Assemblée Générale des théoriciens 2013

Multiparticle-multihole configuration mixing method and nuclear long range correlations

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Outline

- Introduction
- Formalism
- Numerical techniques
- Preliminary results: test cases
- Conclusion, prospects

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Introduction: Different approaches to nuclear structure

→ microscopic methods: search for solution of H|ψ>=E|ψ>

- “ab initio” techniques:
  → ~ Exact solution
  → feasible up to mid-mass nuclei

- “Shell-model”:
  → all correlations treated in restricted valence space
  → uses renormalized interactions in model space
  → no symmetry breaking

- Mean-field and beyond:
  → all nucleons active
  → separate treatment of correlations: Hartree-Fock (HF), HF+BCS / HFB (pairing),RPA (collectives states)...
  → symmetry breaking

✷ Introduction: Different approaches to nuclear structure

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mp-mh Configuration Mixing Method:
Unified treatment of long-range correlations without symmetry breaking

Conserves:
- spherical symmetry
- particle number
- Pauli principle

Already used in atomic physics (MCHF) and quantum chemistry (MCSCF)

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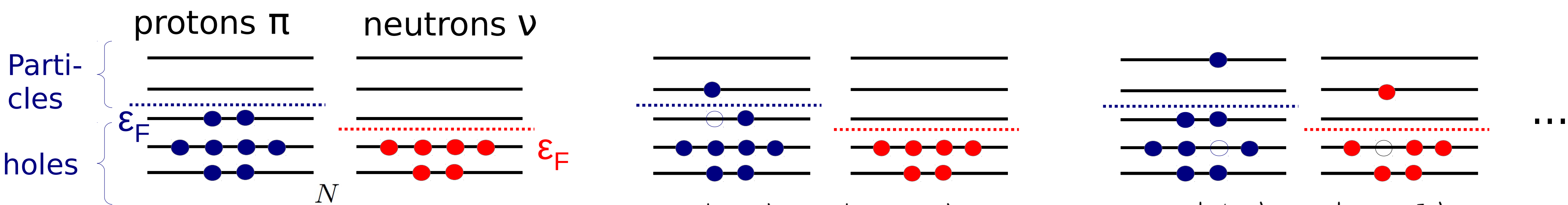
Formalism

- Trial wave function $\left|\Psi\right\rangle$ = superposition of Slater determinants

$$|\Psi\rangle = A_0|\phi\rangle + \sum_{\alpha\in\{1p1h\}} A_\alpha|\phi_\alpha\rangle + \sum_{\alpha\in\{2p2h\}} A_\alpha|\phi_\alpha\rangle + ... + \sum_{\alpha\in\{NpNh\}} A_\alpha|\phi_\alpha\rangle$$



$$|\phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

$$|\phi_\alpha\rangle = |1p1h\rangle$$

$$|\phi_\alpha\rangle = |2p2h\rangle$$

- mp-mh excitation = **Configuration**

- **Unknown quantities ?**

Formalism

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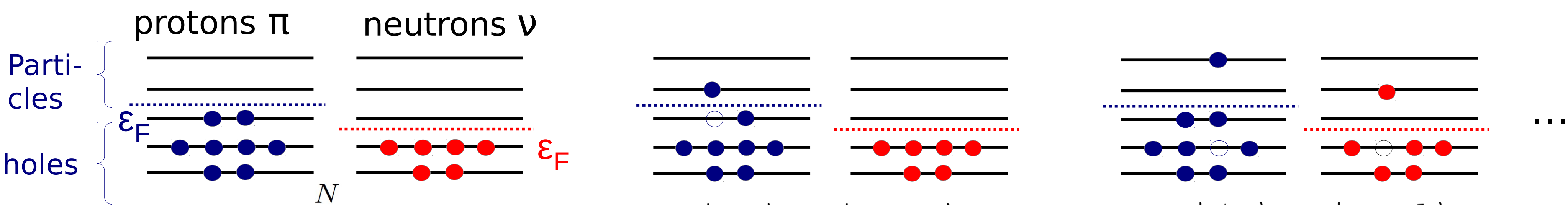

$$|\phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle \qquad |\phi_\alpha\rangle = |1p1h\rangle \qquad |\phi_\alpha\rangle = |2p2h\rangle$$

- mp-mh excitation = **Configuration**

- **Unknown quantities ?** → Mixing coefficients $\{A_\alpha\}$

Formalism

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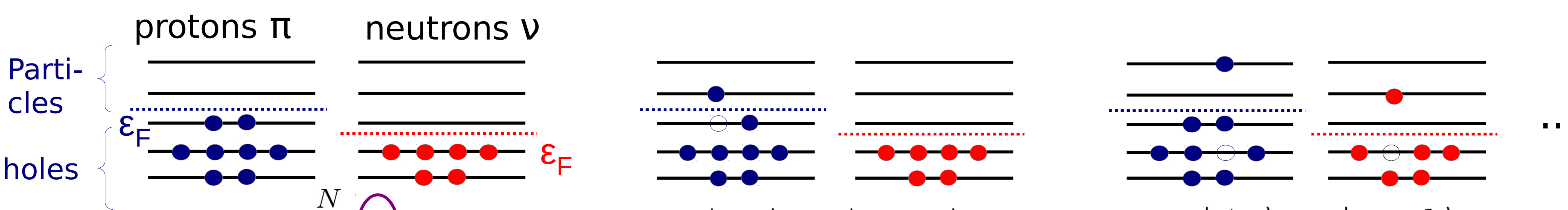

$$|\phi\rangle = \prod_{i=1}^{N} a_i^\dagger|0\rangle \qquad |\phi_\alpha\rangle = |1p1h\rangle \qquad |\phi_\alpha\rangle = |2p2h\rangle$$

- mp-mh excitation = **Configuration**

- **Unknown quantities ?**
  - Mixing coefficients $\{A_\alpha\}$
  - Single-particle orbitals $\{\varphi_i\}$

Formalism

- **Variational principle applied to the energy:** $\delta\mathcal{E}[\Psi] = 0$

- Method can be applied to any N-body (effective) interaction.

- Here, we use the phenomenological density-dependent Gogny force $V^{2N}_{D1S}[\rho]$.

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

+ Hypothesis: Independent variations of coefficients and orbitals

➡ Two coupled equations to solve:

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

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1st variational equation: determining the coefficients

$$\delta\mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0$$

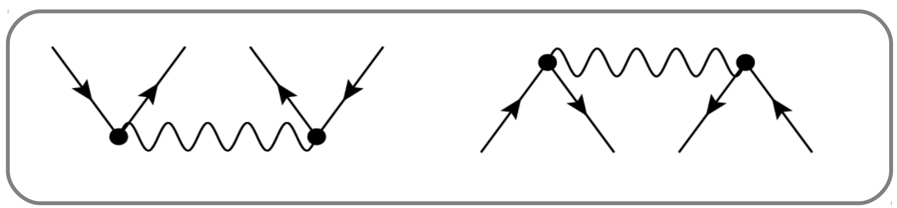
$$\frac{\partial\mathcal{E}[\Psi]}{\partial A^*_\alpha} = 0 \Leftrightarrow \sum_\beta A_\beta \langle\phi_\alpha|\hat{\mathcal{H}}[\rho]|\phi_\beta\rangle = \lambda A_\alpha$$

with $\hat{\mathcal{H}} = \hat{H} + \hat{\mathcal{R}} = \hat{H} + \int d^3r \langle\Psi|\frac{\partial V}{\partial\rho(\vec{r})}|\Psi\rangle\hat{\rho}(\vec{r})$

⟺ Diagonalization of a Hamiltonian matrix in the configuration space

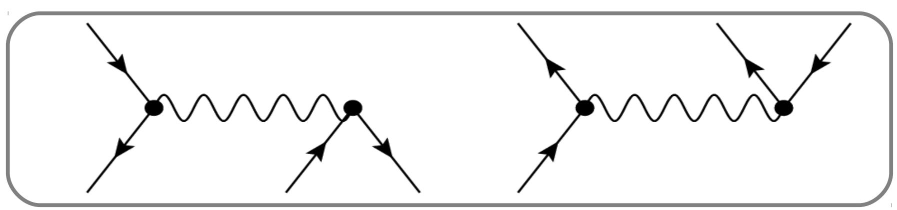
→ Vertex $\langle\phi_\alpha|\hat{V}|\phi_\beta\rangle$:

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



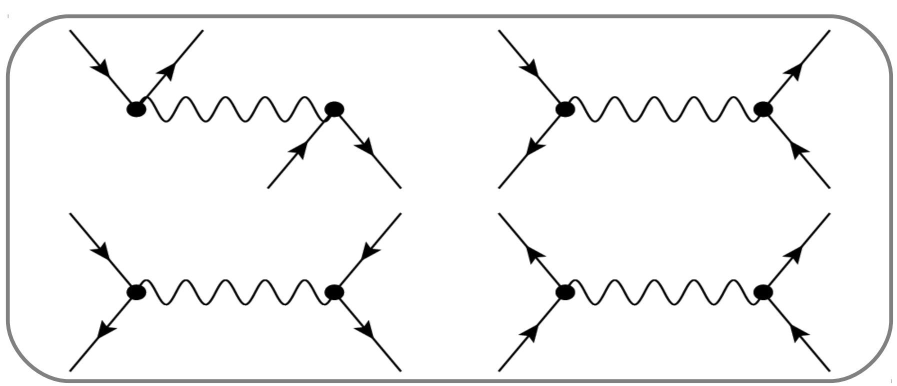
RPA, pairing

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



particle-vibration

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



RPA

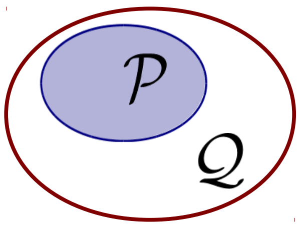
pairing

1st variational equation: determining the coefficients

- Truncation in configuration space:

Possible criteria:

-excitation order of configurations (1p1h, 2p2h...)
-excitation energy of configurations
-single-particle basis (core + valence space)



$$\mathcal{P} + \mathcal{Q} = \mathcal{S}$$

Total N-body configuration space

➡ $\mathcal{P}$ space = configurations included in $|\Psi\rangle$
$\mathcal{Q}$ space = configurations excluded from $|\Psi\rangle$

$$\begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix} \rightarrow \begin{pmatrix} H_{PP} \end{pmatrix}$$

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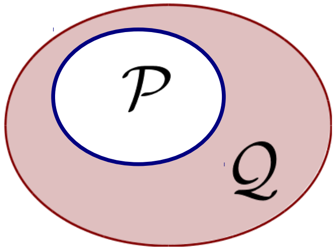
2nd variational equation: determining the orbitals

$$\delta\mathcal{E}[\Psi]_{/\{\varphi_i^*\}} = 0$$



→ Orbital variation:

$$a_i^\dagger \to e^{i\hat{S}} a_i^\dagger e^{-i\hat{S}} \Rightarrow \delta a_i^\dagger = i\left[\hat{S}, a_i^\dagger\right] \quad \text{where} \quad \hat{S} = \sum_{ij} S_{ij} a_i^\dagger a_j$$

+ variation of configurations restricted to $\mathcal{Q}$ space $\Rightarrow |\delta\phi_\alpha\rangle = i\hat{Q}\hat{S}|\phi_\alpha\rangle$

$$\left[\hat{h}[\rho,\sigma], \hat{\rho}\right] = \hat{g}[\sigma]$$

→ $\rho_{ki} = \langle\Psi|a_i^\dagger a_k|\Psi\rangle$ → (correlated) 1-body density

→ $h[\rho,\sigma]_{ij} = T_{ij} + \sum_{kl} \langle ij|\widetilde{V}|kl\rangle \rho_{lk} + \frac{1}{4} \sum_{klmn} \langle kl|\frac{\partial \widetilde{V}}{\partial \rho_{ji}}|mn\rangle \langle\Psi|a_k^\dagger a_l^\dagger a_n a_m|\Psi\rangle$ → Mean-field

$$\equiv T_{ij} + \Gamma_{ij}[\rho,\sigma]$$

→ $\sigma_{ikmn} = \langle\Psi|a_i^\dagger a_m^\dagger a_n a_k|\Psi\rangle - \rho_{ki}\rho_{nm} + \rho_{km}\rho_{ni}$ → 2-body correlation matrix

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

2nd variational equation: determining the orbitals

$$\rightarrow \quad \boxed{\left[\hat{h}[\rho,\sigma],\hat{\rho}\right] = \hat{g}[\sigma]}$$

- General equation in physics:

→ can be obtained from the dynamical equation relating the 1- and 2-body Green's functions, in the limit of equal time (with $G^{(3)} \sim G^{(2)} G^{(1)}$).

Self-energy — Static part — Dynamical part

$$\Sigma(t_1 - t_2) = \Sigma^{(0)}\delta(t_1 - t_2) + \Sigma'(t_1 - t_2)$$

- $\Sigma^{(0)} = \Gamma[\rho,\sigma]$ ← average potential

- $\lim_{t_2 \to t_1^+} \int dt \left[G^{(1)}(t - t_2), \Sigma'(t_1 - t)\right] = g[\sigma]$

1-body GF — Source term

- Roles:

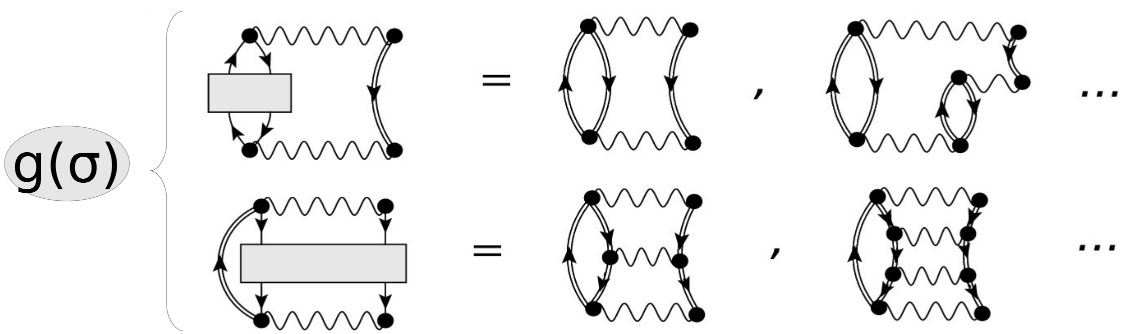
→ Includes effect of correlations into the mean-field through g(σ)
→ Compensates (partially) P/Q truncations

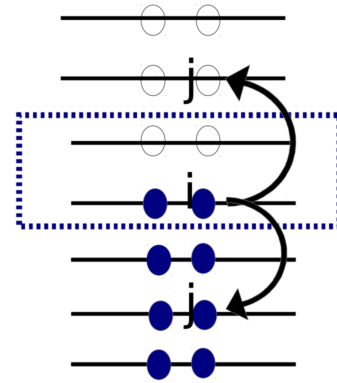
2nd variational equation: determining the orbitals

- Propagation of the effect of correlations outside valence space

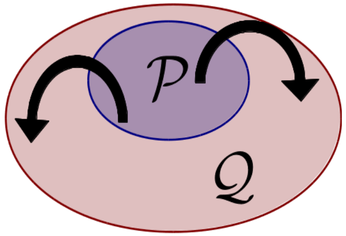
$$g_{ij}(\sigma) = \frac{1}{2}\sum_{klm} \widetilde{V}_{kmjl}\,\sigma_{ki,ml} - \frac{1}{2}\sum_{klm} \widetilde{V}_{kiml}\,\sigma_{jl,km}$$

j: $\in$ whole basis; i: $\in$ valence





- Effect on the correlated wave function



Orbital renormalization: $a_i^\dagger = e^{i\hat{S}'} a_{i_{HF}}^\dagger e^{-i\hat{S}'}$

➡ $|\phi\rangle = e^{iS'}|HF\rangle$

$$= |HF\rangle + i\sum_{ph} S'_{ph} a_p^\dagger a_h |HF\rangle - \frac{1}{2}\sum_{php'h'} S'_{ph} S'_{p'h'} a_p^\dagger a_h a_{p'}^\dagger a_{h'} |HF\rangle + \ldots$$

→ New reference state = superposition of mp-mh excitations on top of |HF>.

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Numerical techniques: general algorithm

- Global self-consistent process:

Starting point: Hartree-Fock orbitals

Solve the 1st equation:

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

→ Mixing coefficients $\{A_\alpha\}$

Calculation of the quantity of interest:

-one-body density $\rho_{ki} = \langle \Psi | a_i^\dagger a_k | \Psi \rangle$

-two-body density $\langle \Psi | a_i^\dagger a_m^\dagger a_n a_k | \Psi \rangle$

$\rightarrow \sigma_{ikmn} = \langle \Psi | a_i^\dagger a_m^\dagger a_n a_k | \Psi \rangle - \rho_{ki}\rho_{nm} + \rho_{km}\rho_{ni}$

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

Solve the 2nd equation:

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

→ New single-particle orbitals

… → until convergence

Numerical techniques: solving the equations

- Secular equation: solved with shell-model-type algorithm

- Orbital equation:

$$\left[\hat{h}[\rho,\sigma],\hat{\rho}\right] = \hat{g}[\sigma] \quad \Longleftrightarrow \quad \left[\hat{h}[\rho,\sigma] - \hat{Q}[\rho,\sigma],\hat{\rho}\right] = 0$$

New "Correlation field"

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

$$\begin{cases} Q[\rho,\sigma]_{\mu\nu} = \dfrac{g[\sigma]_{\mu\nu}}{n_\nu - n_\mu} & \text{, if } \quad n_\mu \neq n_\nu \\ Q[\rho,\sigma]_{\mu\nu} = 0 & \text{, otherwise.} \end{cases}$$

Solution {φ} = eigenfunctions of h-Q
→ non-linear problem → iterative solution

Orbitals $\varphi^{(1)}$, 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 $\rho^{(n)}=\rho^{(n+1)}$ → Back to 1st equation...

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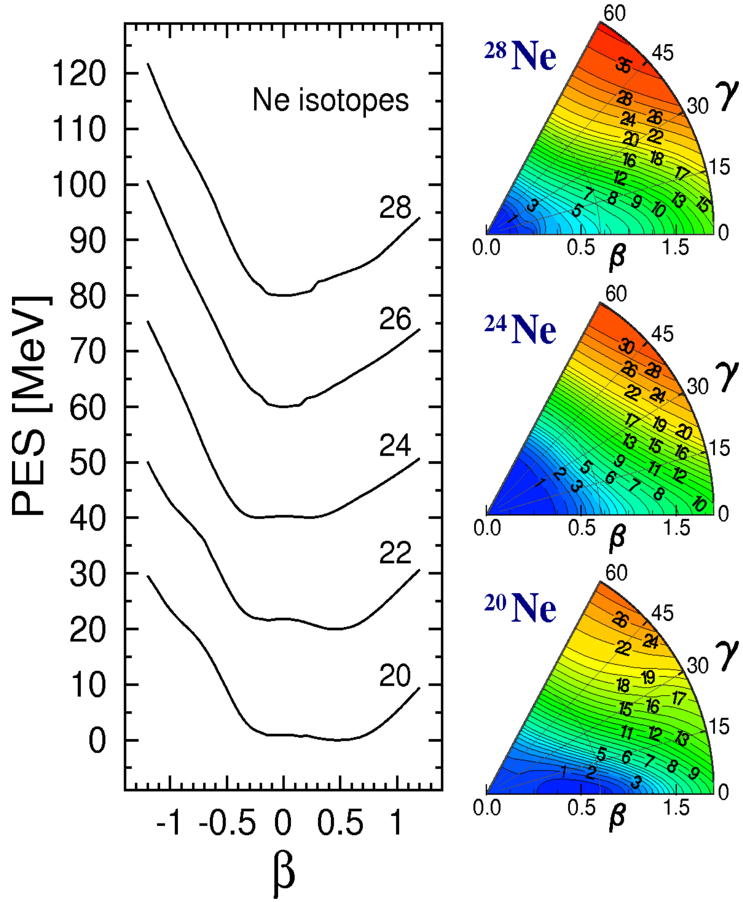
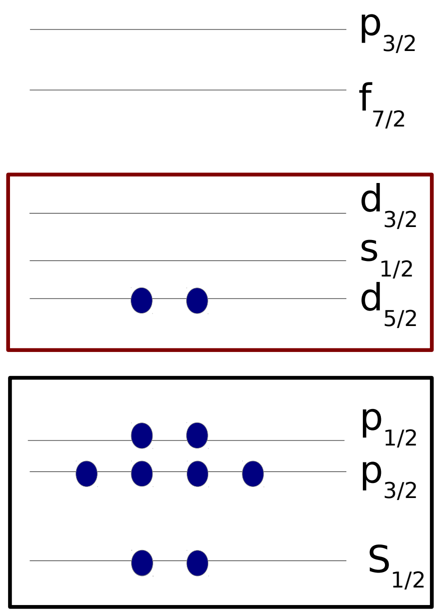
Preliminary results...

... for the **ground-state** of ^{28}Ne and ^{20}Ne



Courtesy of N.Pillet

correlations



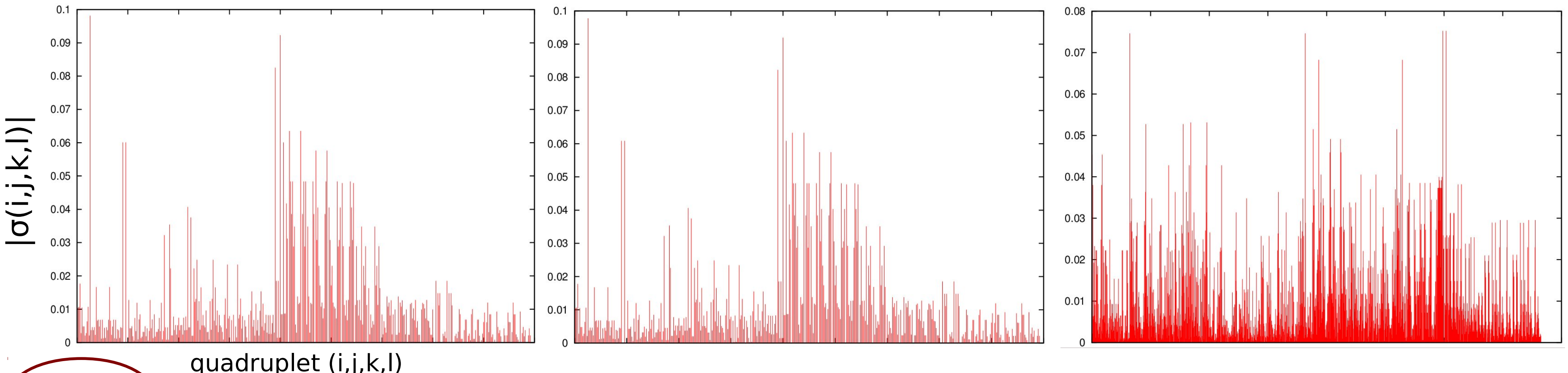
Valence space = s-d shell

core

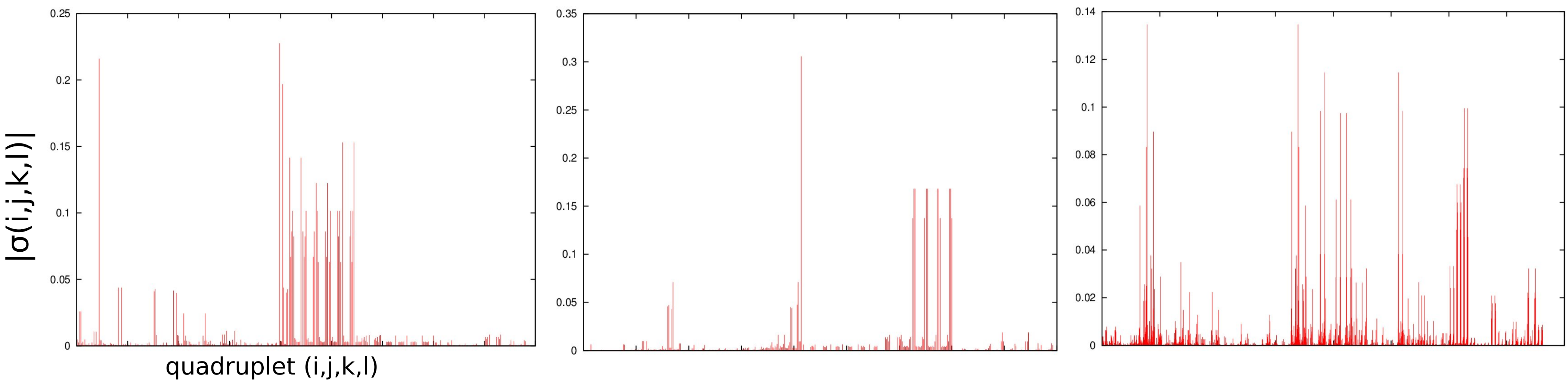
✷ Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Two-body correlation matrix: $\sigma_{ikmn} = \langle \Psi | a_i^\dagger a_m^\dagger a_n a_k | \Psi \rangle - \rho_{ki}\rho_{nm} + \rho_{km}\rho_{ni}$

$^{20}Ne_{10}$ Proton correlations — Neutron correlations — Proton/Neutron correlations



$^{28}Ne_{18}$

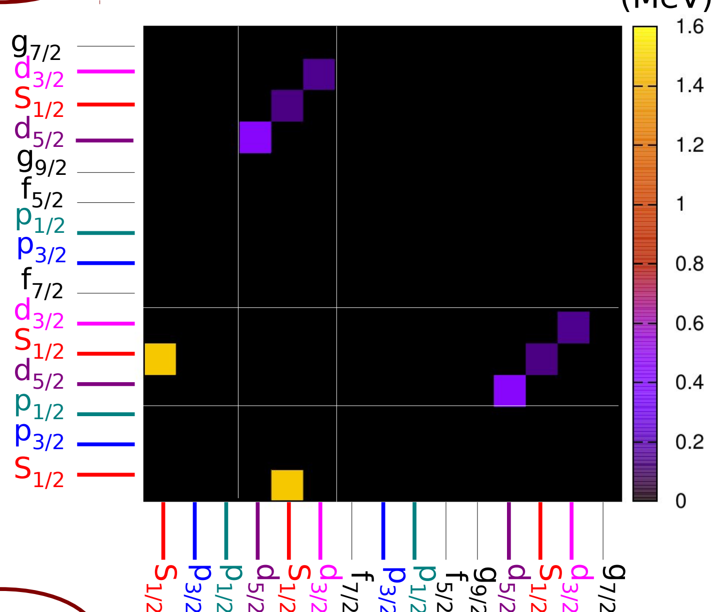


✷ Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

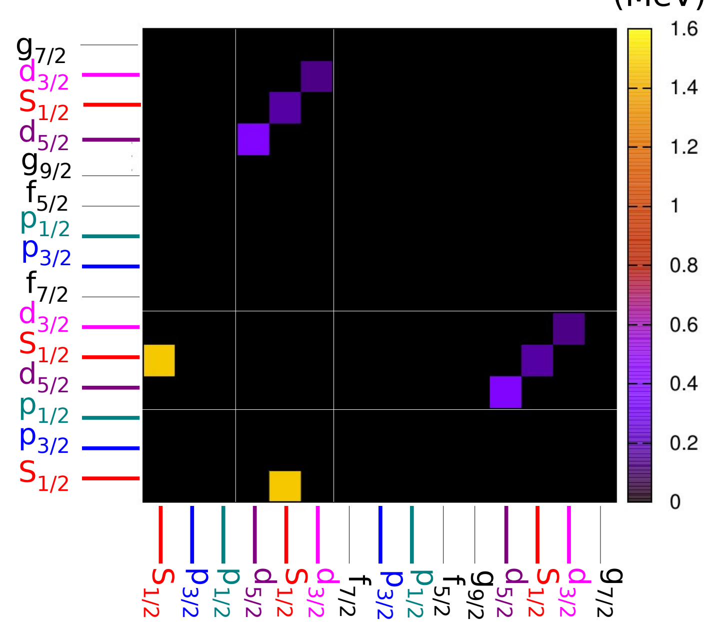
- **Source term g(σ):** $$g_{ij}(\sigma) = \frac{1}{2}\sum_{klm} \widetilde{V}_{kmjl}\,\sigma_{ki,ml} - \frac{1}{2}\sum_{klm} \widetilde{V}_{kiml}\,\sigma_{jl,km}$$

$^{20}Ne_{10}$

Proton term



Neutron term



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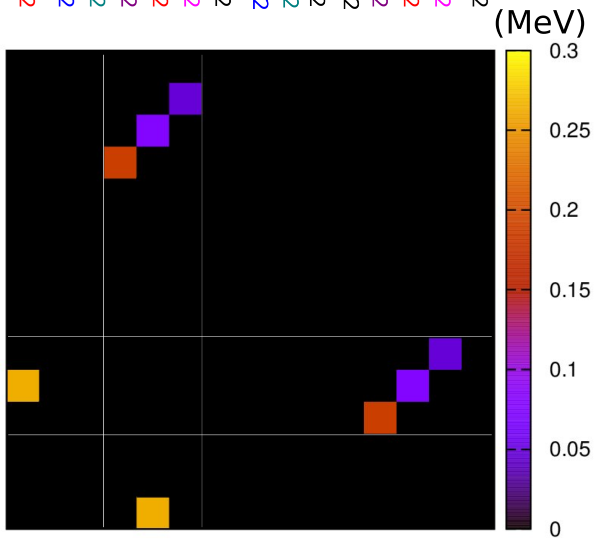
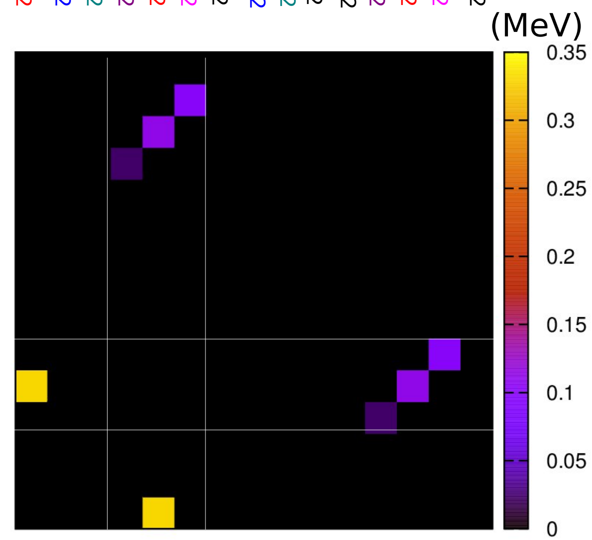
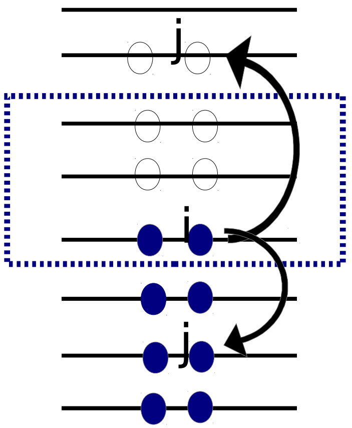






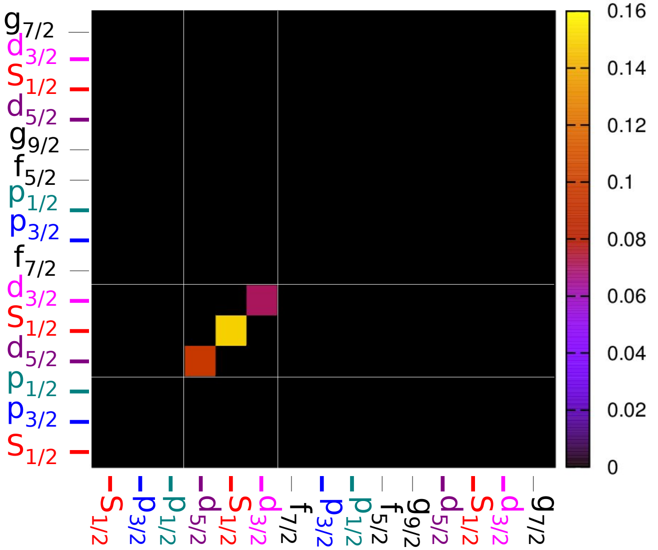
Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Evolution of the neutron one-body density matrix:

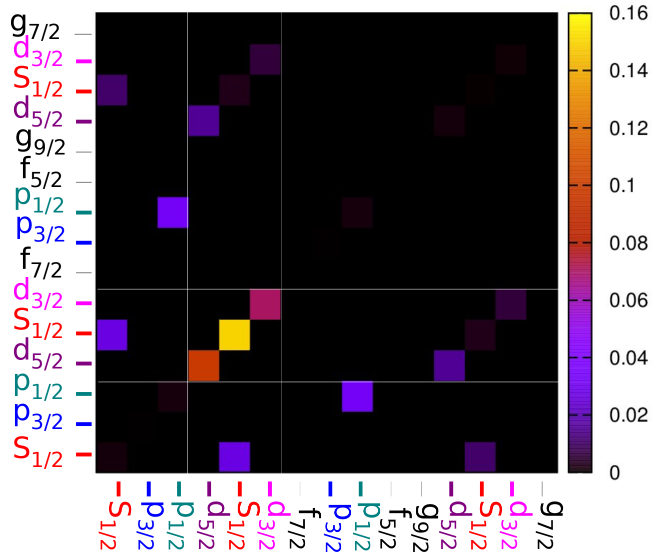
Representation of $\Delta\rho=|\rho_{HF}-\rho_{correlated}|$ in HF basis

$^{20}Ne_{10}$

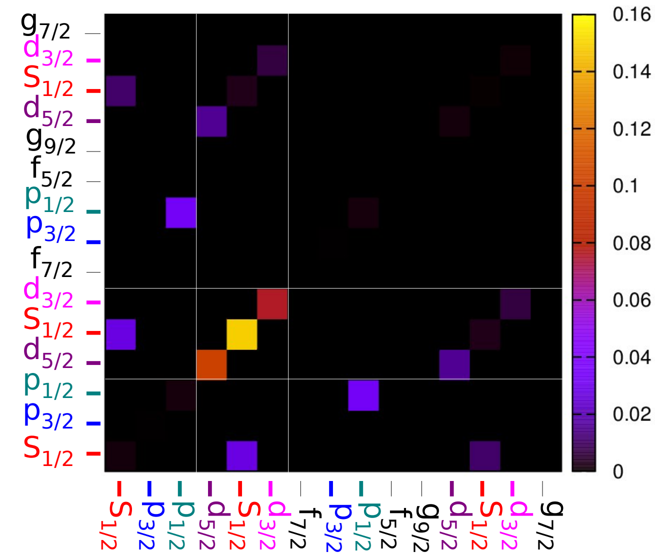
Global iteration 1, after equation 1



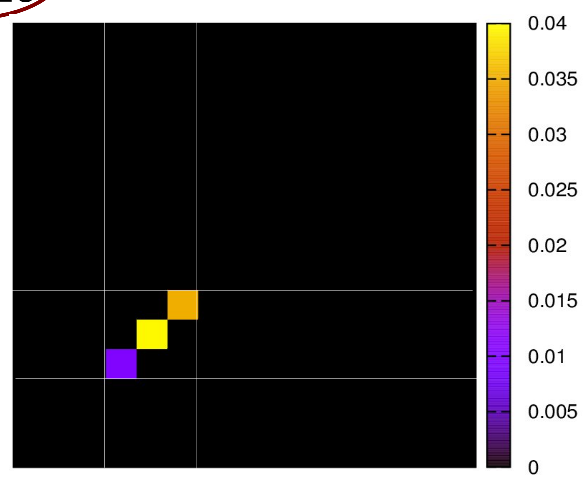
Global iteration 1, after equation 2

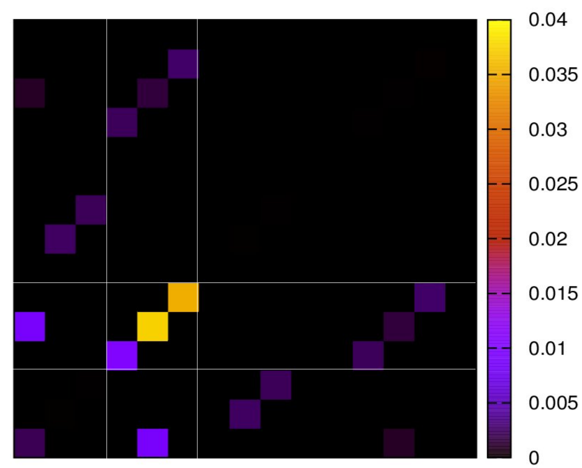


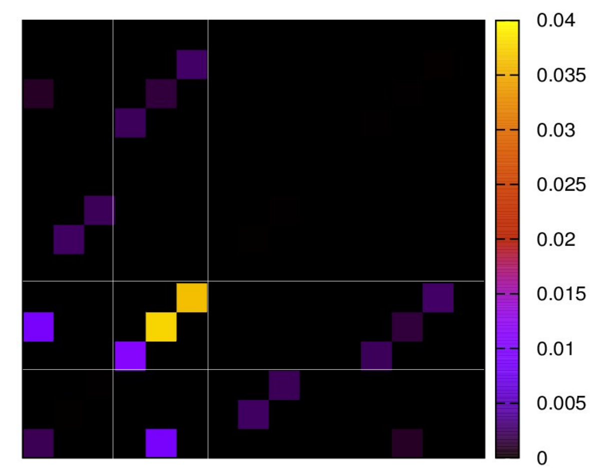
Global iteration 2, after equation 1



$^{28}Ne_{18}$



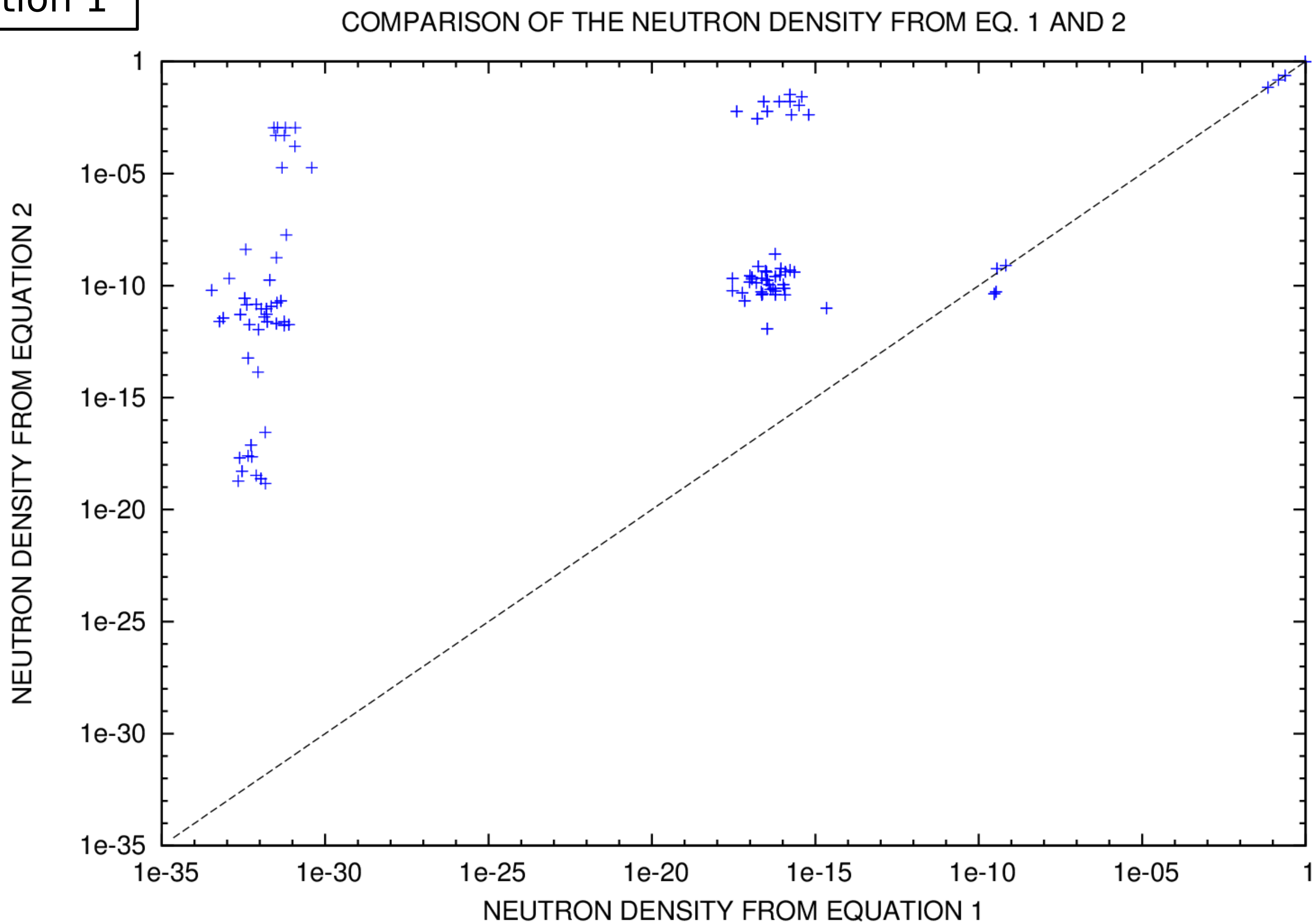




✷ Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

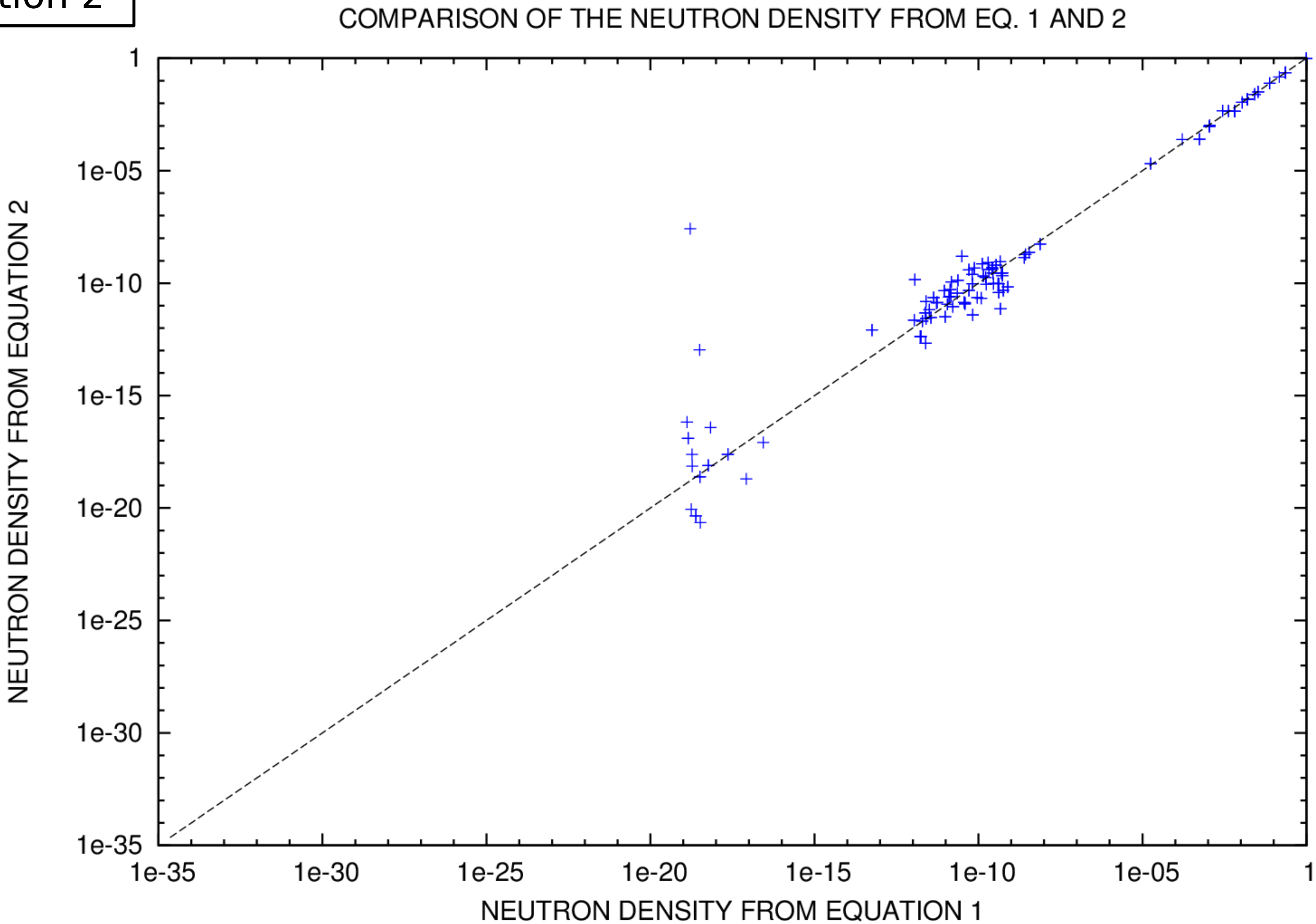
Iteration 1



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

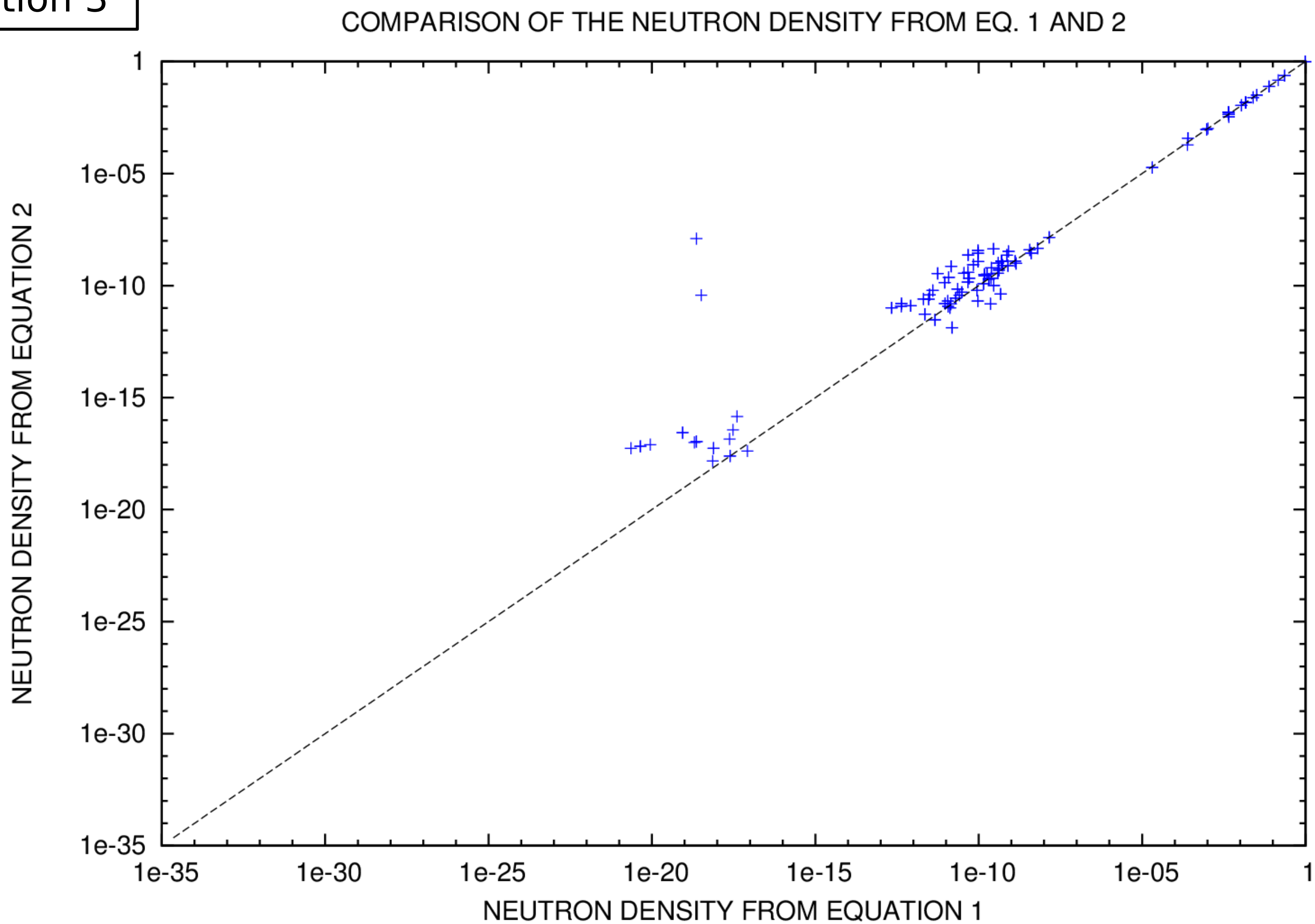
Iteration 2



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

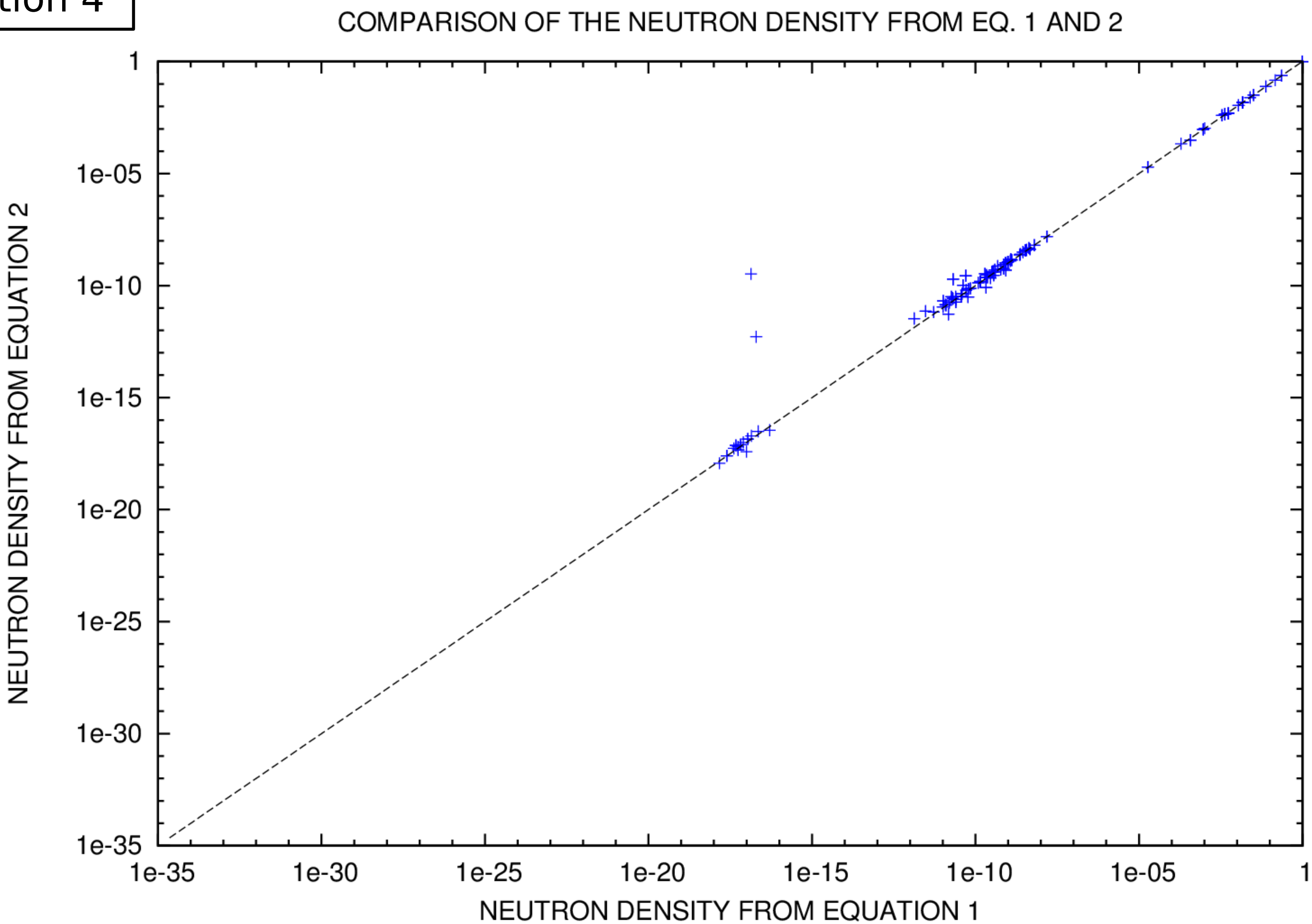
Iteration 3



Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

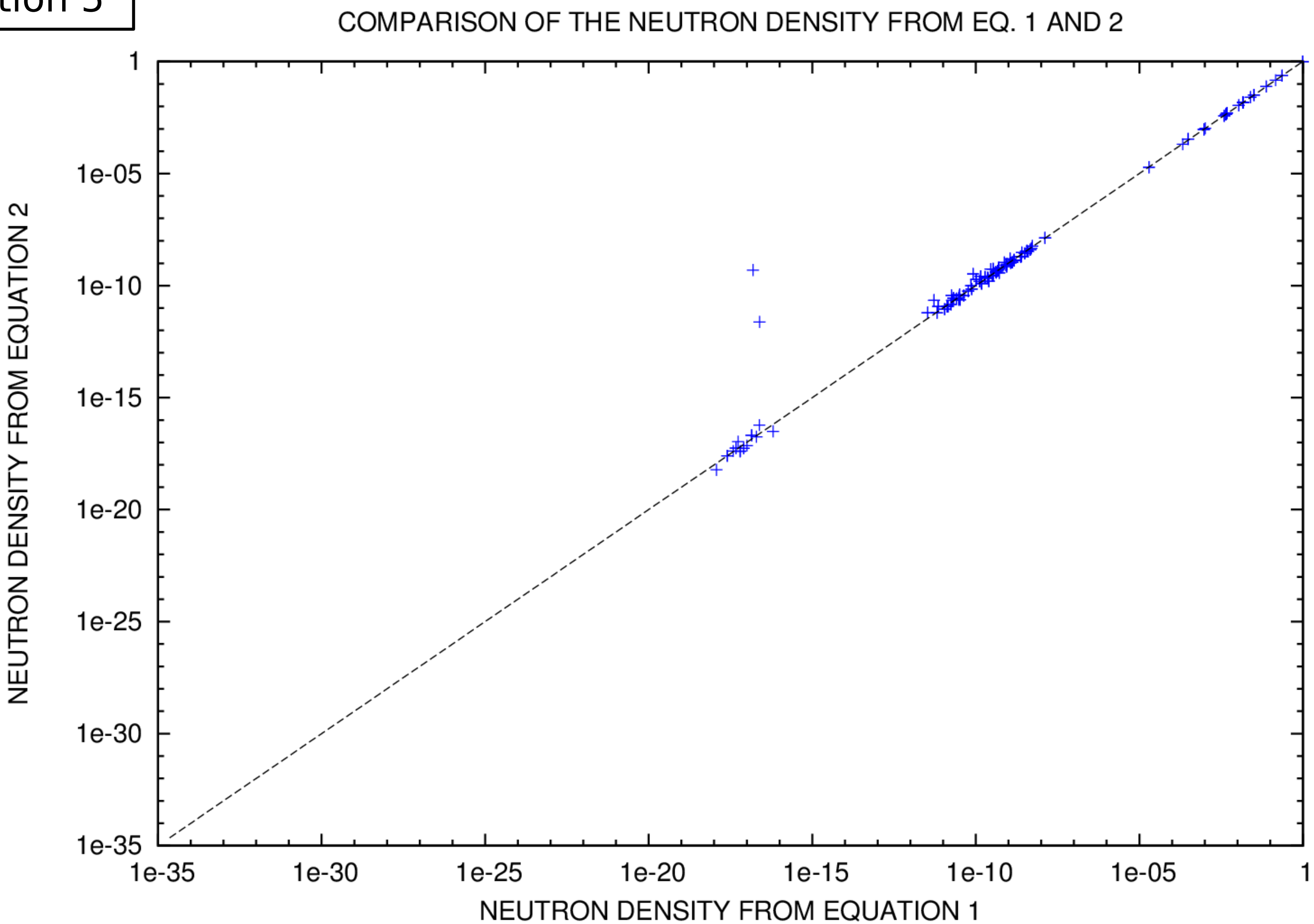
Iteration 4



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

Iteration 5



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

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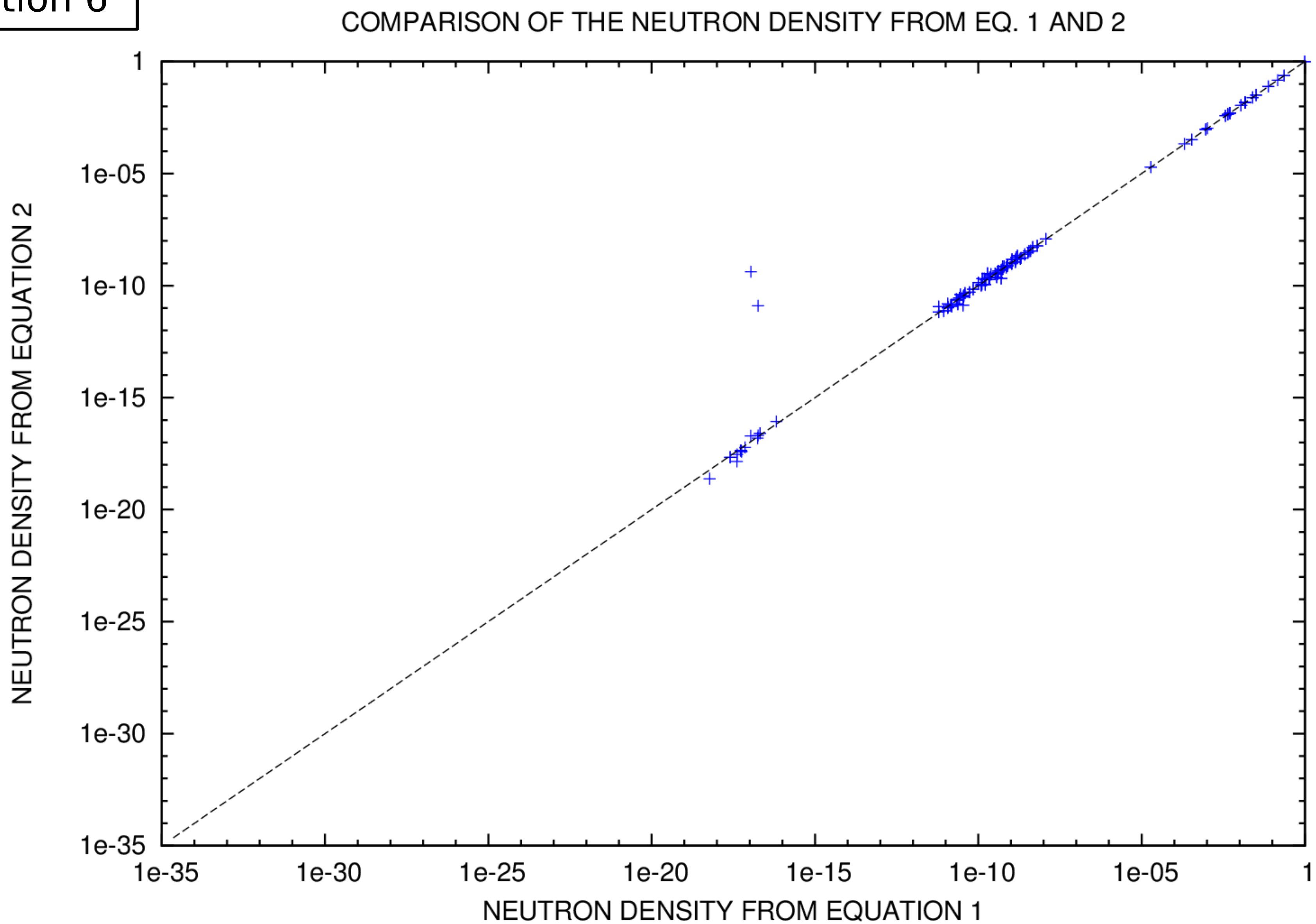
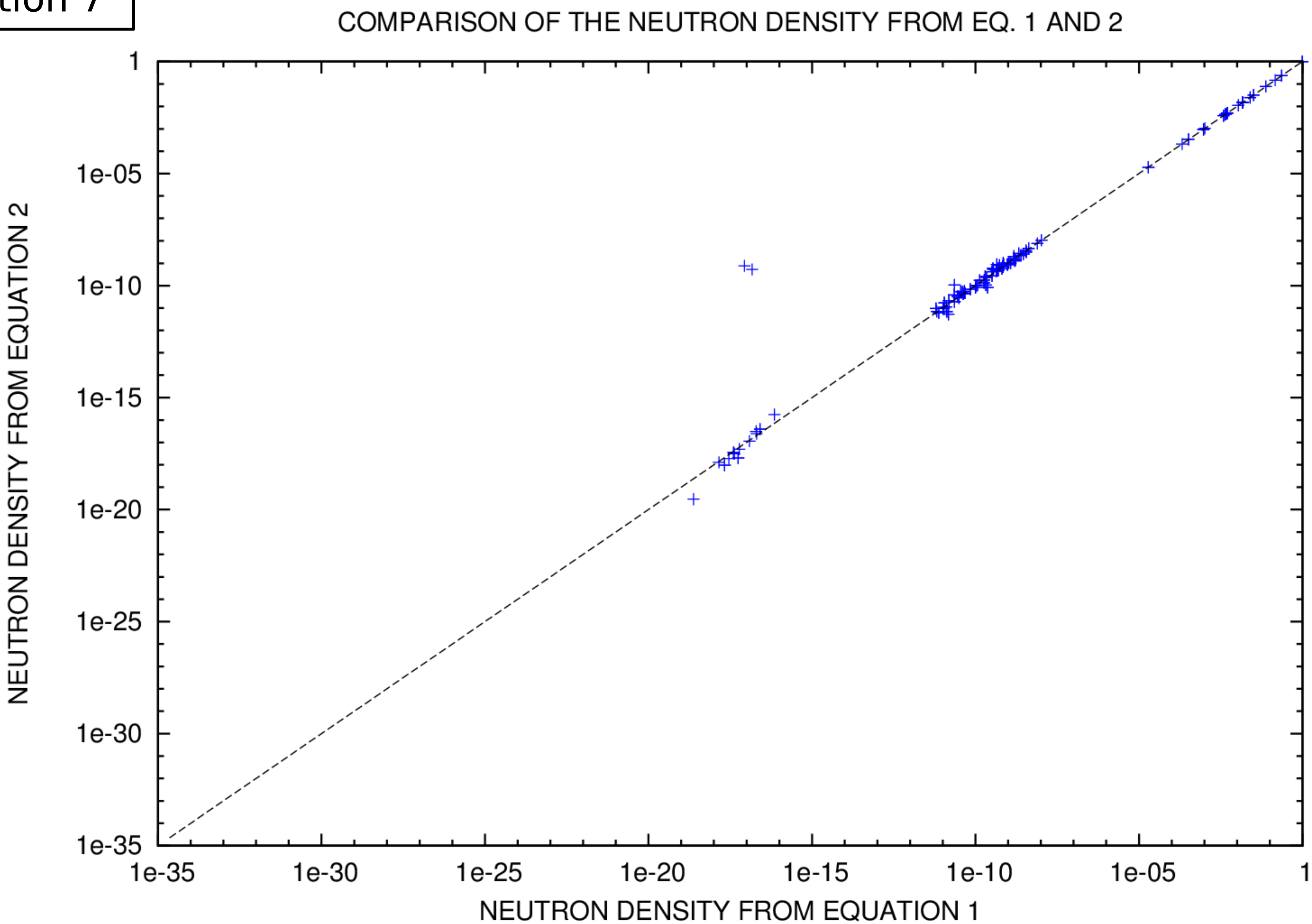
Iteration 6



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

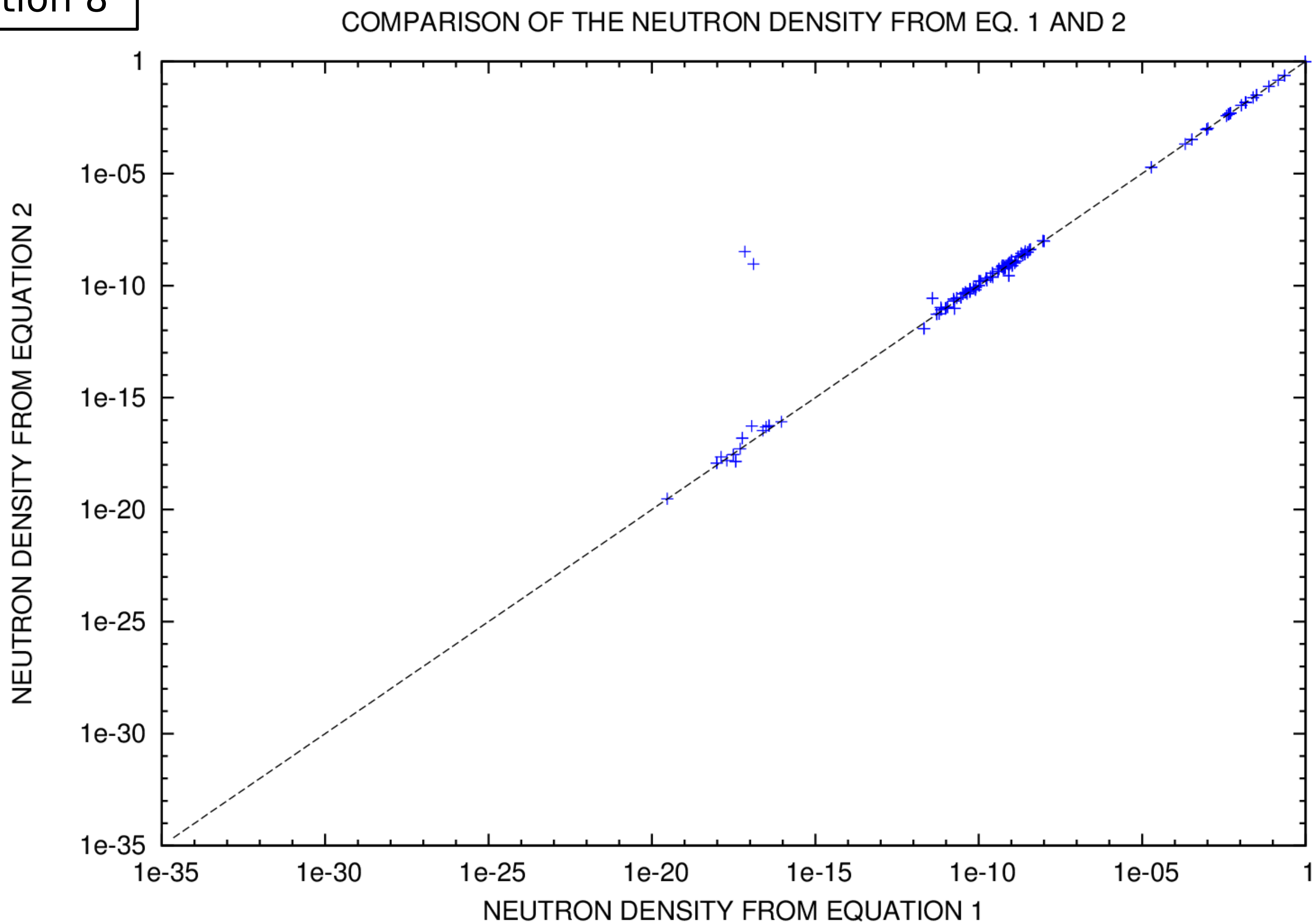
Iteration 7



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

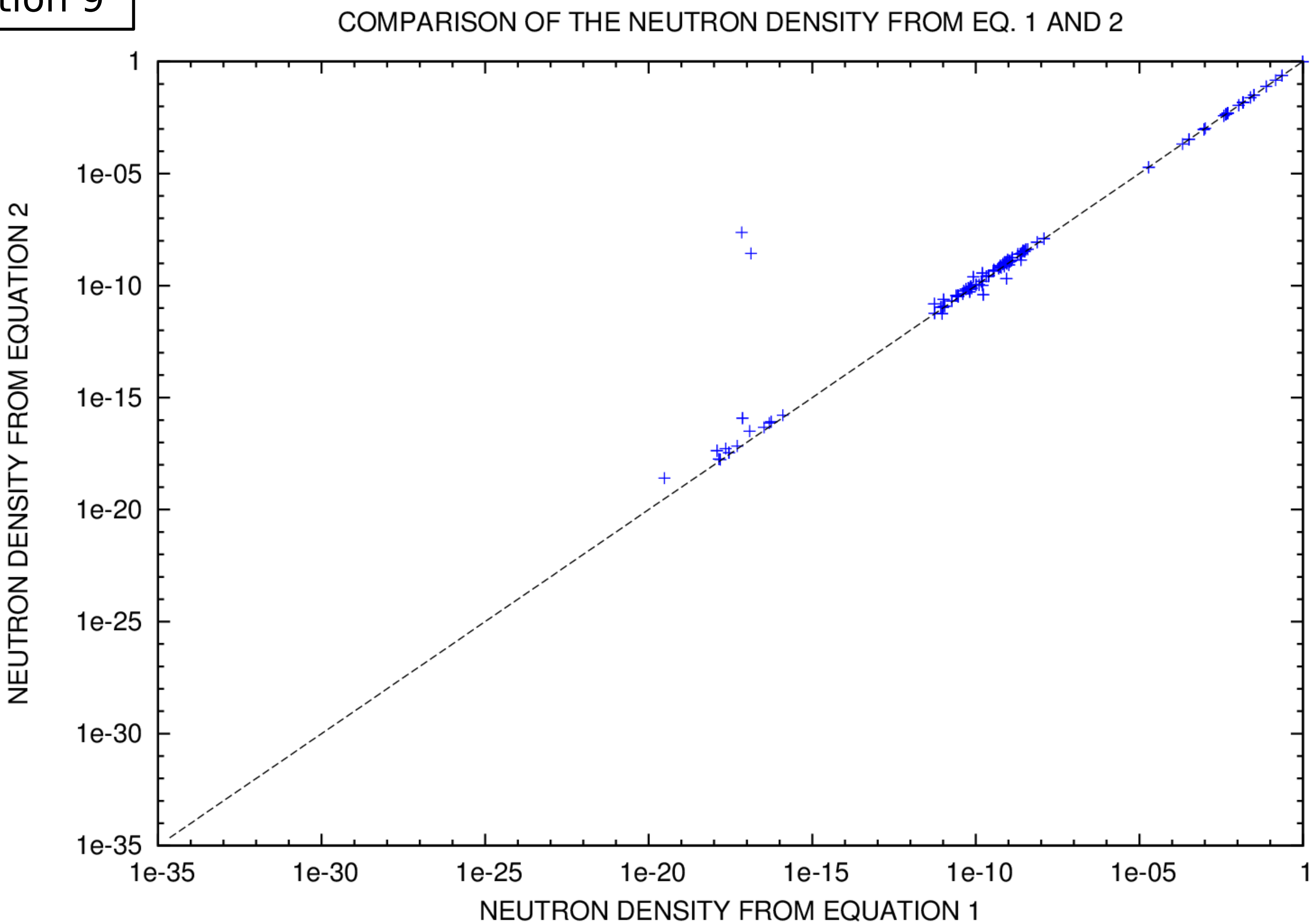
Iteration 8



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

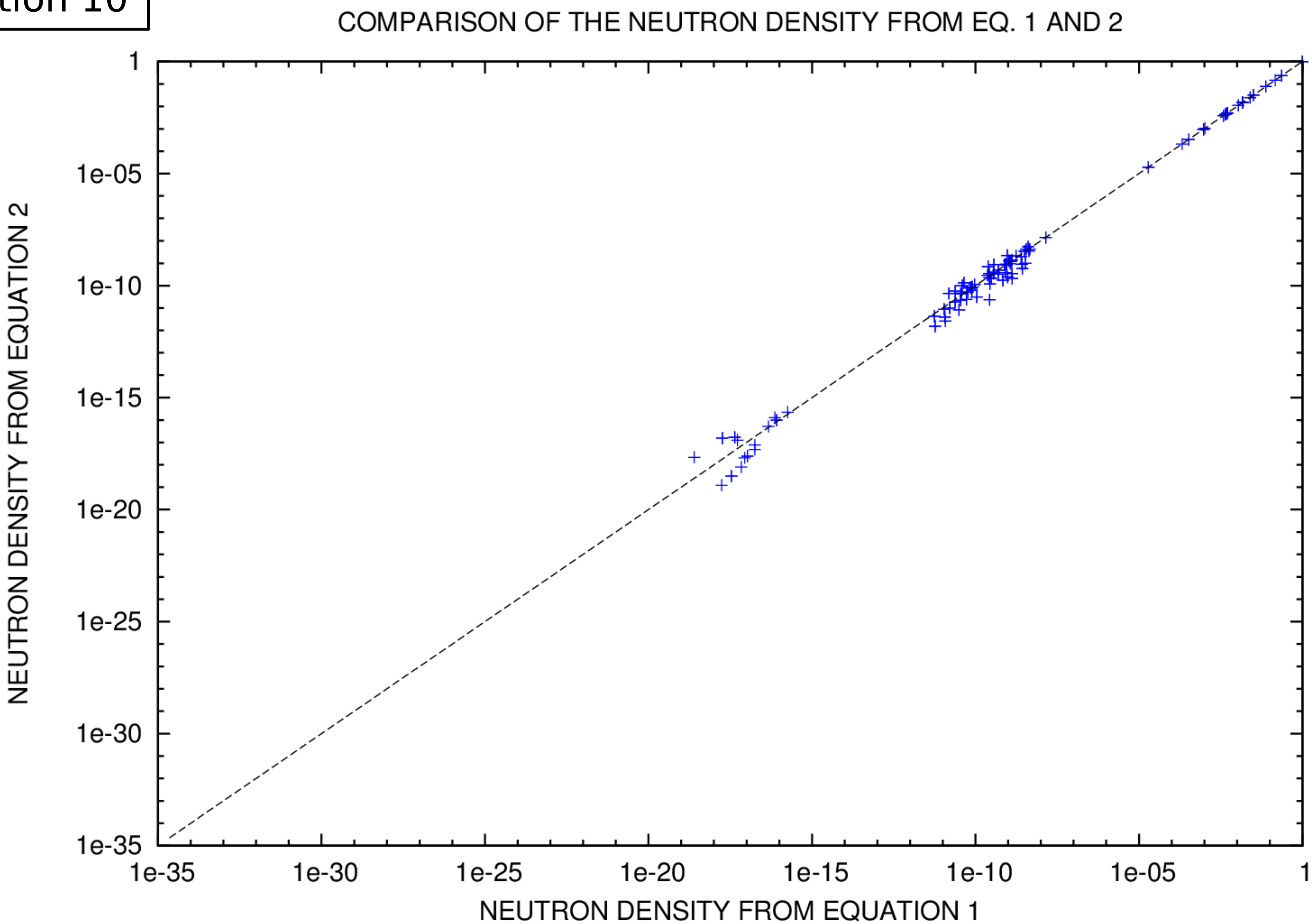
Iteration 9



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

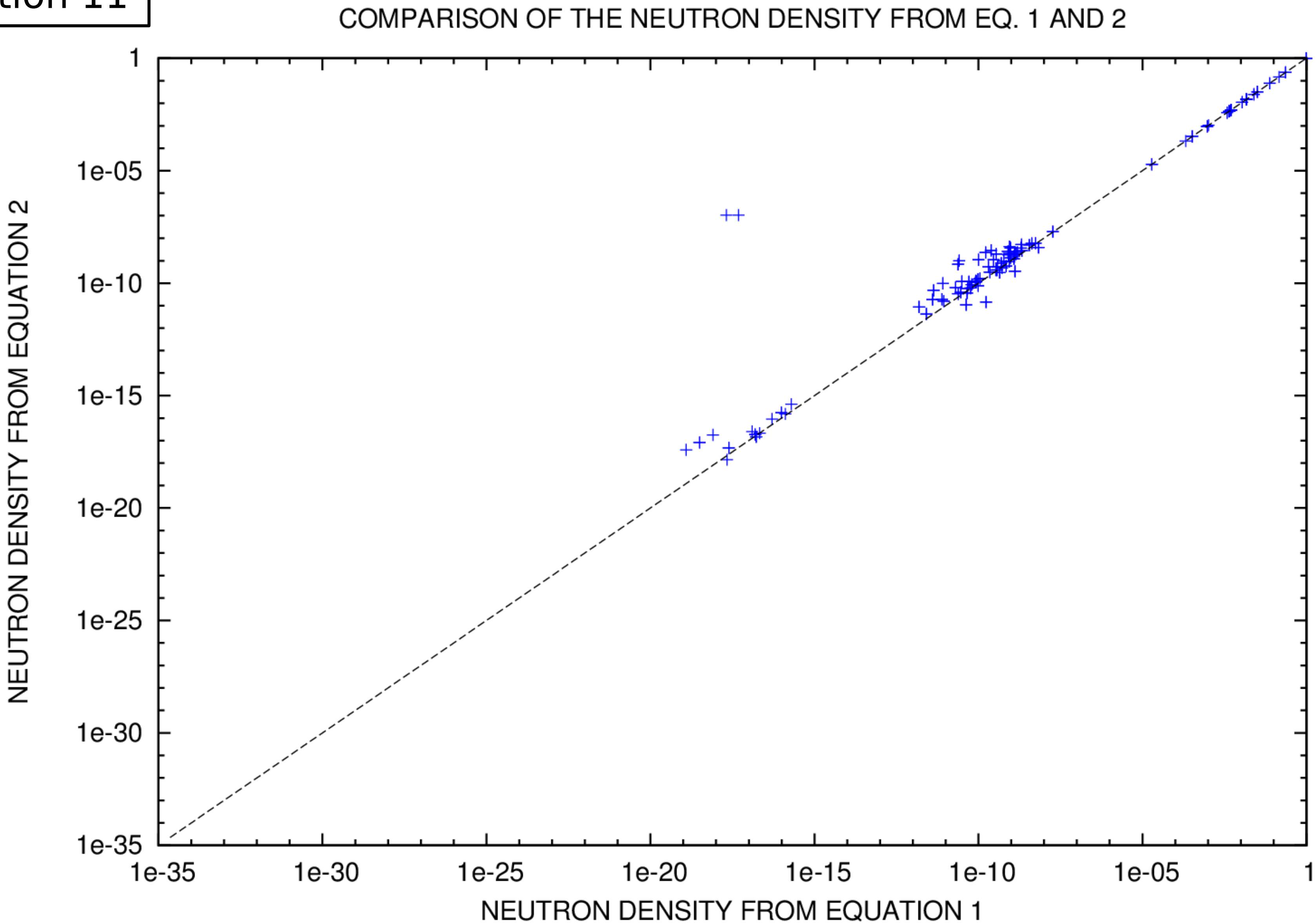
Iteration 10



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

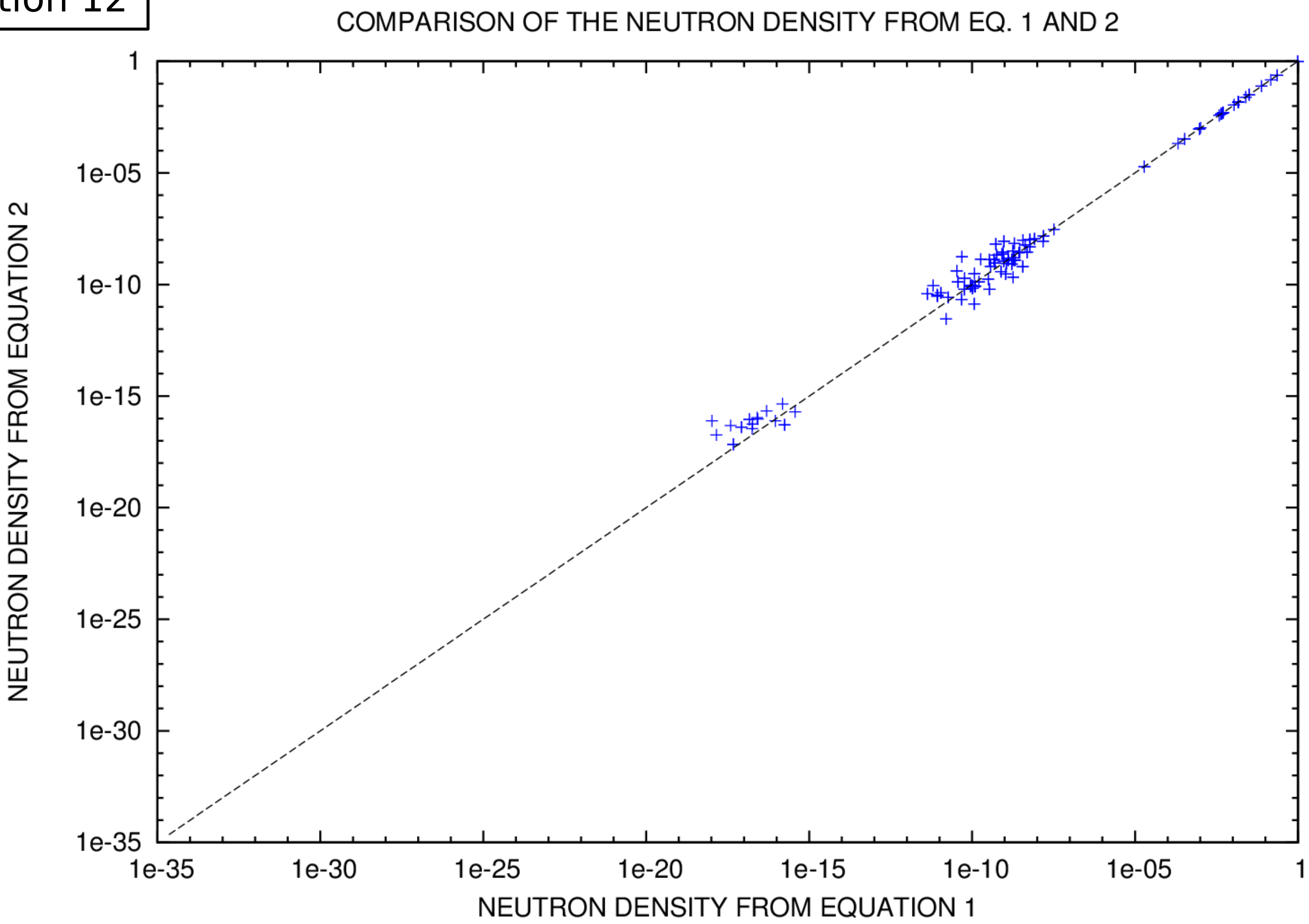
Iteration 11



Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

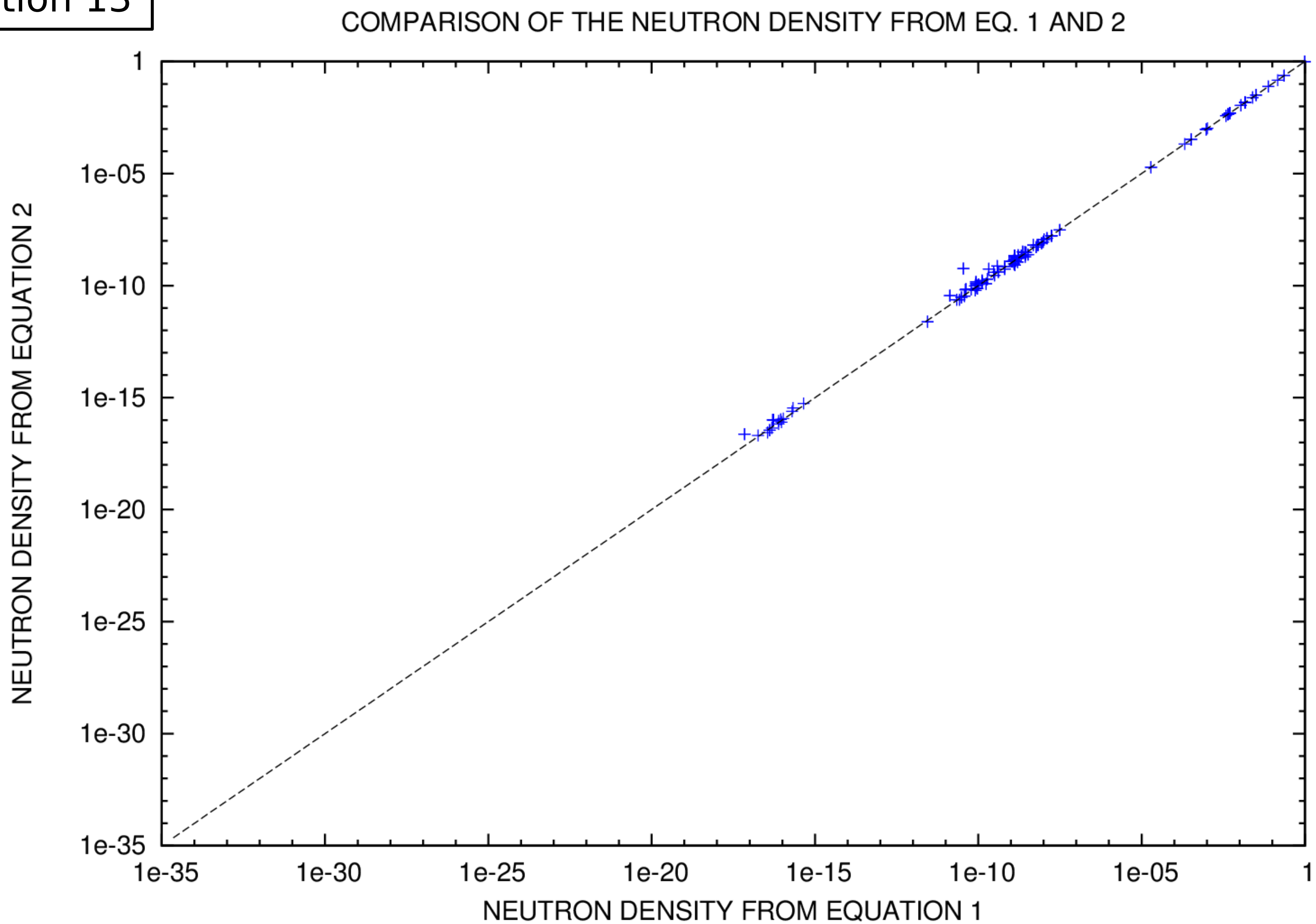
Iteration 12



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

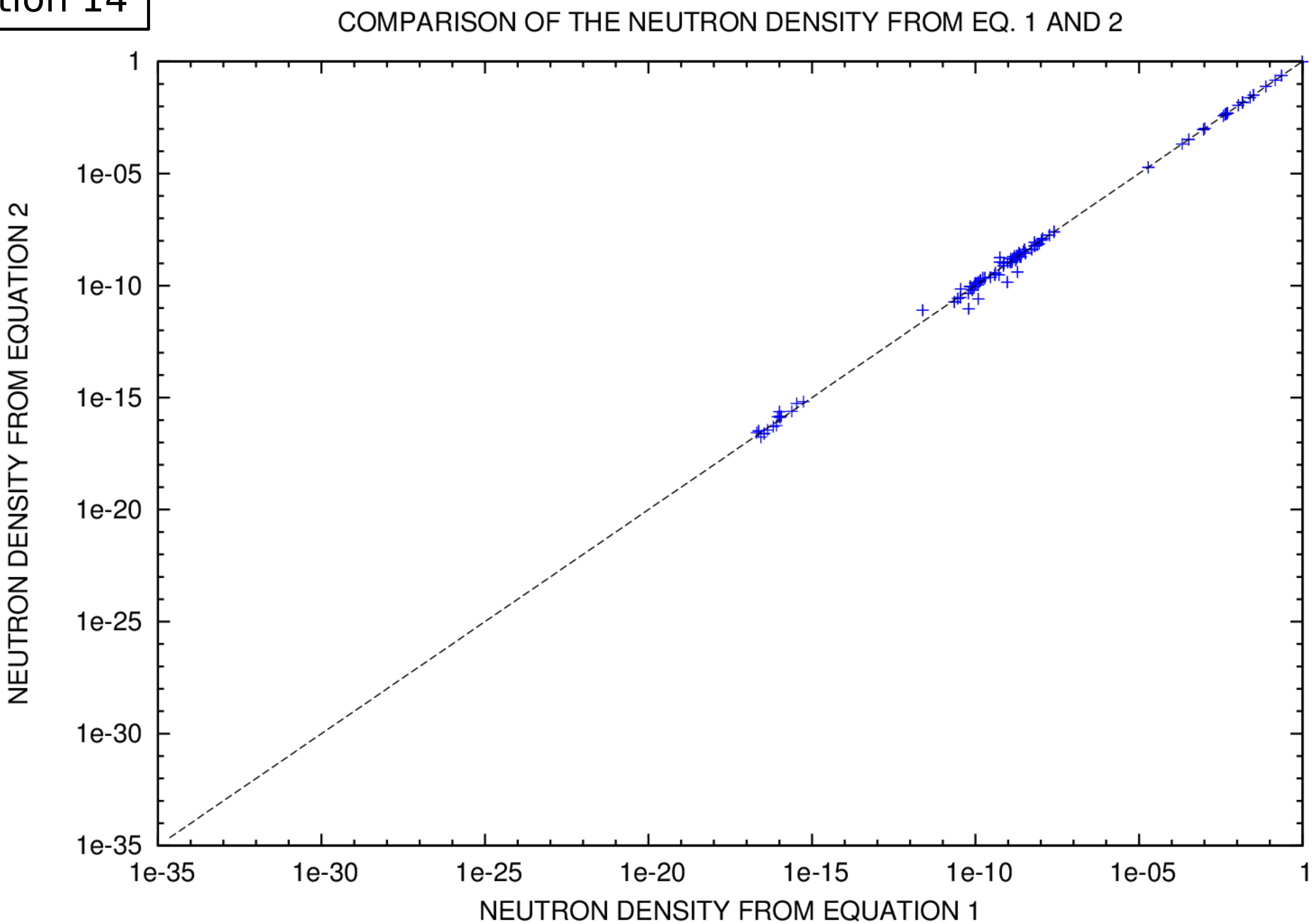
Iteration 13



✷ Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

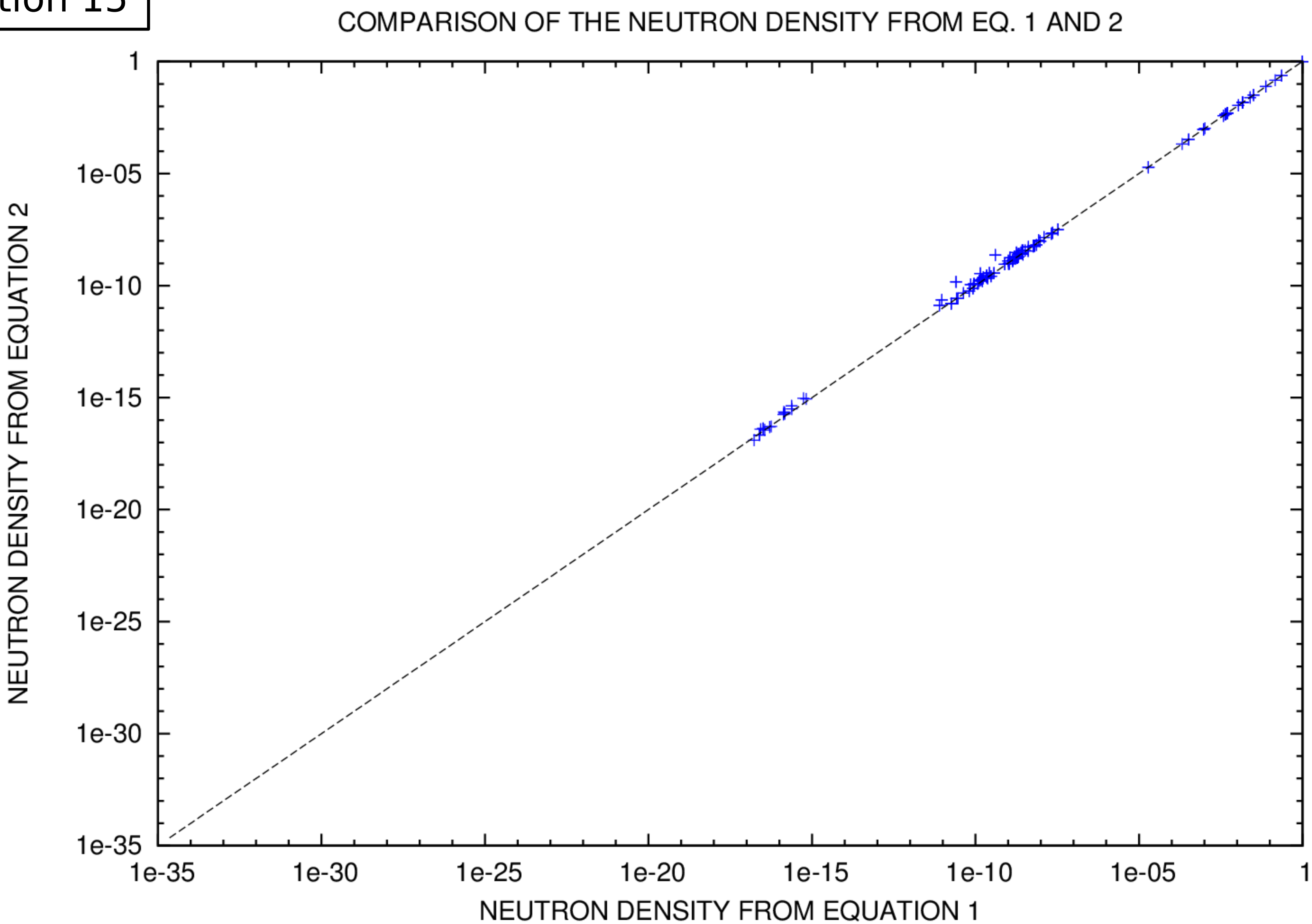
Iteration 14



Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

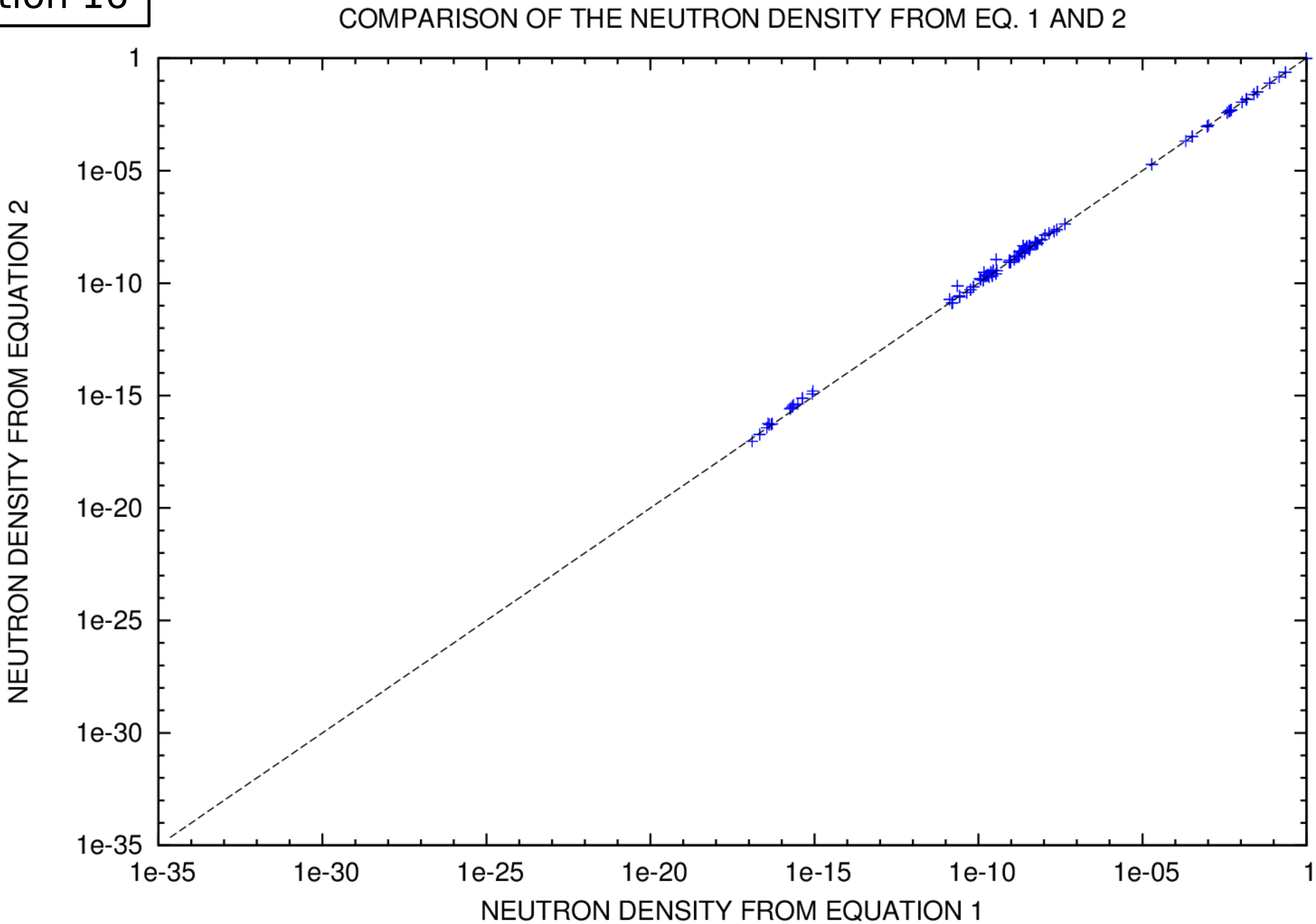
Iteration 15



✷ Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

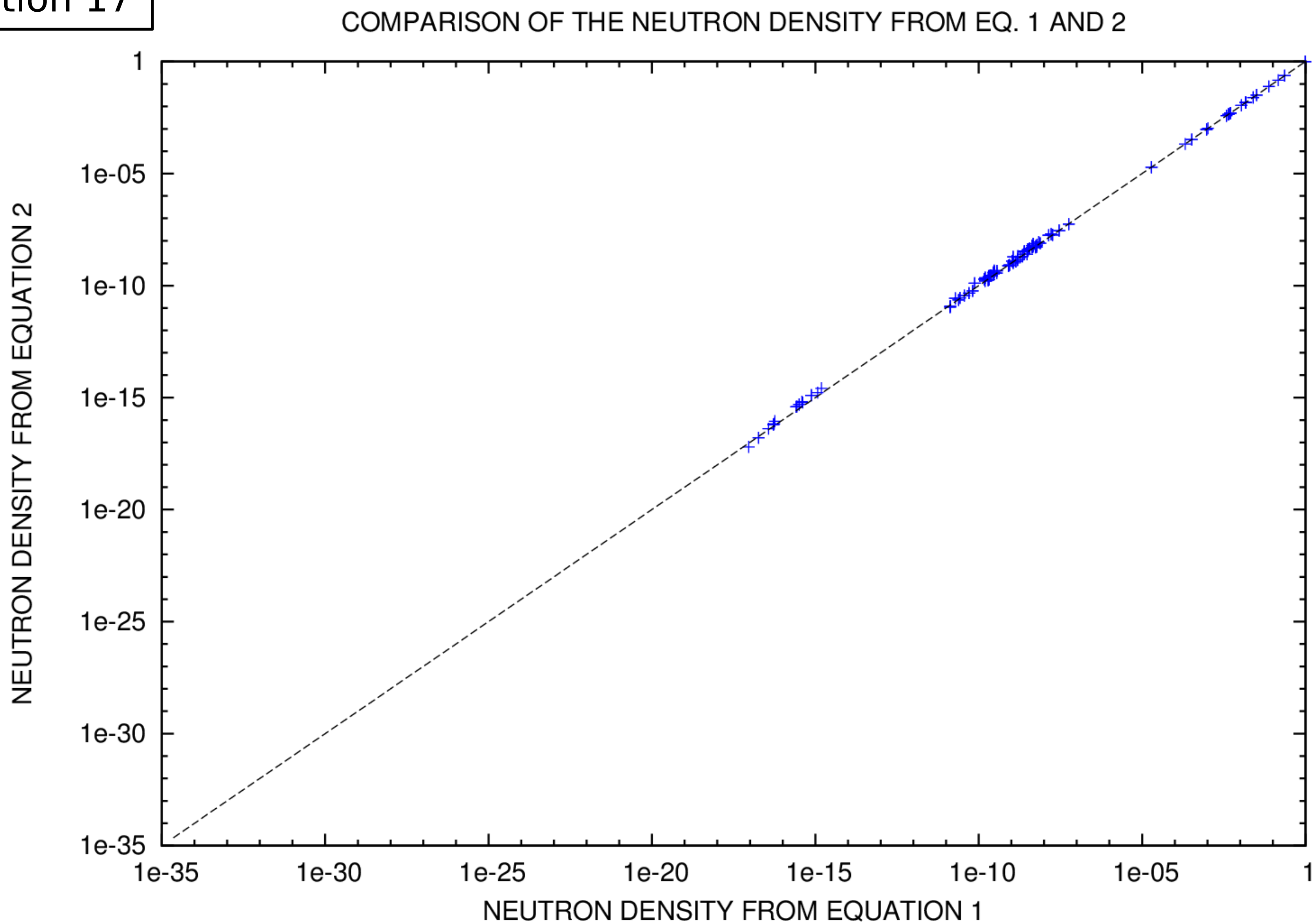
Iteration 16



✷ Preliminary results for the 2nd equation: [h(ρ,σ),ρ]=g(σ)

- Convergence of the density matrix: (Case of ^{20}Ne)

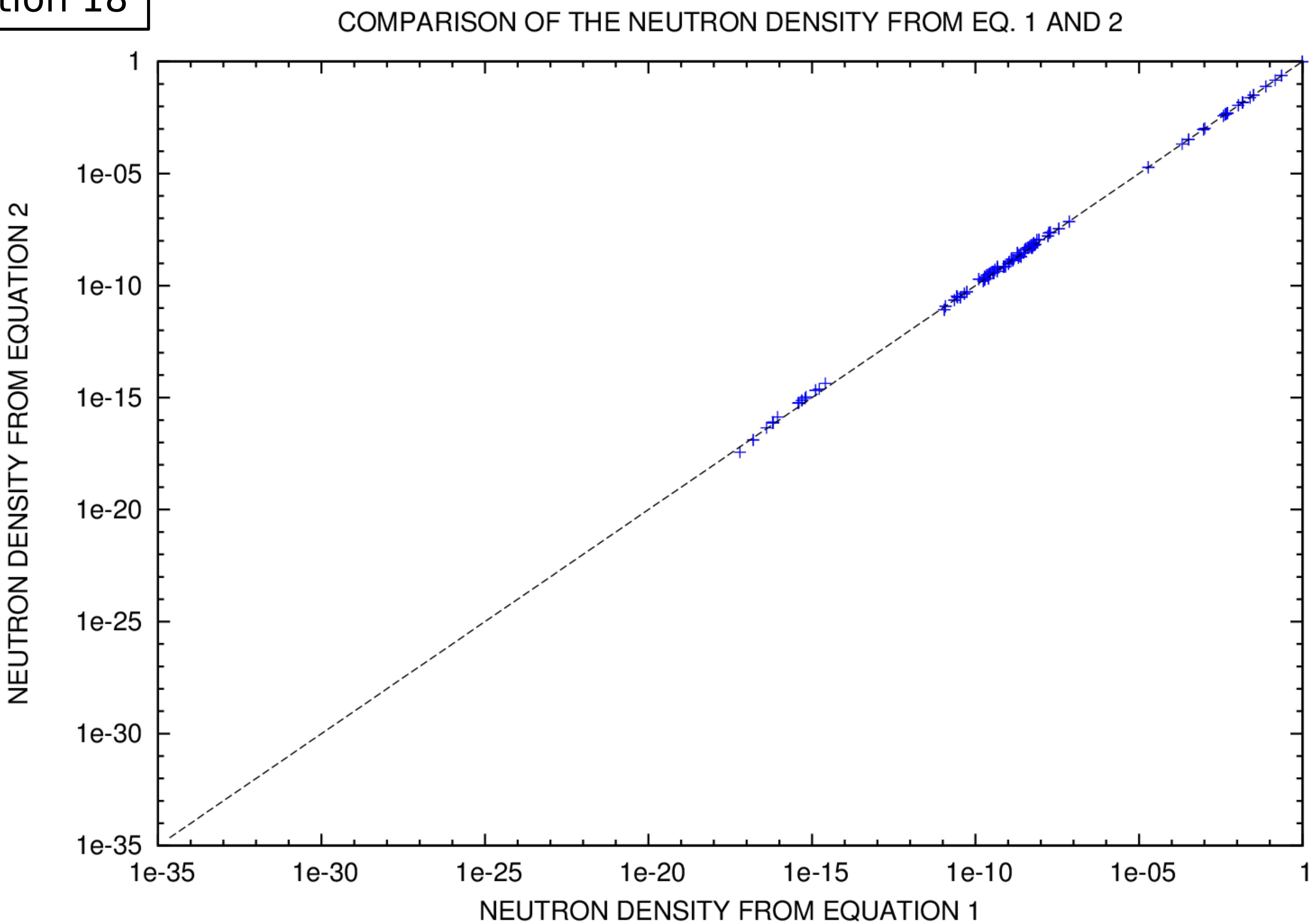
Iteration 17



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

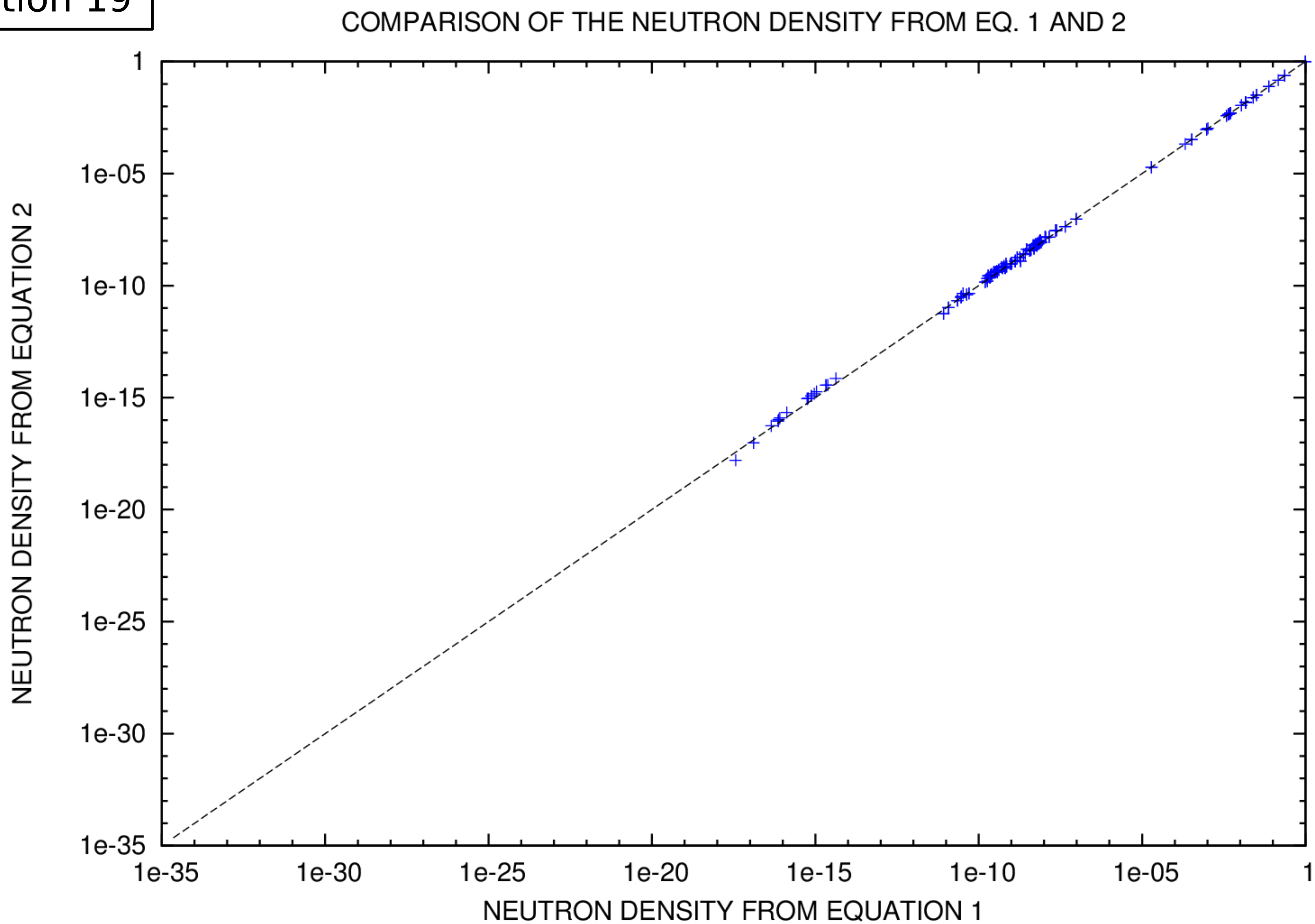
Iteration 18



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

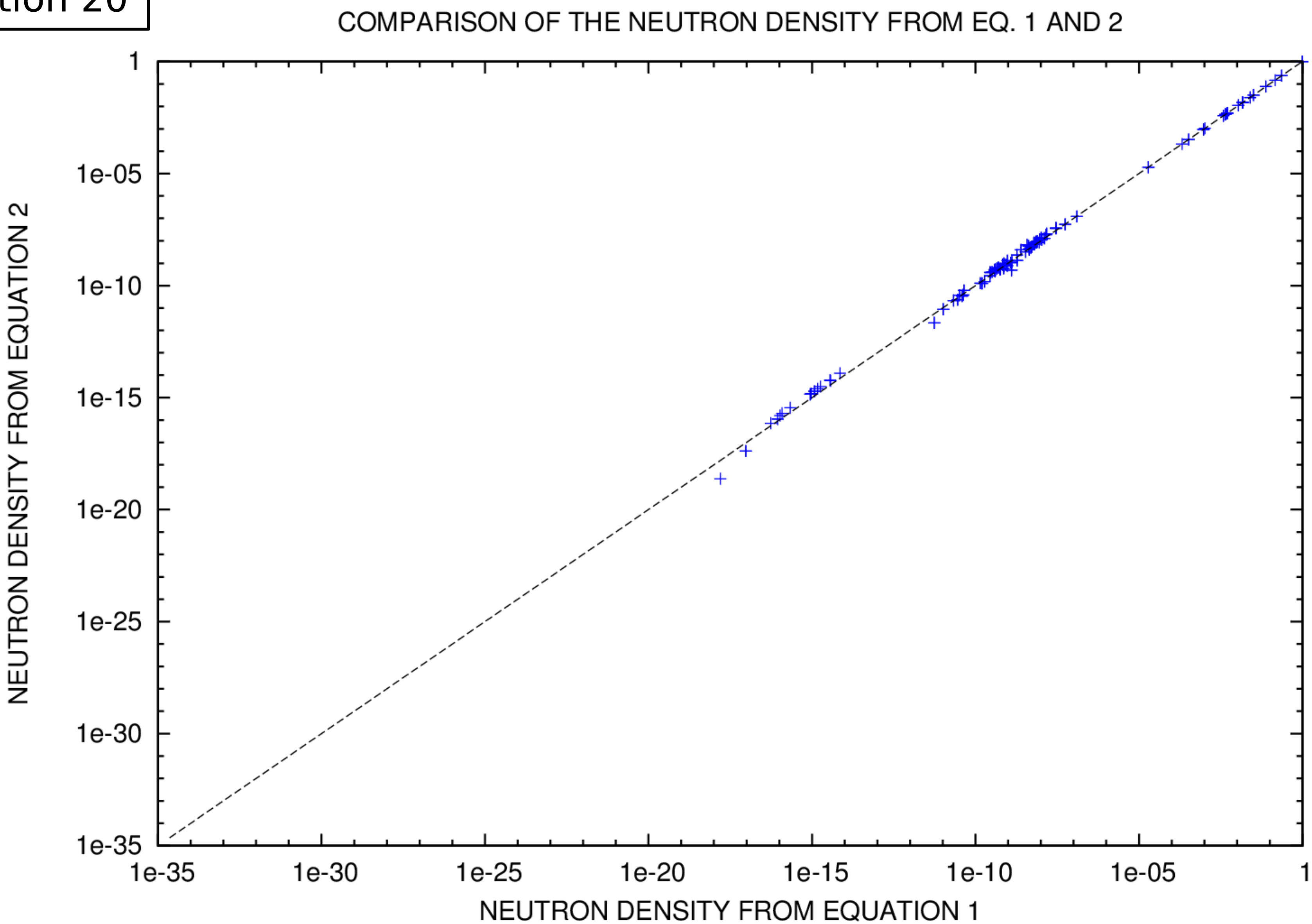
Iteration 19



✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

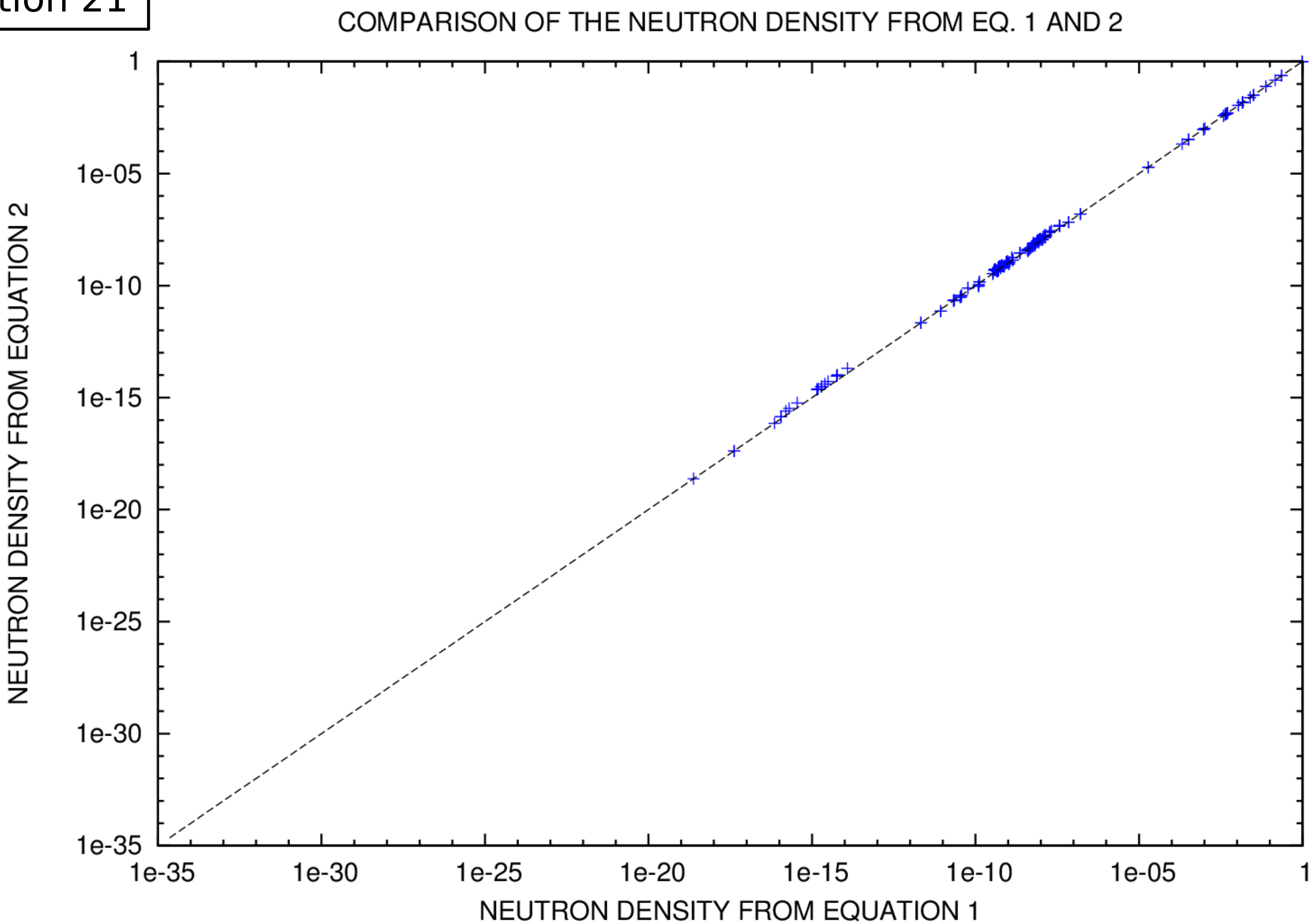
Iteration 20



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence of the density matrix: (Case of ^{20}Ne)

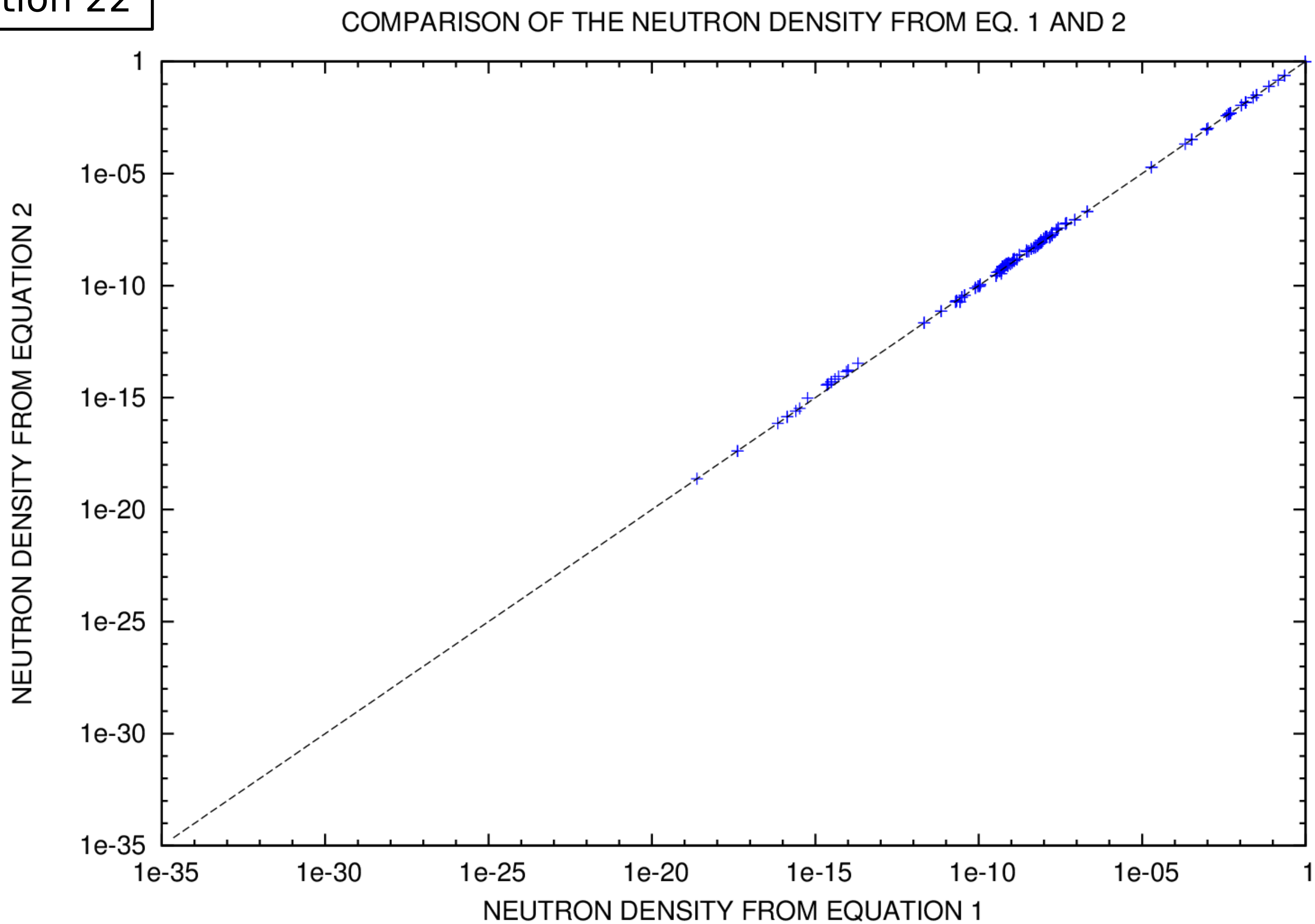
Iteration 21



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

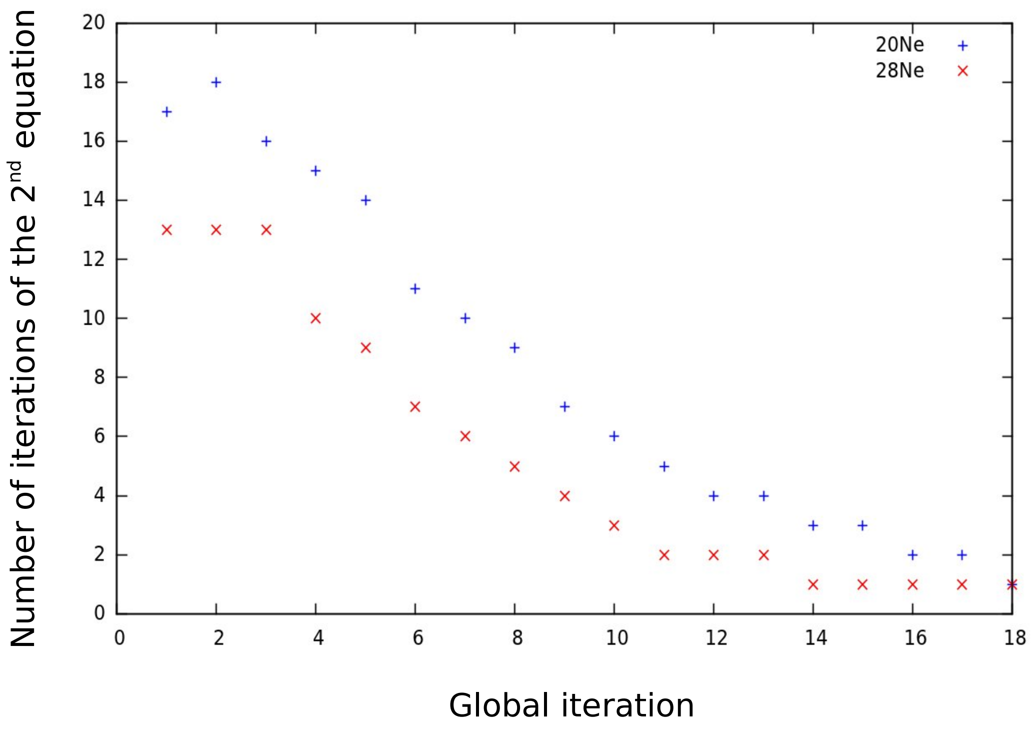
- Convergence of the density matrix: (Case of ^{20}Ne)

Iteration 22



Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Convergence process:



Global iteration	# iterations 2nd equation	
	^{20}Ne	^{28}Ne
1	17	13
2	18	13
3	16	13
4	15	10
5	14	9
6	11	7
7	10	6
8	9	5
9	7	4
10	6	3
11	5	2
12	4	2
13	4	2
14	3	1
15	3	1
16	2	1
17	2	1
18	1	1

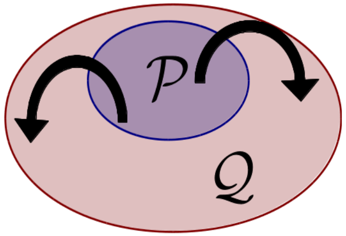
✷ Preliminary results for the 2nd equation: $[h(\rho,\sigma),\rho]=g(\sigma)$

- Consideration of the Q space:

Each configuration in the final valence space can be expanded on the full basis of Slater determinants built on the HF orbitals:

$$|\phi_\alpha^{final}\rangle = \sum_{\beta\in(\mathcal{P}+\mathcal{Q})} C_{\alpha\beta}|\phi_\beta^{HF}\rangle$$

~10^{14}-10^{16} terms!
(5 HO shells)



➡ ~10^3 configurations (^{20}Ne) in the new s-d valence space simulates ~10^{17}-10^{19} Slaters built on the whole HF basis

Outline

- Introduction
- Formalism
  - First equation: Mixing coefficients
  - Second equation: Single-particle orbitals
- Resolution technique
- Preliminary results: test cases
- Conclusion, prospects

Conclusion, prospects

Today:

- Self-consistent solution obtained with convergence criteria $\Delta\rho \sim 10^{-7}$
- 2^{nd} orbital equation promising:

  → Propagation of correlations outside valence through the source term g(σ)
  → Absorption of correlations by the mean-field quite fast (cf # iterations)
  → Avoids diagonalization of too big matrices

To do next:

- Optimize/parallelize the code
- Impact of orbital renormalization on the description of ground and excited states, and on the collectivity (cf Julien Le Bloas' talk):

  → binding energies
  → quadrupole moments
  → Electric and magnetic transition probabilities

Later:

- Study of giant and pygmy resonances in calcium nuclei

Conclusion, prospects

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Thank you !

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