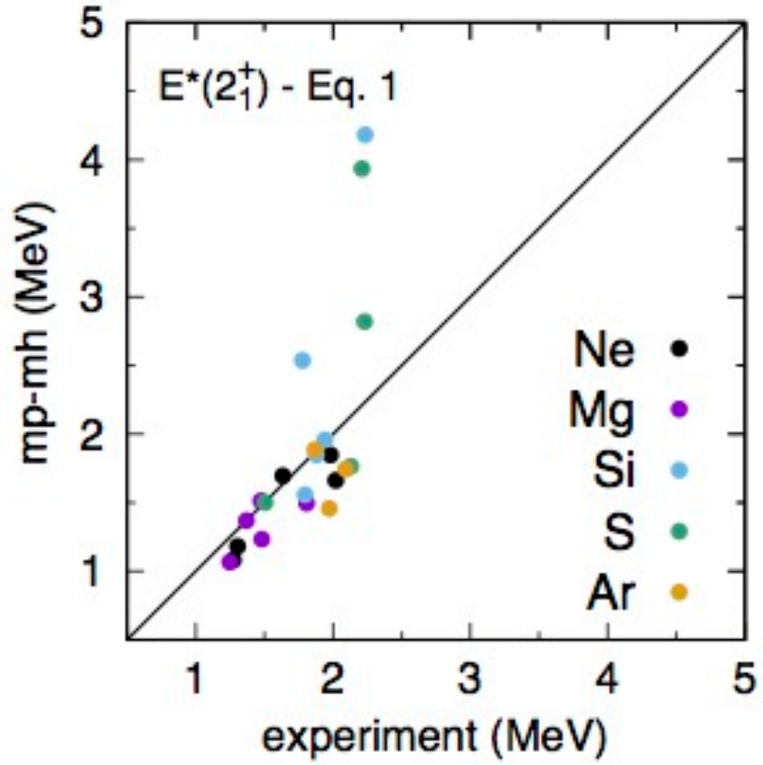




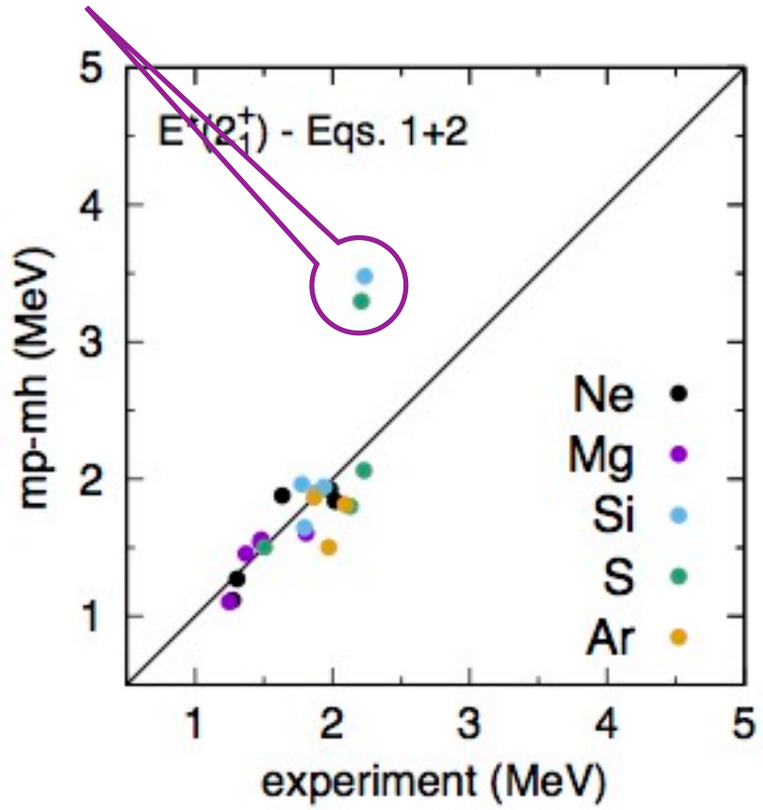
Application to sd-shell nuclei with the Gogny force

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

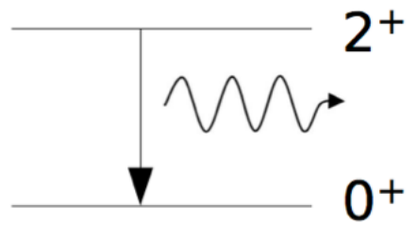
^{30}S & ^{30}Si excluded
$$\begin{cases} \langle \Delta E^* \rangle = 226 \text{keV} \\ \sigma(\Delta E^*) = 214 \text{ keV} \end{cases}$$

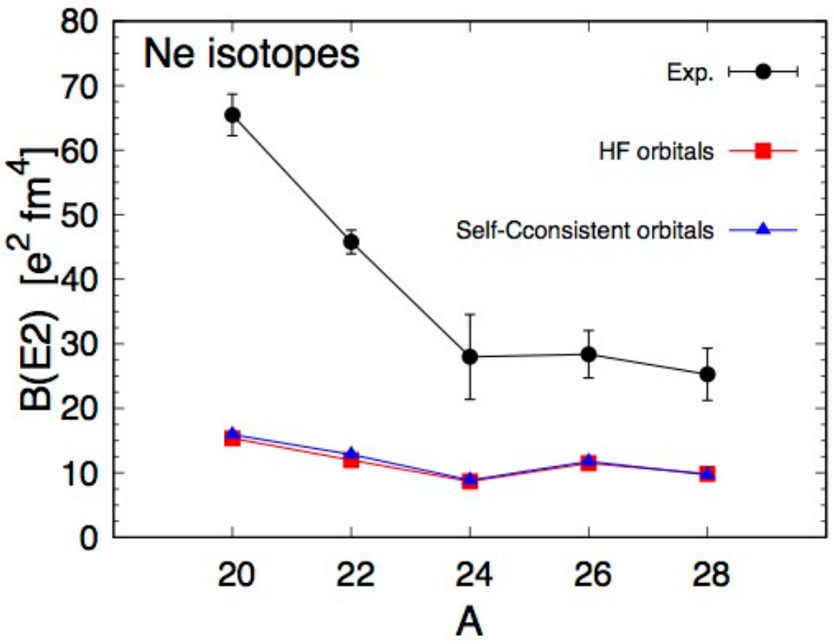
All
$$\begin{cases} \langle \Delta E^* \rangle = 235 \text{ keV} \\ \sigma(\Delta E^*) = 323 \text{ keV} \end{cases}$$

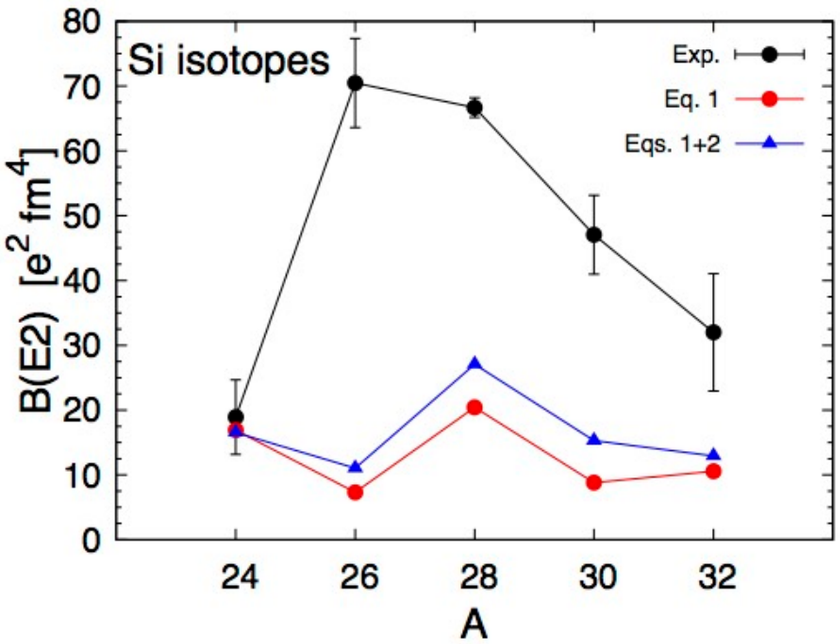
^{30}S & ^{30}Si excluded
$$\begin{cases} \langle \Delta E^* \rangle = 142 \text{ keV} \\ \sigma(\Delta E^*) = 122 \text{ keV} \end{cases}$$

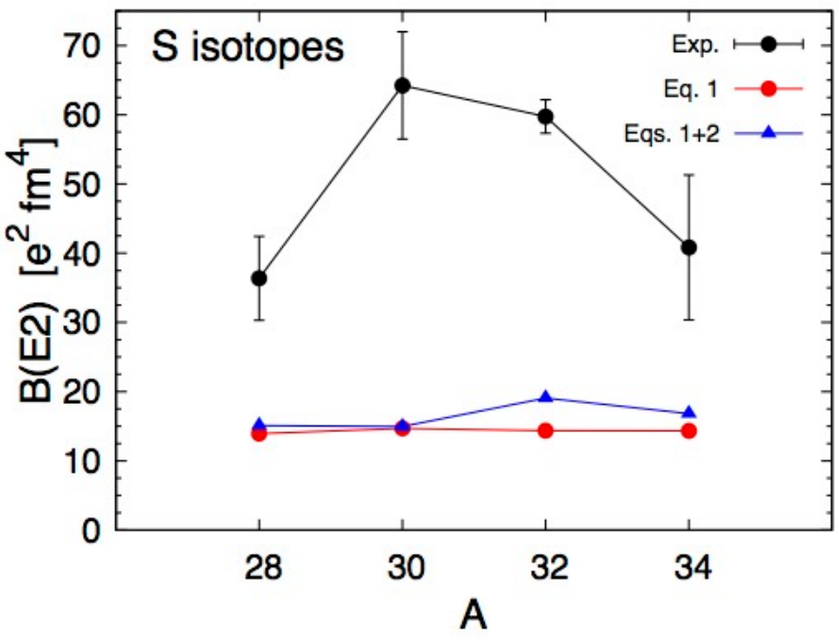
Application to sd-shell nuclei with the Gogny force

✦ Transition probabilities B(E2)









- 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)

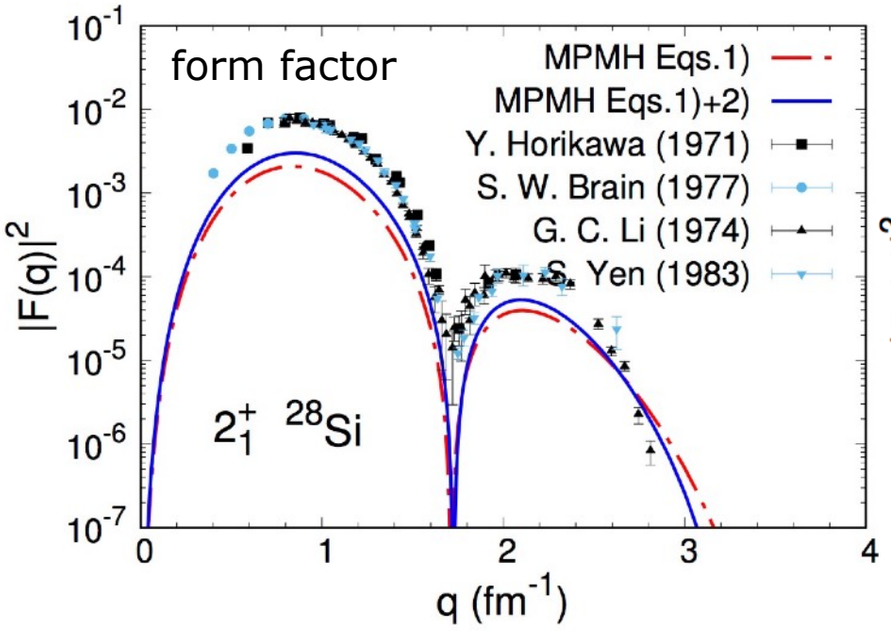
No effective charges

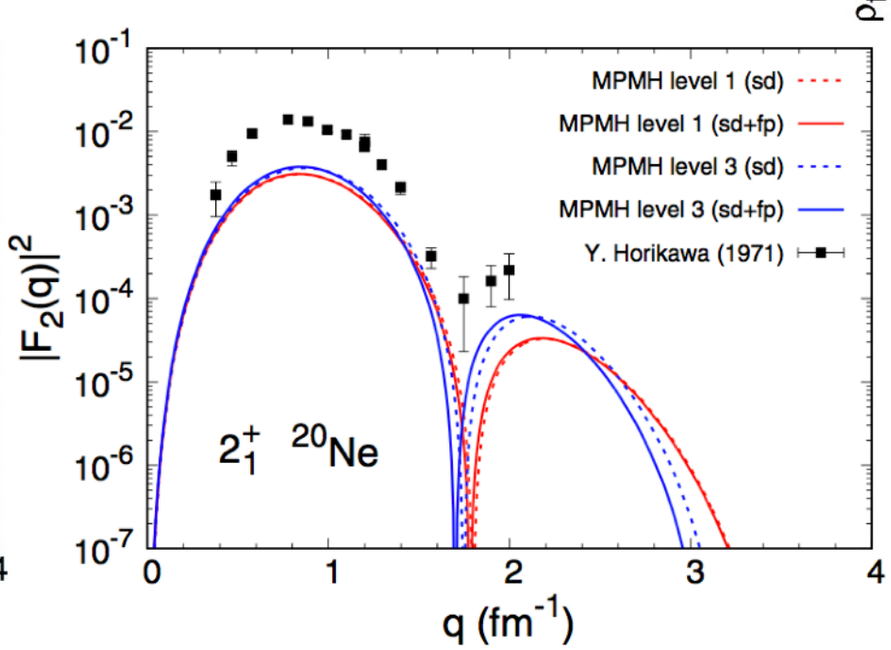
Application to sd-shell nuclei with the Gogny force

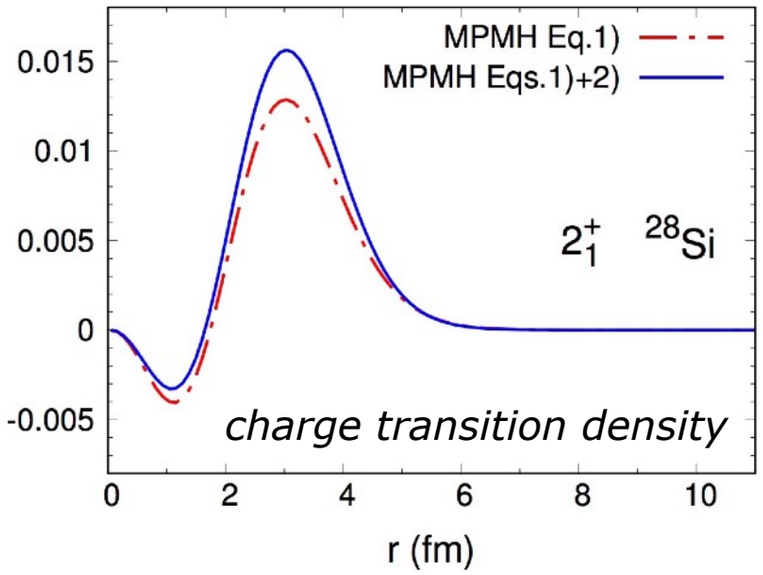
➡ *Electron inelastic scattering on discrete states*

Form factor: $F_\lambda(q) = \frac{\sqrt{4\pi}}{Z}\sqrt{\frac{2J_f+1}{2J_i+1}}\int_0^\infty r^2\, dr\; j_\lambda(qr)\rho_{tr}(r)$

From MPMH:





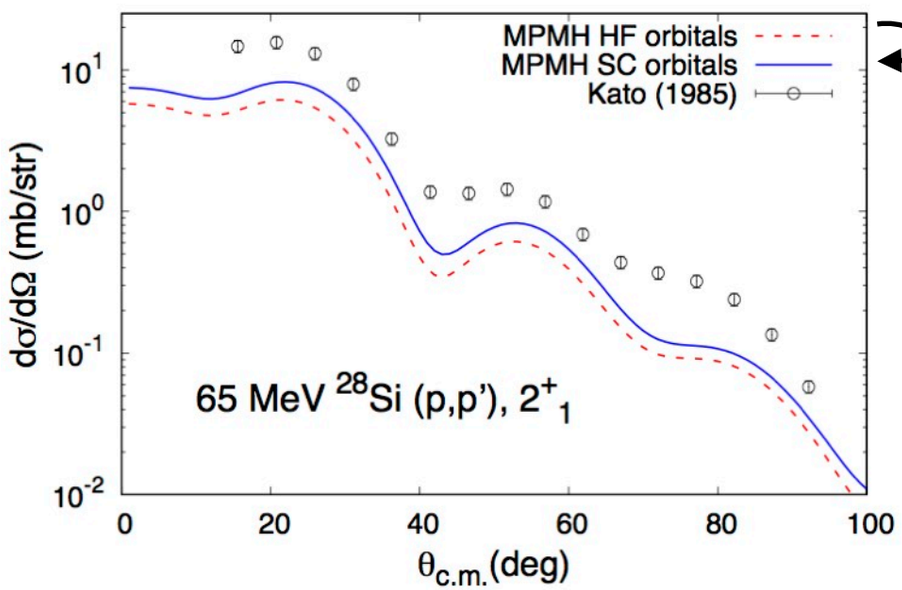


With optimized states:

- Small increase of the magnitude
- Improvement of the trend at high q

➡ *Proton inelastic scattering on discrete states*

In the framework of the DWBA,
with optical and transition potentials
calculated using transition densities from MPMH



factor ~1.3

In collaboration with M. Dupuis, CEA,DAM,DIF

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 orbital equation for each state

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

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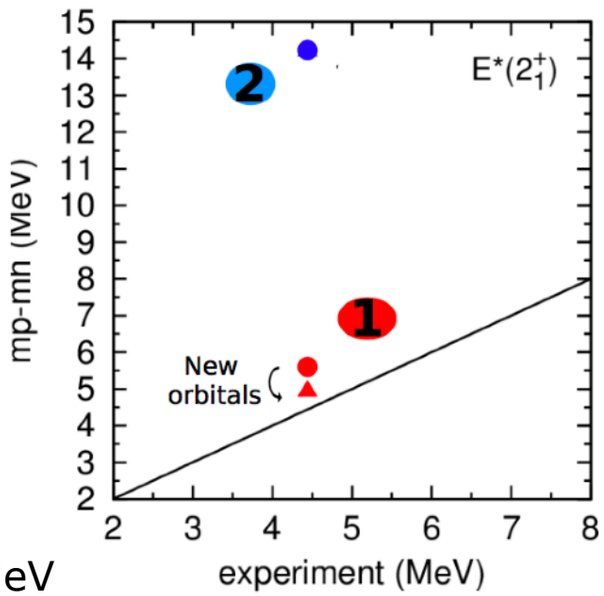
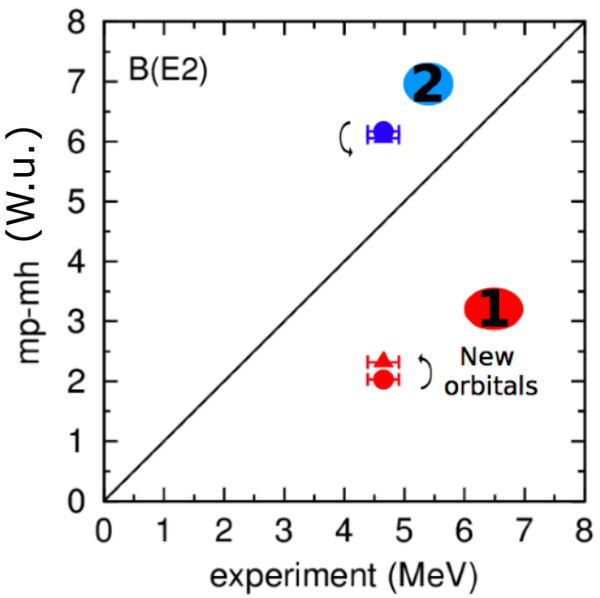
➡ try truncation schemes involving larger single-particle spaces
(excitation order, excitation energy, symmetry-constrained combinations etc.)

✱ 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 0ħω space

collectivity ✗, excitation energies ✓, overbinding ~ 6 MeV

2 Nħω space

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

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➡ 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:

1 0ħω space

collectivity ✗,excitation energies ✓, overbinding ~ 6 MeV

2 Nħω space

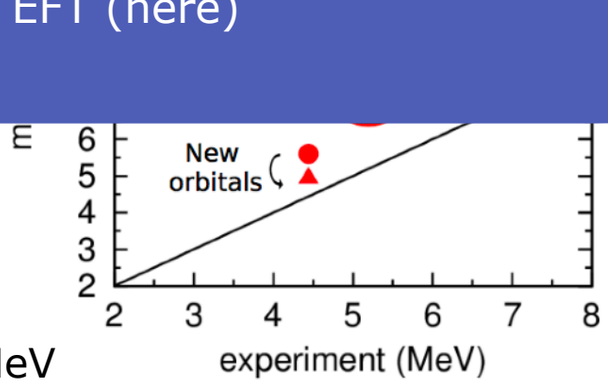
collectivity ✓, excitation energies ✗, overbinding ~ 60 MeV!

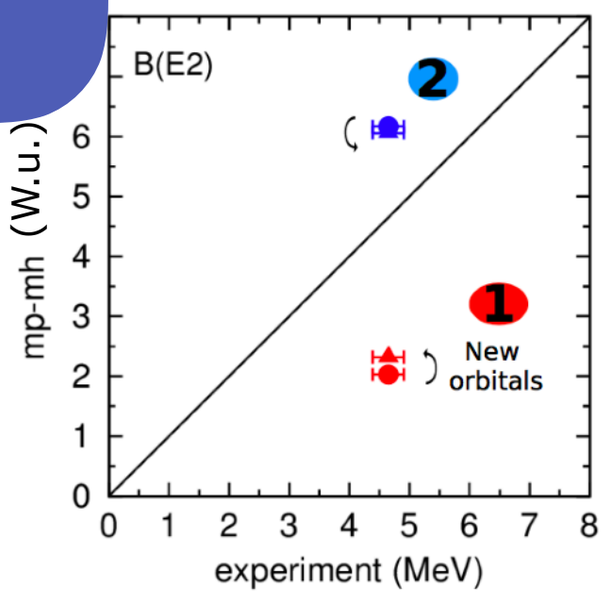
Need a better suited interaction

- fully finite-range, better constrained Gogny interaction with tensor (see Nathalie Pillet's talk)

or

- interaction derived from chiral EFT (here)





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, have to do the CI diagonalization and calculation of the mean field 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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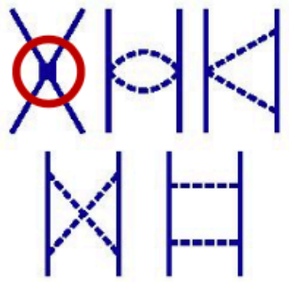
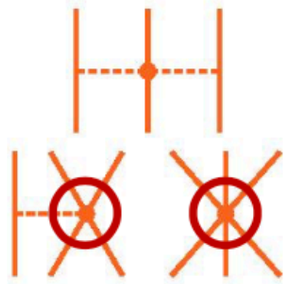
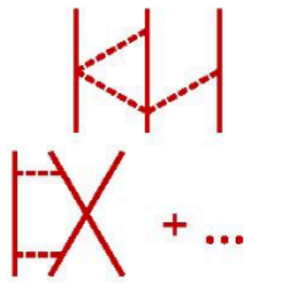
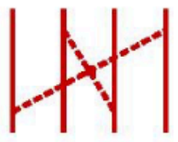
See e.g. A. Gezerlis, I. Tews, E. Epelbaum et al., Phys. Rev. C 90, 054323 (2014)

At each order:

contact terms
+
long-range pion-exchange terms

Chiral expansion:

	NN	3N	4N
LO $O\left(\frac{Q^0}{\Lambda^0}\right)$ 2 LECs		—	—
NLO $O\left(\frac{Q^2}{\Lambda^2}\right)$ 7 LECs		—	—
N²LO $O\left(\frac{Q^3}{\Lambda^3}\right)$ 2 LECs			—
N³LO $O\left(\frac{Q^4}{\Lambda^4}\right)$ 15 LECs	 + …	 + …	 + …

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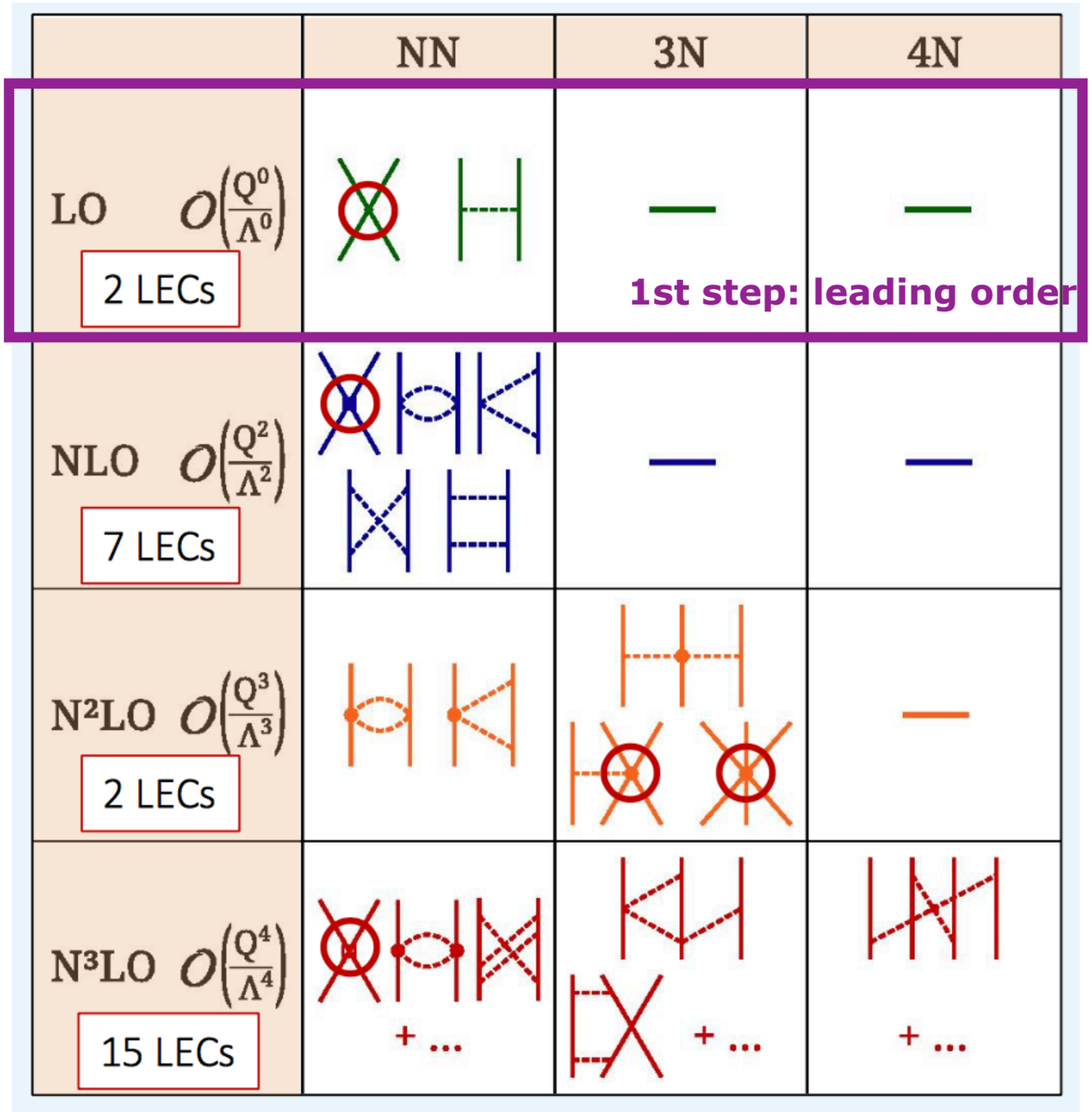
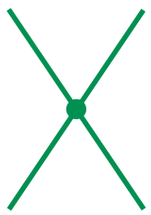


Application of the MPMH method with a chiral interaction

★ Chiral interaction at leading order with Gaussian regulators:

cut-off R_0= 1 fm

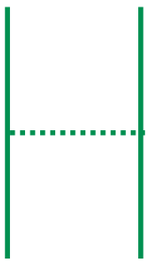
✦ contact term:



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

↠ purely gaussian

✦ long-range one-pion exchange:



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

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

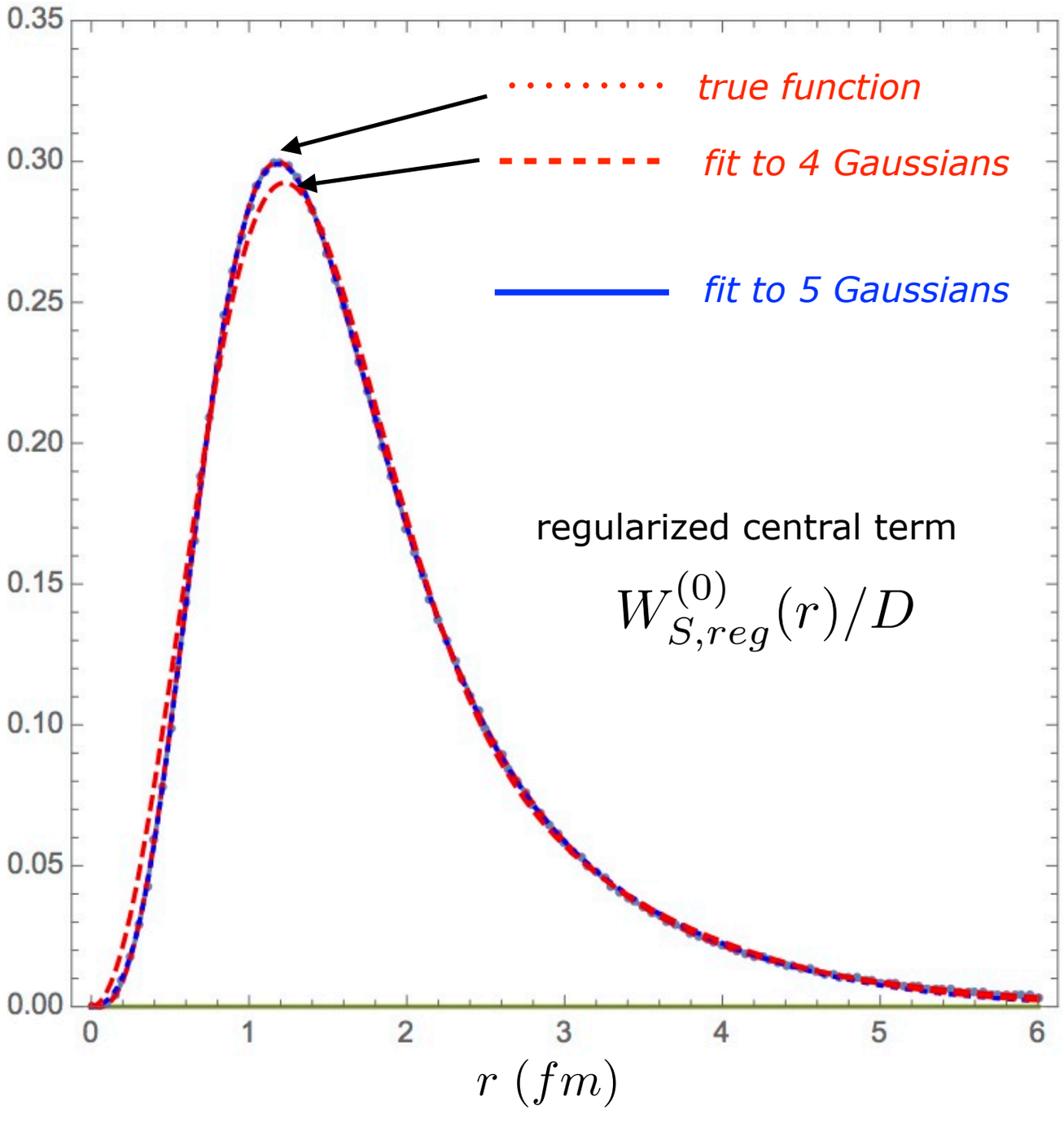
Note:
such fits of Yukawa to Gaussians already applied in *J. Dobaczewski & J. Engel, Phys. Rev. Lett. 94, 232502 (2005), or more recently in e.g. R. Navarro Perez et al. PRC 97, 054304 (2018).*

Application of the MPMH method with a chiral interaction

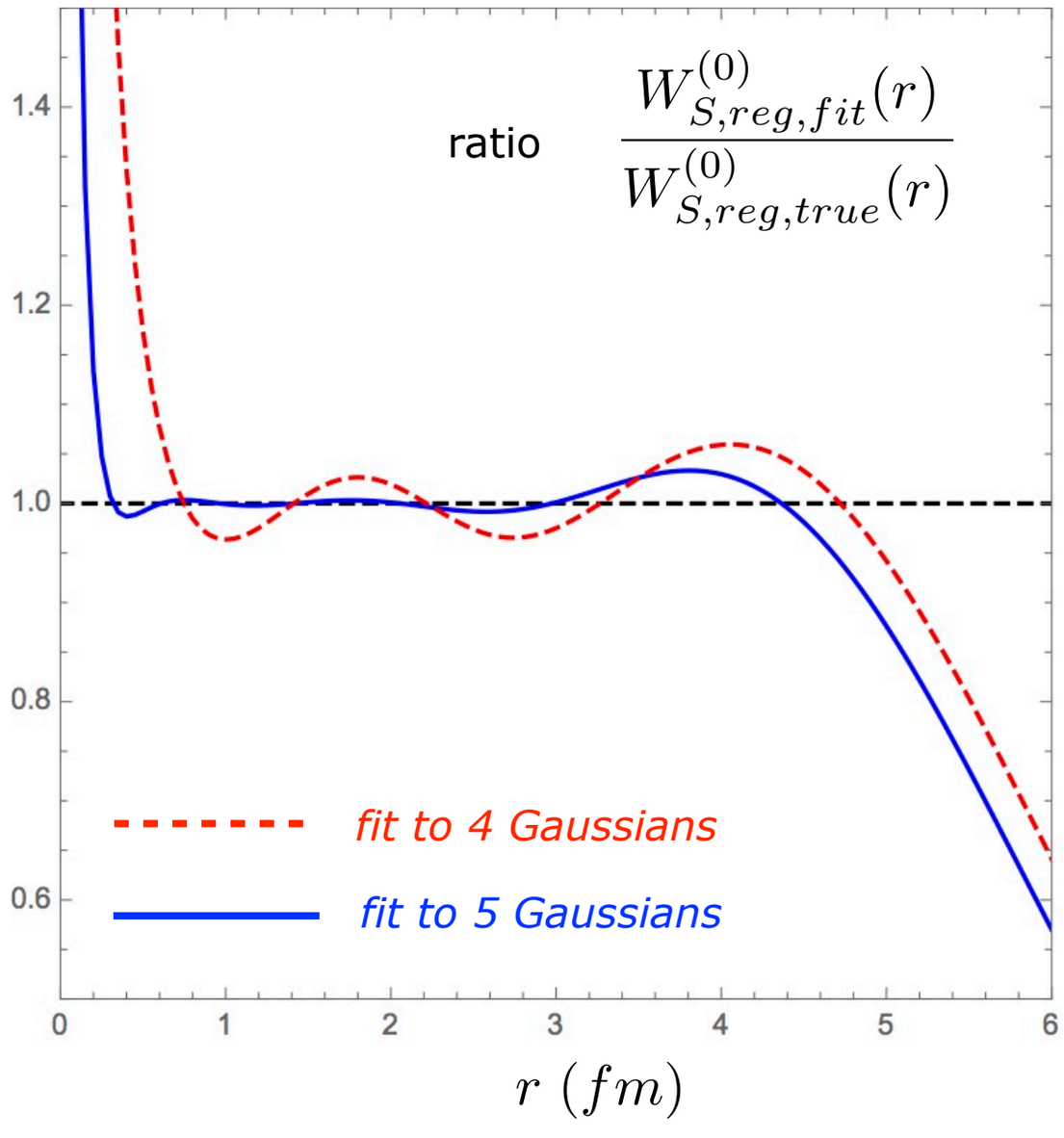
➠ **Central term:**

Very preliminary!

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



Choose 5 Gaussians



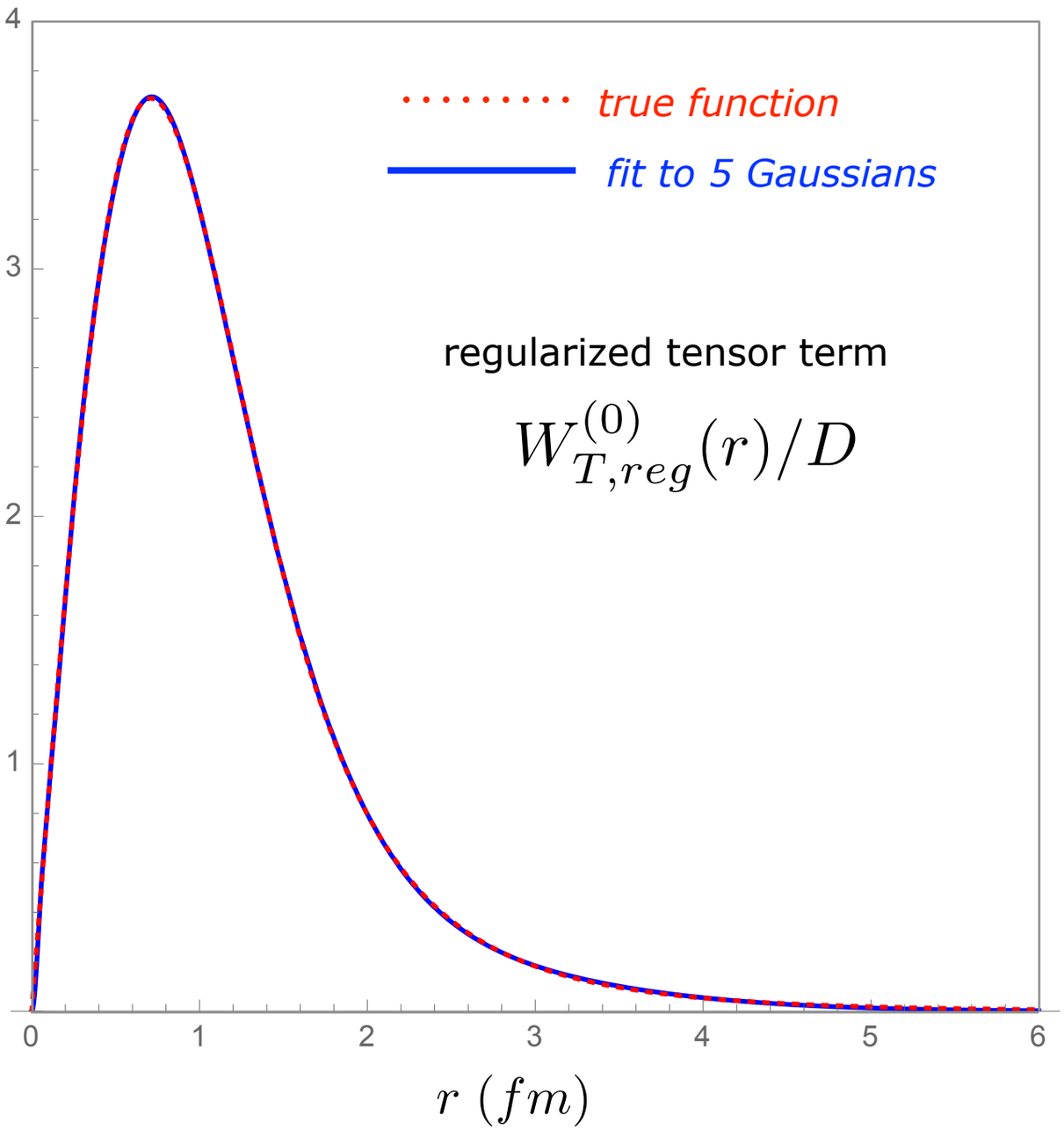
Courtesy of I. Tews

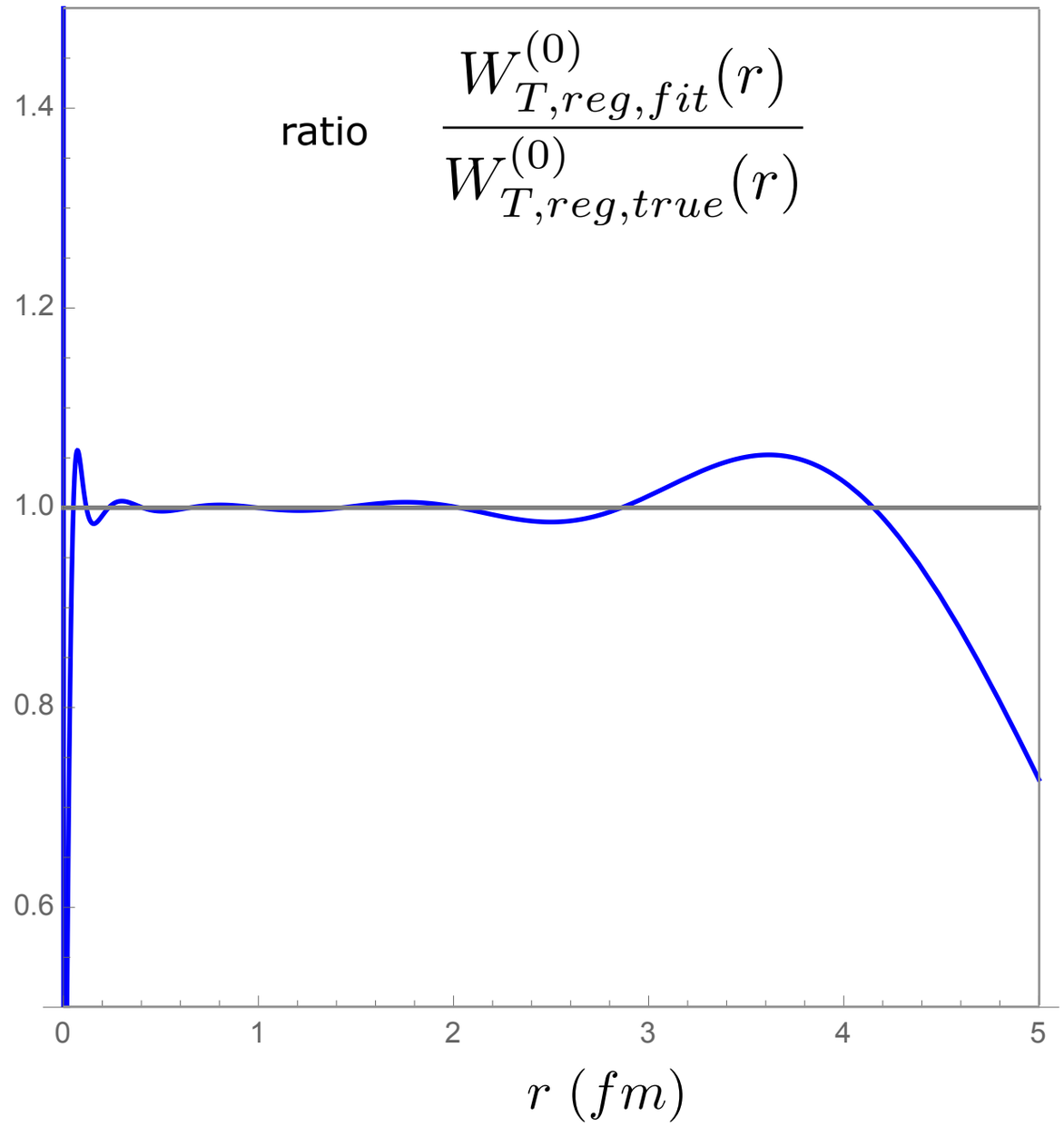
Application of the MPMH method with a chiral interaction

➠ **Tensor term:**

Very preliminary!

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





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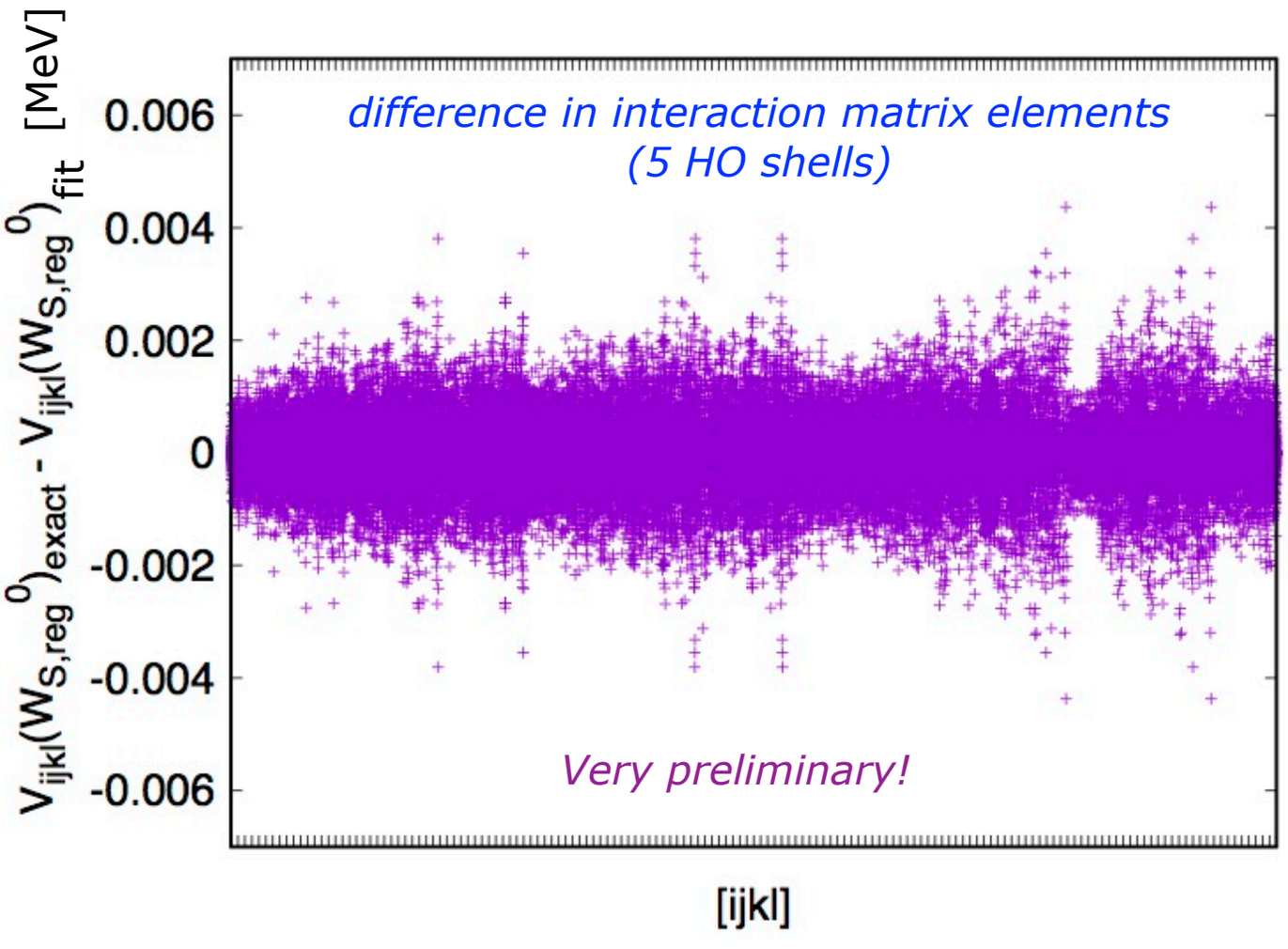
Application of the MPMH method with a chiral interaction

↠ ***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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