

Inizializzazione

ρ^{in}

v_{eff}

$$\{H^{KS}\}_{ij} = \langle \psi_i | \left[-\frac{\nabla^2}{2} + \hat{v}_{eff} \right] | \psi_j \rangle$$

$$\det(H^{KS} - \varepsilon I) = 0$$

$\{\psi_i\}^{out}$

ρ^{out}

$\rho^{out} \rightarrow \rho^{in}$

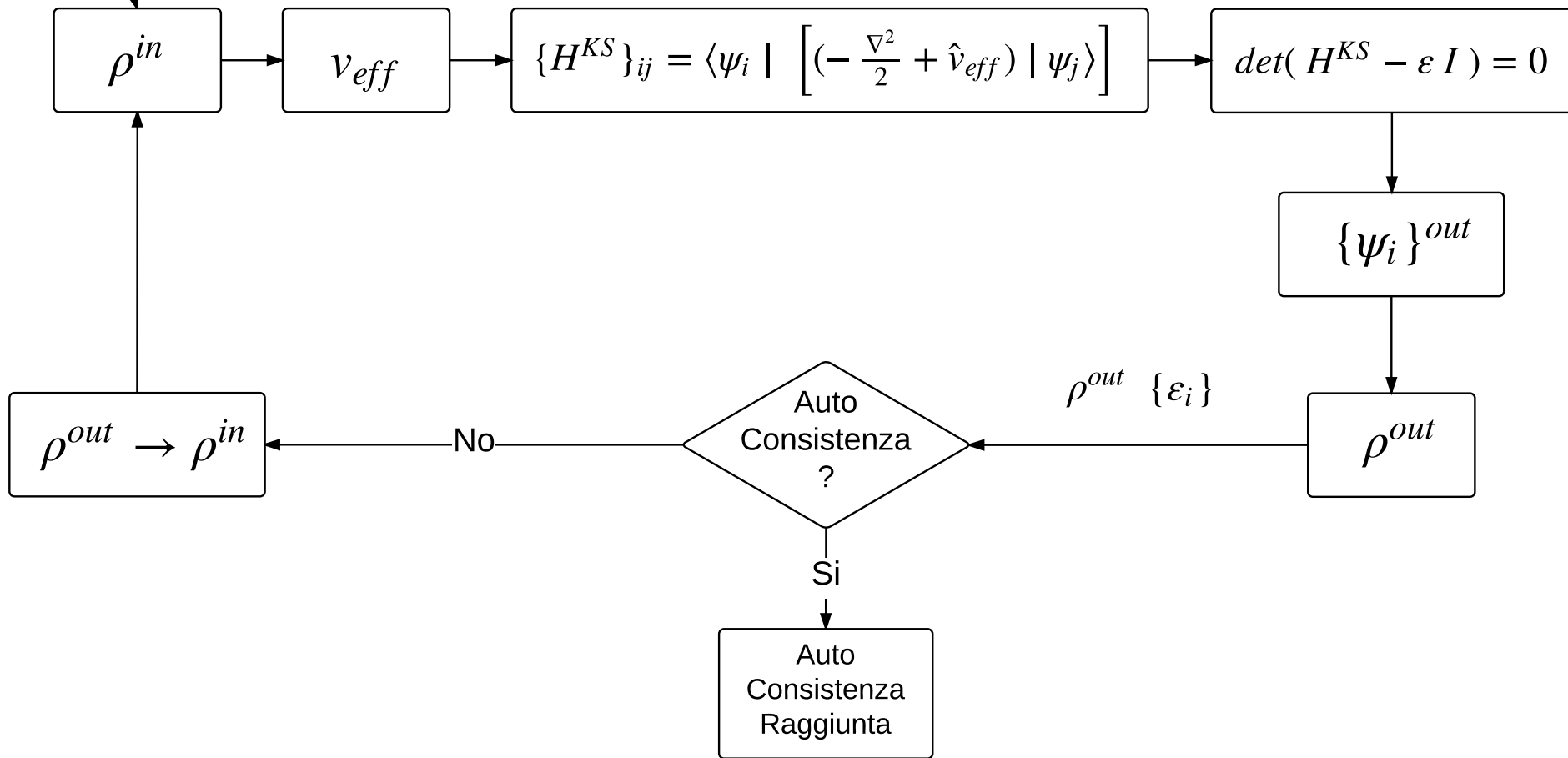
No

Auto
Consistenza
?

$\rho^{out} \quad \{\varepsilon_i\}$

Sì

Auto
Consistenza
Raggiunta



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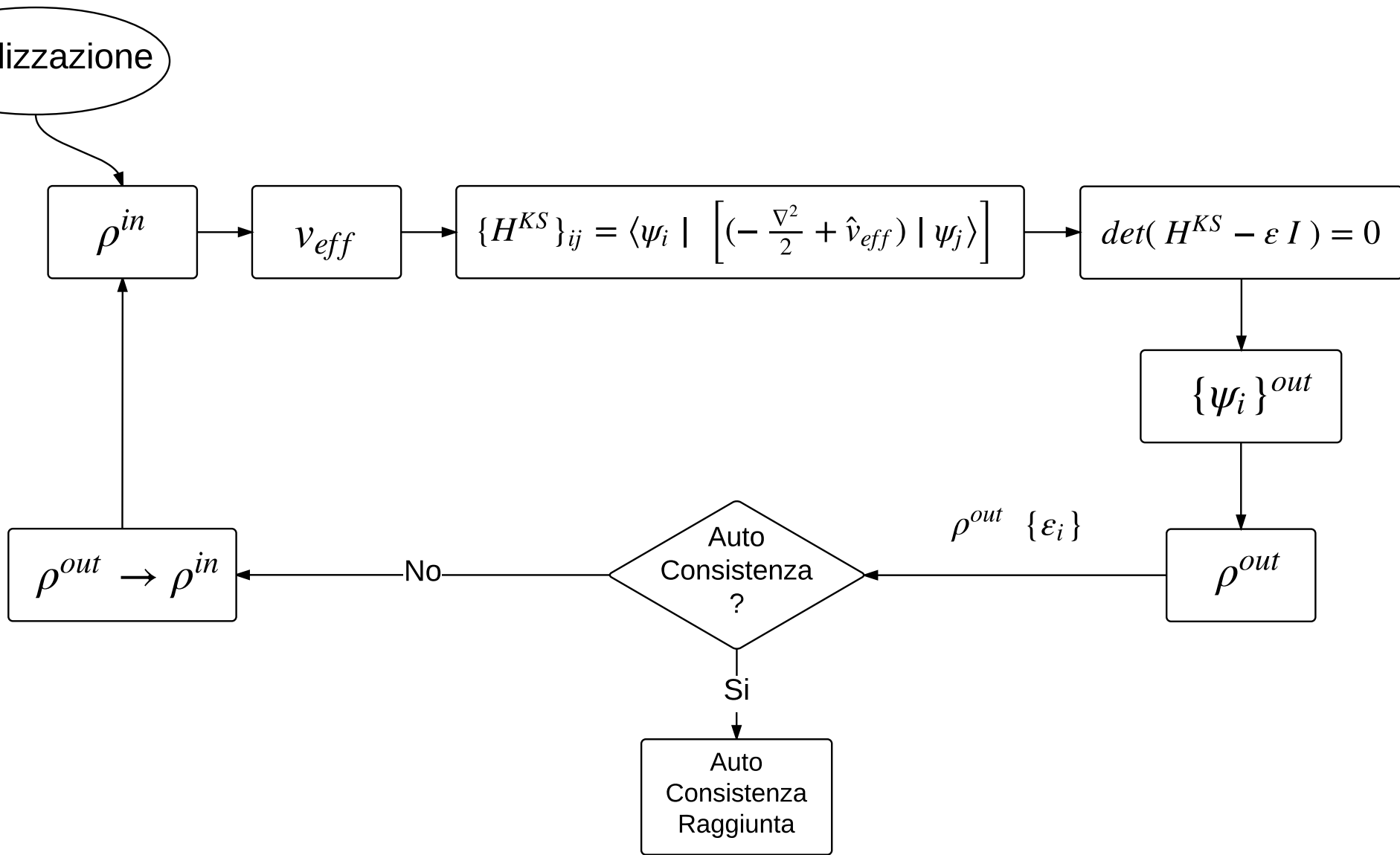
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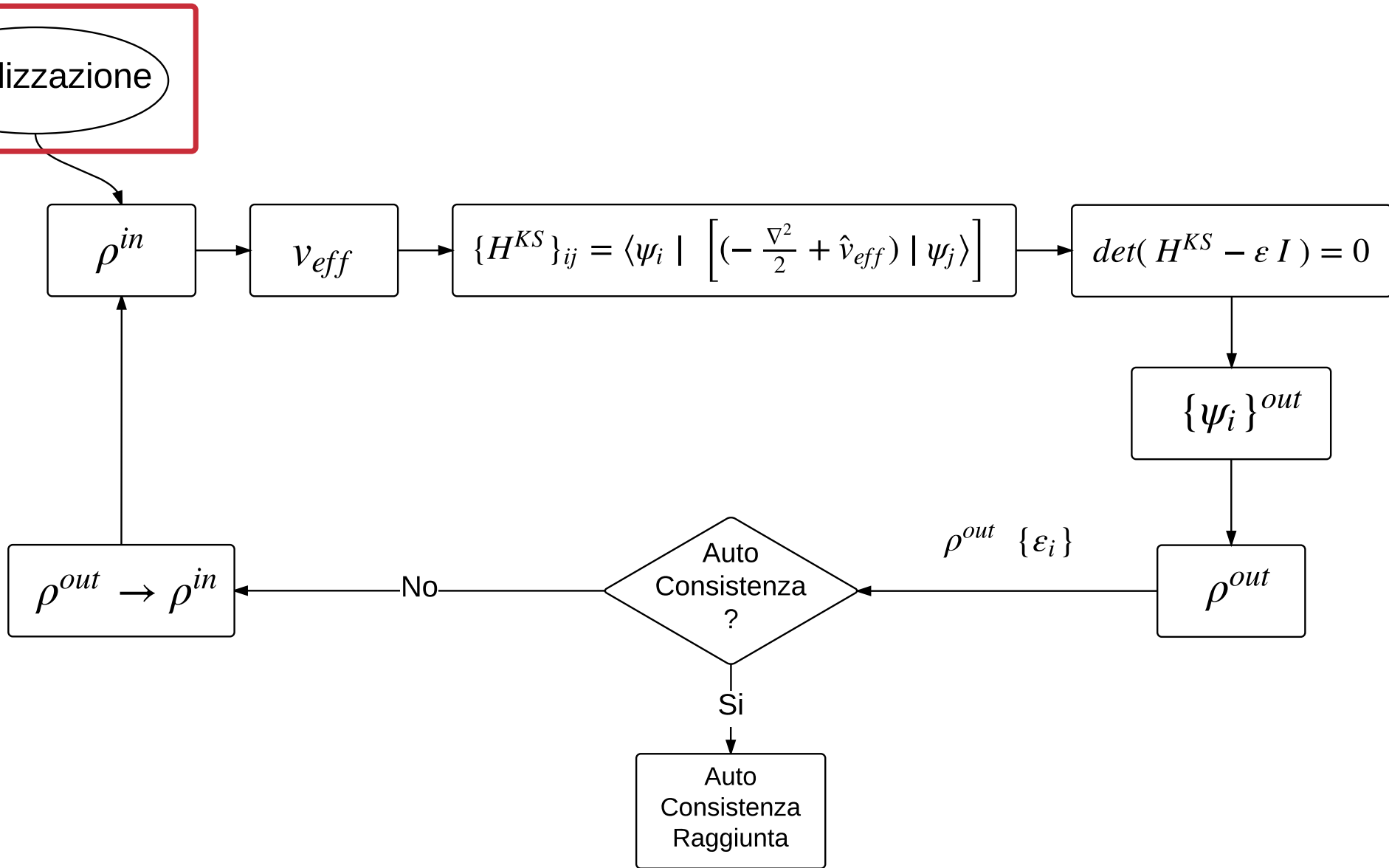
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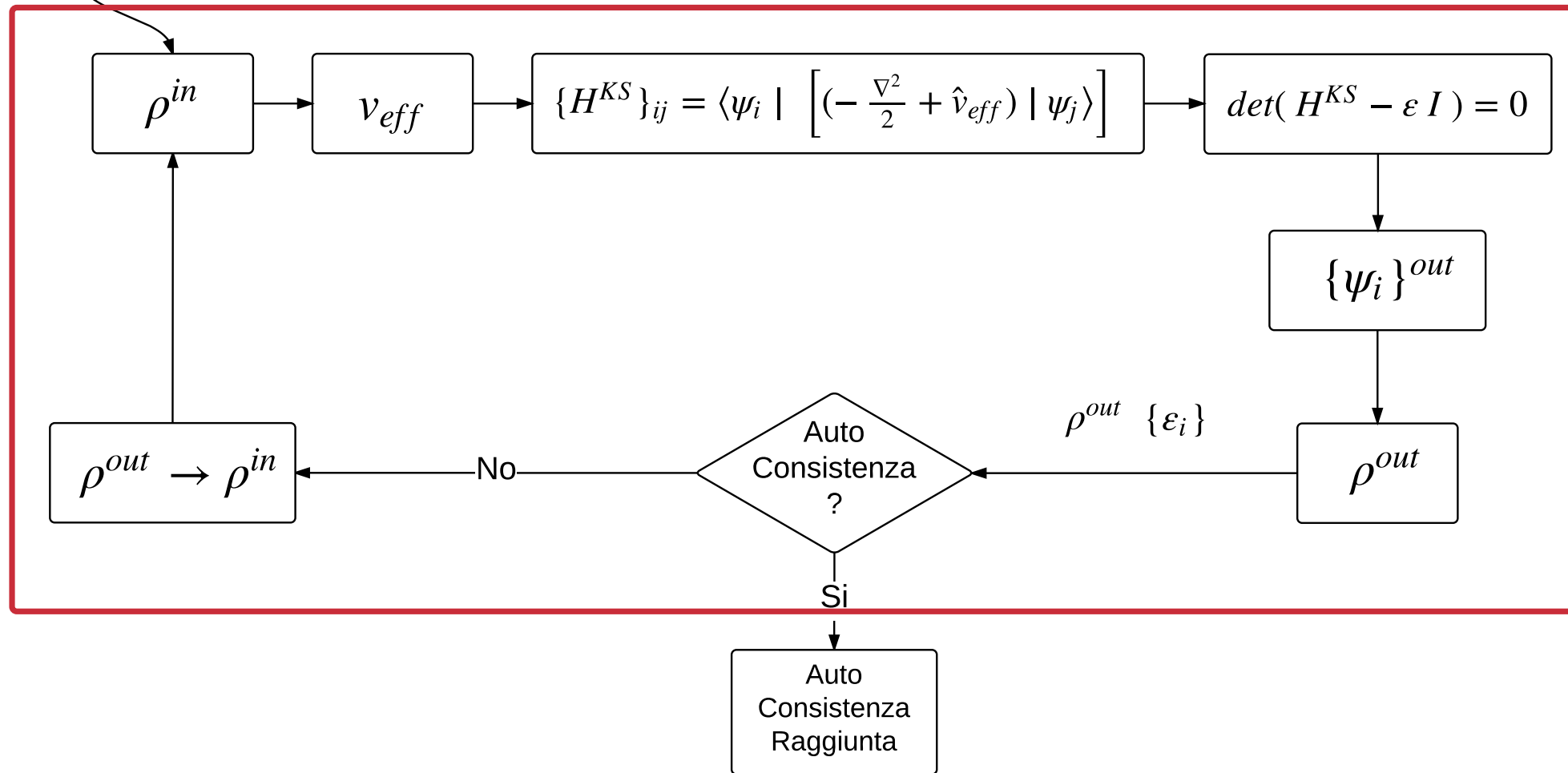
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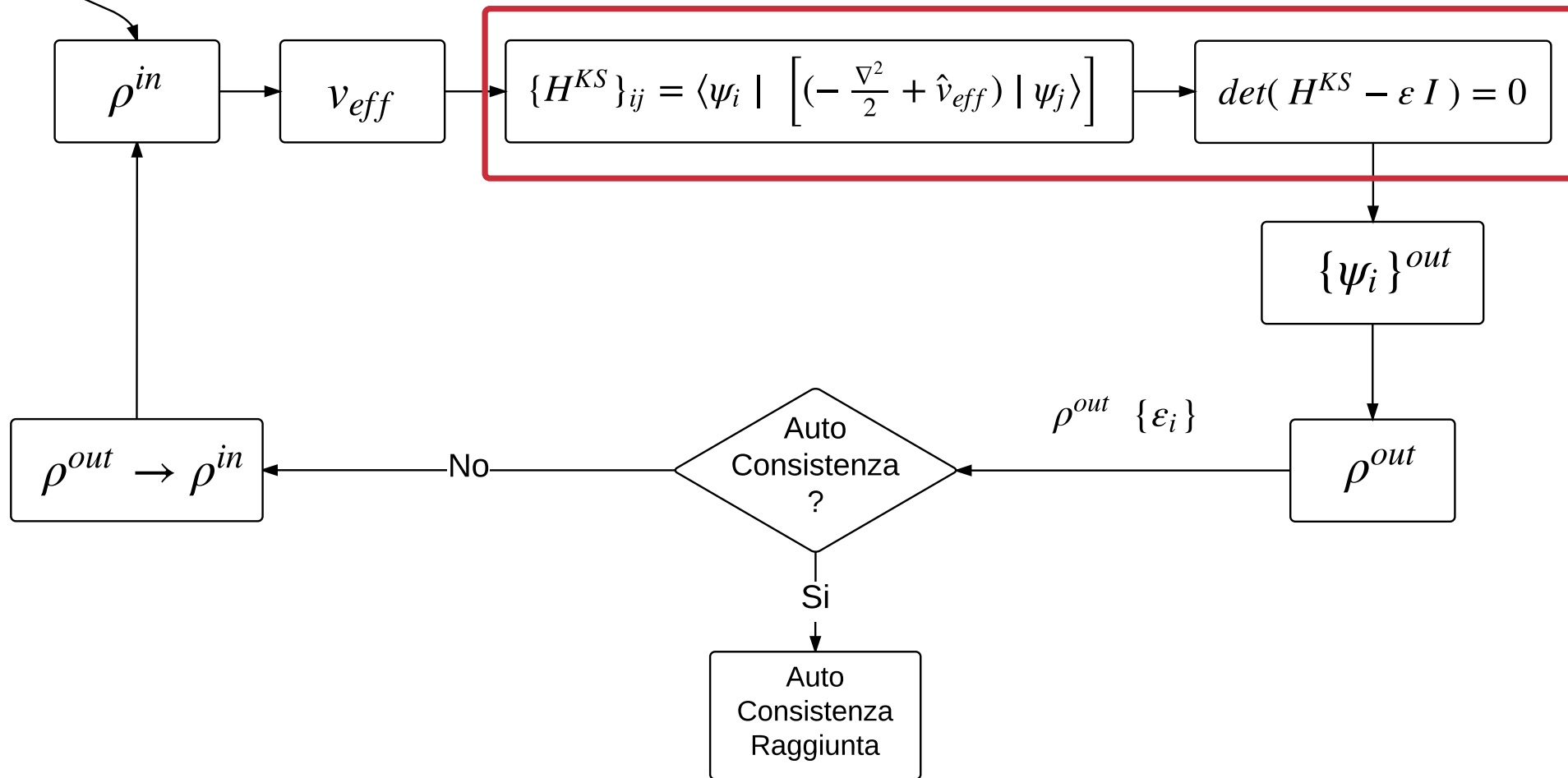
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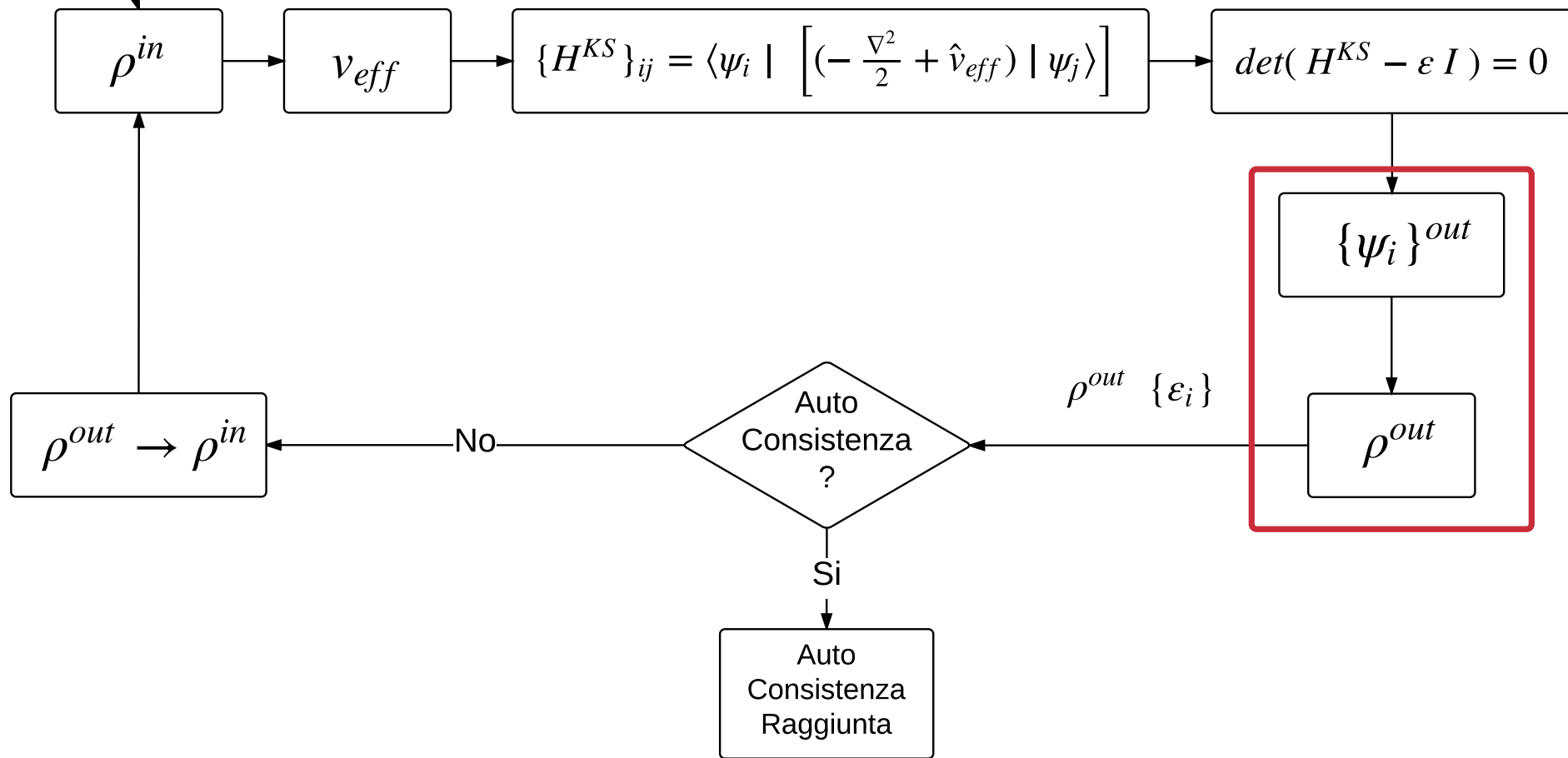
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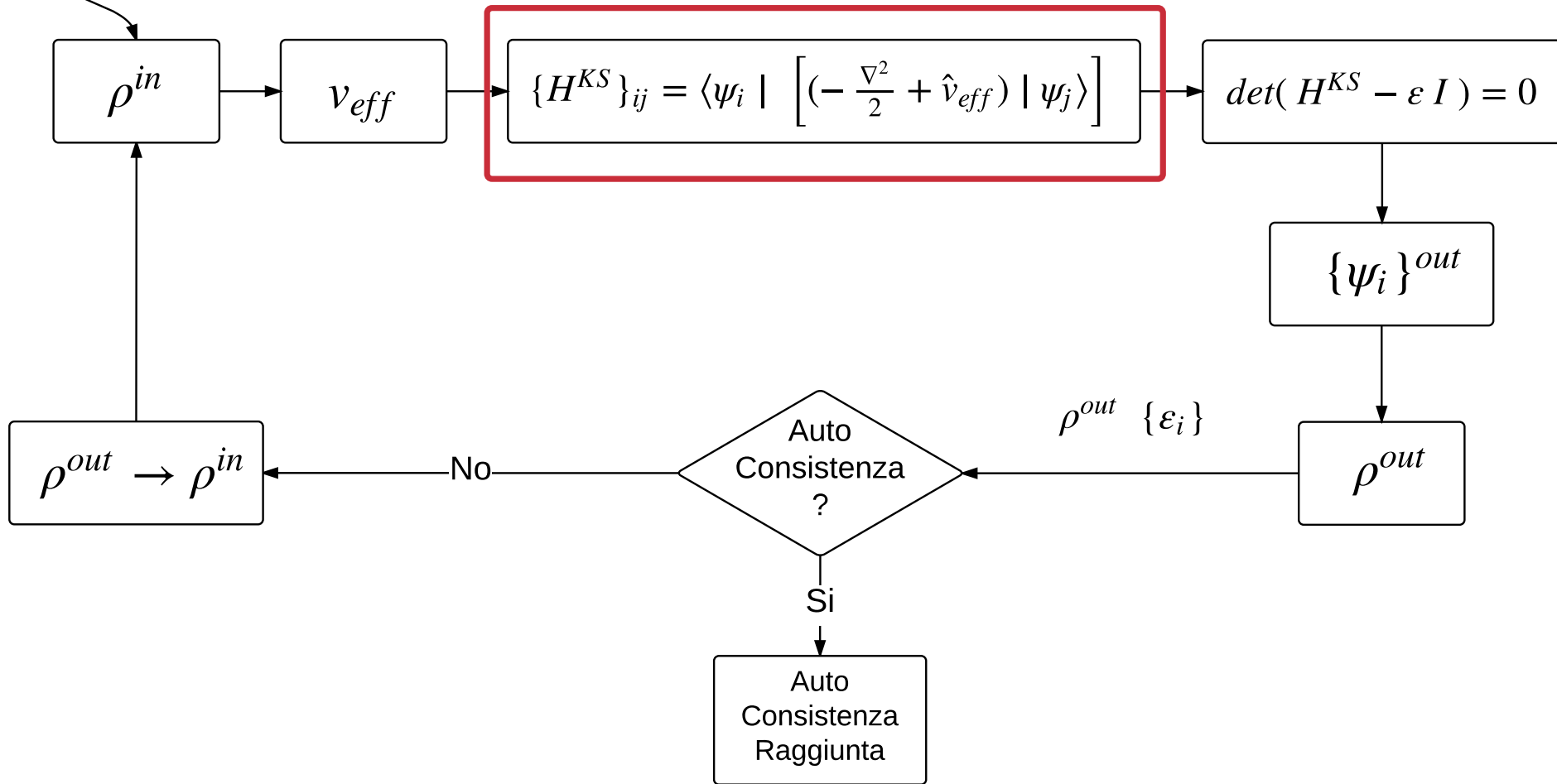
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