Dynamical Mean Field Theory for strongly correlated electrons

TOOLbox series, nov 2021

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Monday 22

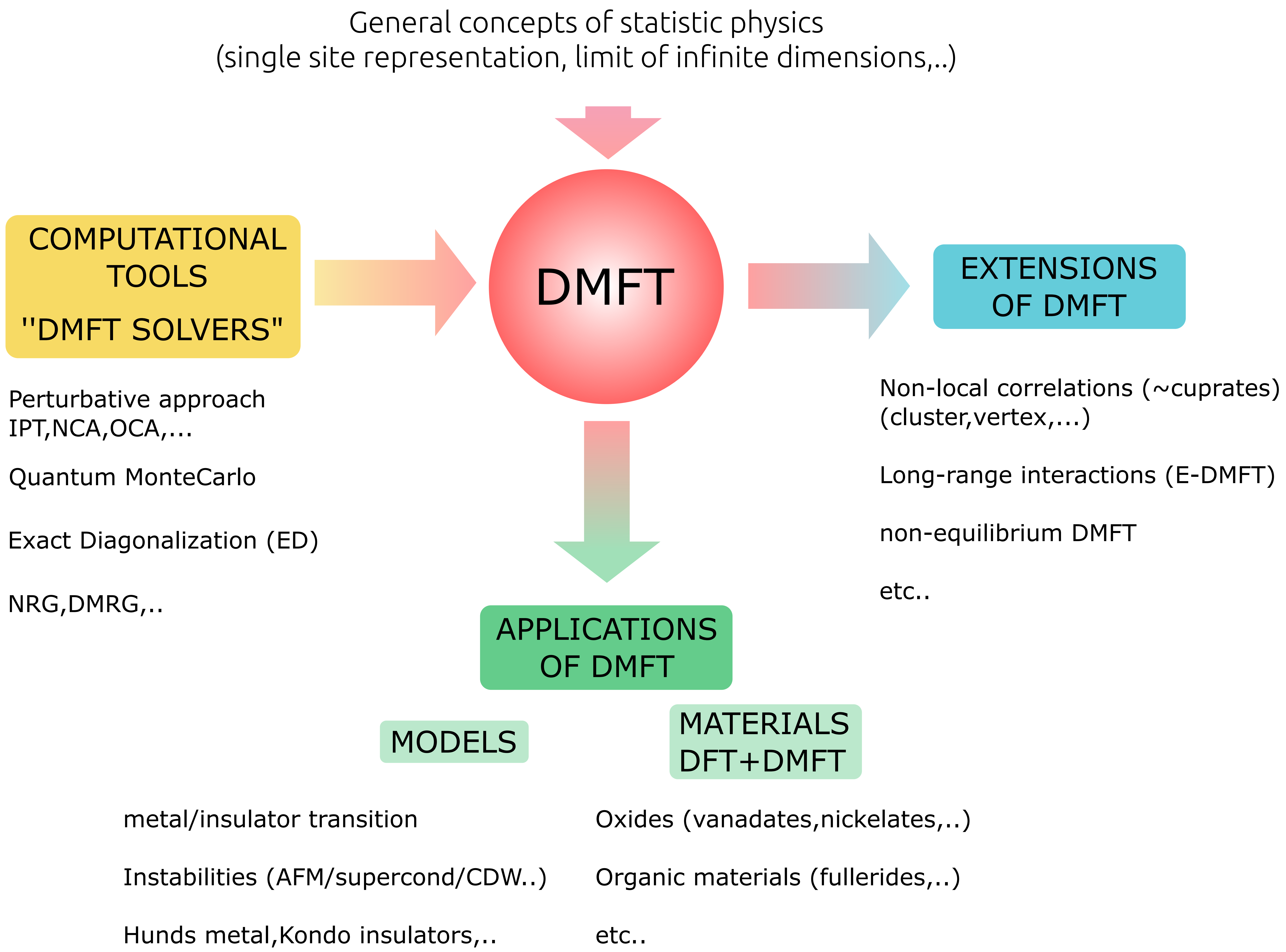
Introduction to the basics concepts of the Dynamical Mean Field Theory

(instruction for the hands-on tutorial)

Tuesday 23

Hands-on tutorial

- Mott transition with iterated perturbation theory
- Weak to strong coupling superconductivity using Exact Diagonalization methods

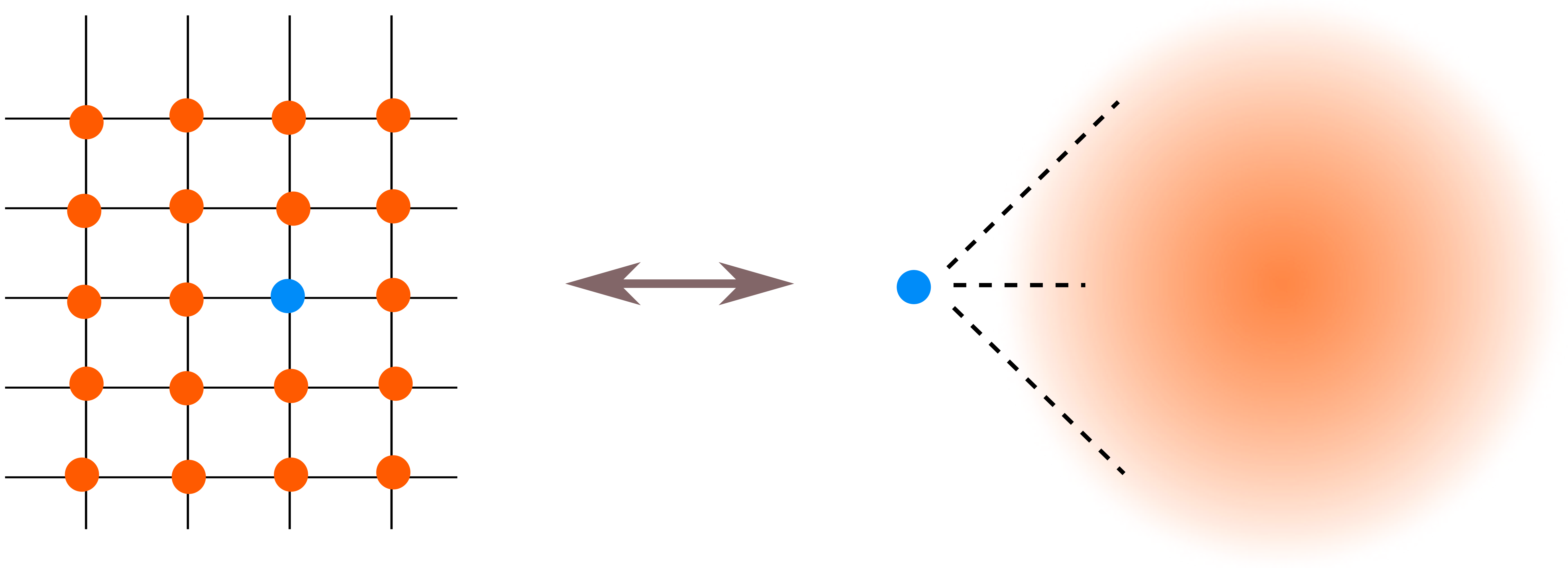


Adapted from A. Georges
Fermions en interaction: Introduction a la theorie du champ moyen dynamique. College de France, 2019 (online)

$$H_{\mathrm{Hubbard}} = -t \sum_{\langle \mathbf{R}\mathbf{R}' \rangle \sigma} c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow} - \mu \sum_{\mathbf{R}\sigma} c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}\sigma},$$

Lattice problem

Single-site representation



Compare with static mean-field

$$H_{\mathrm{Ising}} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - \sum_i h_i \sigma_i$$

	STATIC MeanField	DYNAMICAL MeanField
LOCAL OBSERVABLE	local magnetization $m_i = \langle \sigma_i \rangle$	
LOCAL REPRESENTATION	spin in a magnetic field $m_i = \tanh\left(\beta h_i^{\mathrm{eff}}\right)$	
SELF CONSISTENCY RELATION	$h_i^{\mathrm{eff}} = h_i + J \sum_{\langle ij \rangle} m_j$	

	STATIC MeanField	DYNAMICAL MeanField
LOCAL OBSERVABLE	local magnetization $m_i = \langle \sigma_i \rangle$	local Greens function $G_{ii}(\tau) = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{i\sigma}(0) \rangle$
LOCAL REPRESENTATION	spin in a magnetic field $m_i = \tanh\left(\beta h_i^{\text{eff}}\right)$	atom in a bath $G^{-1}_{ii}(\tau) = \mathcal{G}^{-1}_0(\tau) - \Sigma_{\text{imp}}[\mathcal{G}_0]$
SELF CONSISTENCY RELATION	$h_i^{\text{eff}} = h_i + J \sum_{\langle ij \rangle} m_j$	$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{imp}(\omega)$

$$\mathcal{S}_{\text{imp}}^{(i)} = \int d\tau d\tau' c_{i\sigma}^{\dagger} \mathcal{G}_0^{-1}(\tau - \tau') c_{i\sigma}(\tau') + \int d\tau H_{int}^{(i)}(\tau)$$

$$H_{int}^{(i)} = U n_{i\uparrow} n_{i\downarrow}$$

$$\mathcal{G}_0^{-1}(\tau - \tau') = G_{at,0}^{-1}(\tau - \tau') - \Delta(\tau - \tau').$$

$$G_{at,0}(i\omega_n) = i\omega_n + \mu$$

$$G_{ii,\sigma}(\tau - \tau') = -\langle T_\tau c_{i\sigma}(\tau) c_{i\sigma}^{\dagger}(\tau') \rangle_{\text{imp}[\mathcal{G}_0]}$$

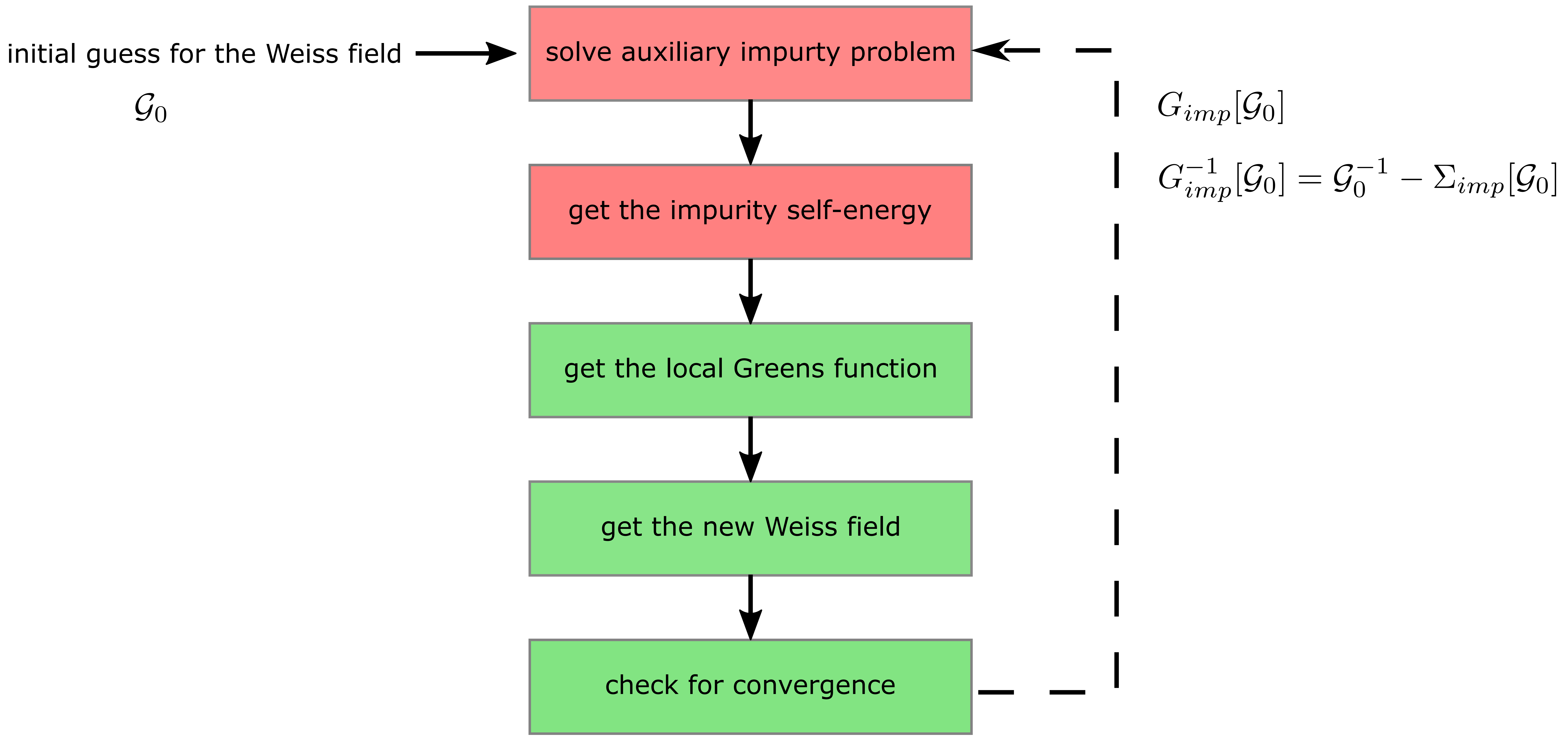
$$G_{ii\sigma}^{-1}(\tau - \tau') = \mathcal{G}_0^{-1}(\tau - \tau') - \Sigma_{\text{imp}}[\mathcal{G}_0]$$

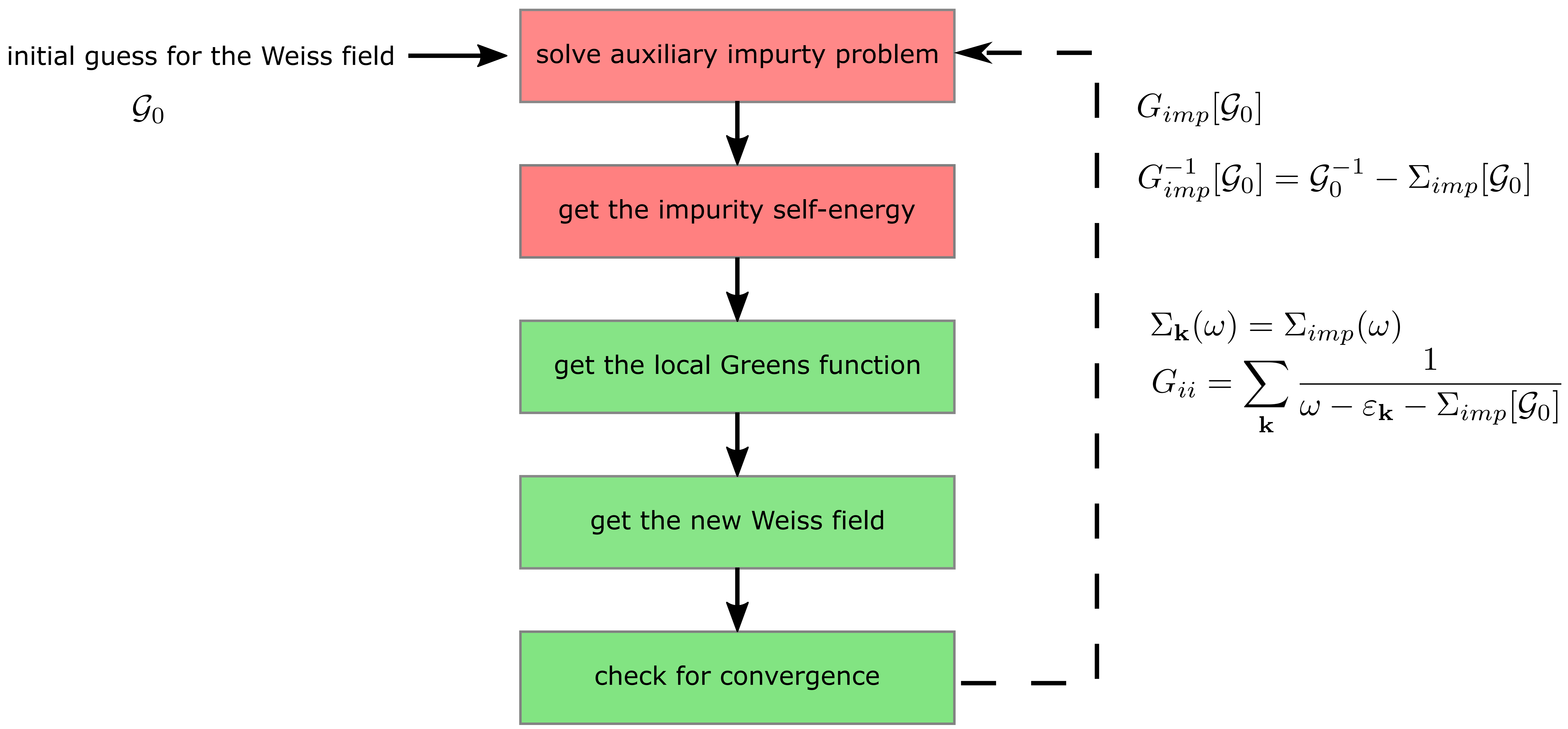
$$G_{ii}(\omega) = \sum_{\mathbf{k}} \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)}$$

DMFT approximation

$$\boxed{\Sigma_{\mathbf{k}} = \Sigma_{\text{imp}}[\mathcal{G}_0]}$$

exact for $z \to \infty$


initial guess for the Weiss field
$\mathcal{G}_0$
solve auxiliary impurty problem
get the impurity self-energy
get the local Greens function
get the new Weiss field
check for convergence
$G_{imp}[\mathcal{G}_0]$
$G_{imp}^{-1}[\mathcal{G}_0] = \mathcal{G}_0^{-1} - \Sigma_{imp}[\mathcal{G}_0]$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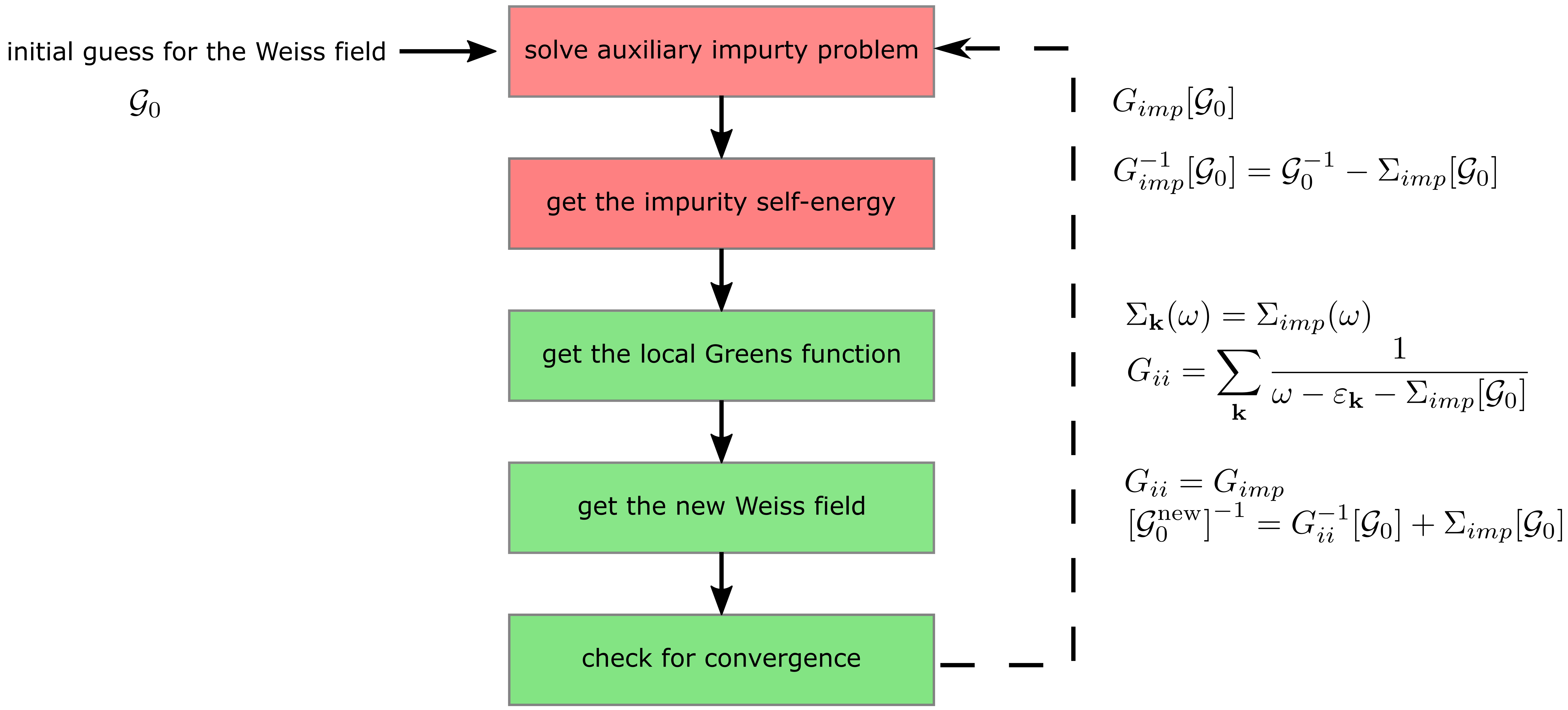

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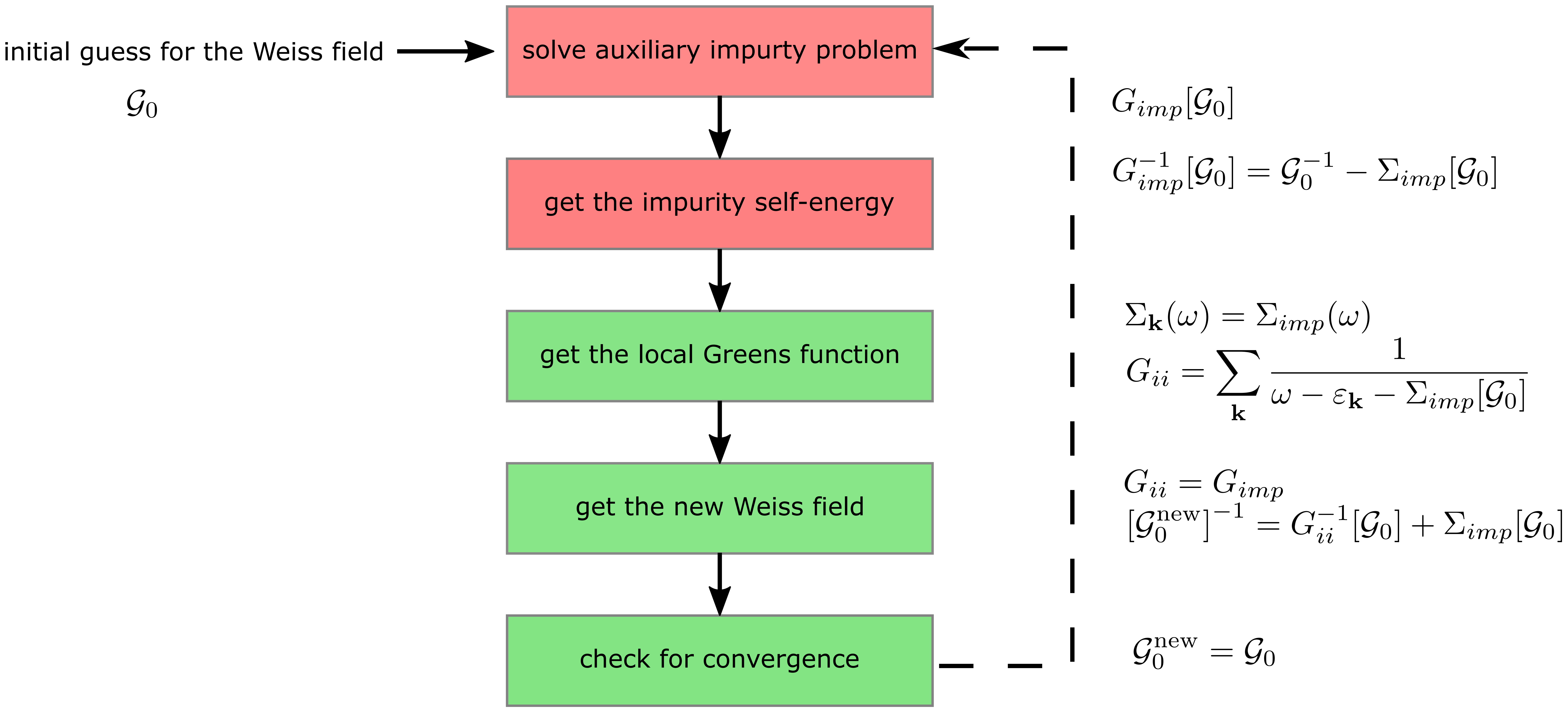
$[\mathcal{G}_0^{\mathrm{new}}]^{-1} = G_{ii}^{-1}[\mathcal{G}_0] + \Sigma_{imp}[\mathcal{G}_0]$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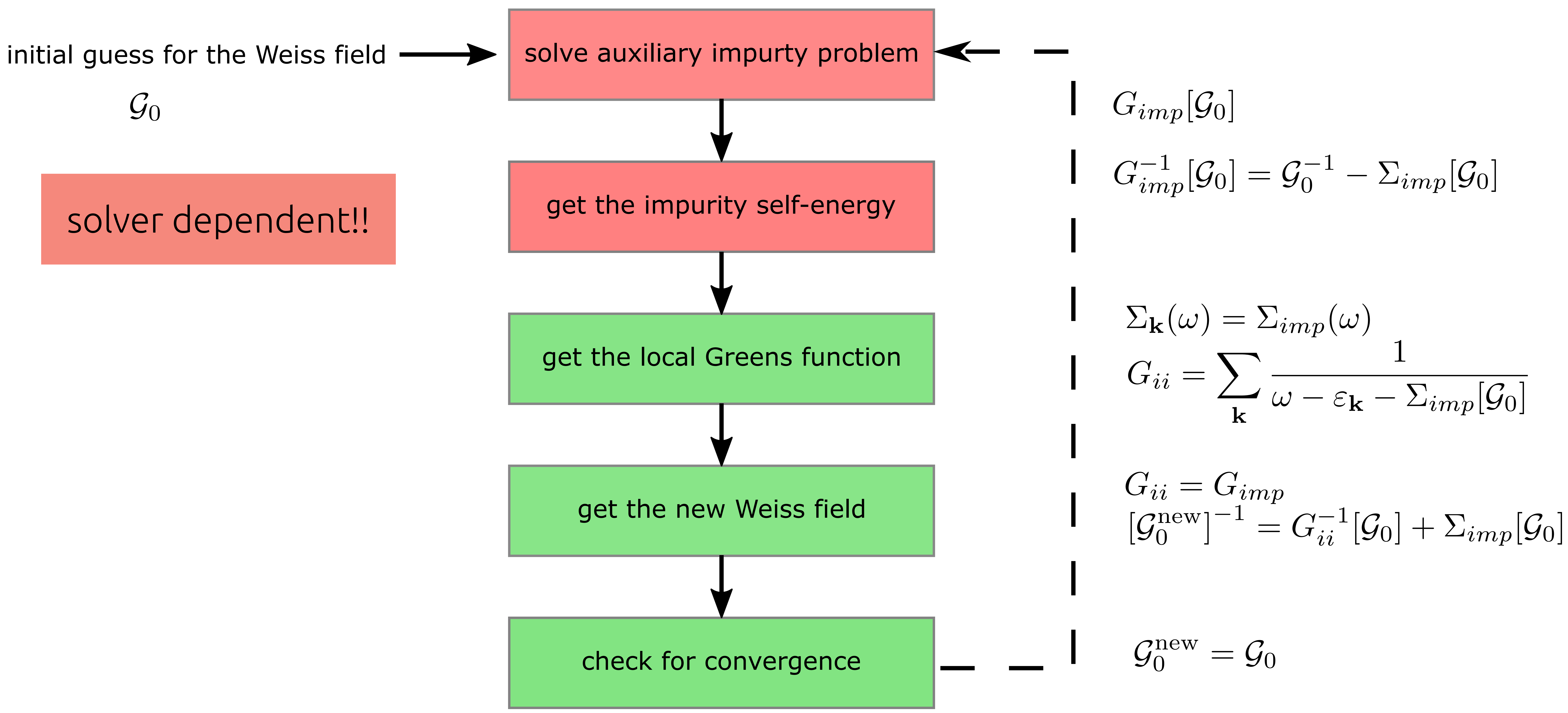
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solver dependent!!
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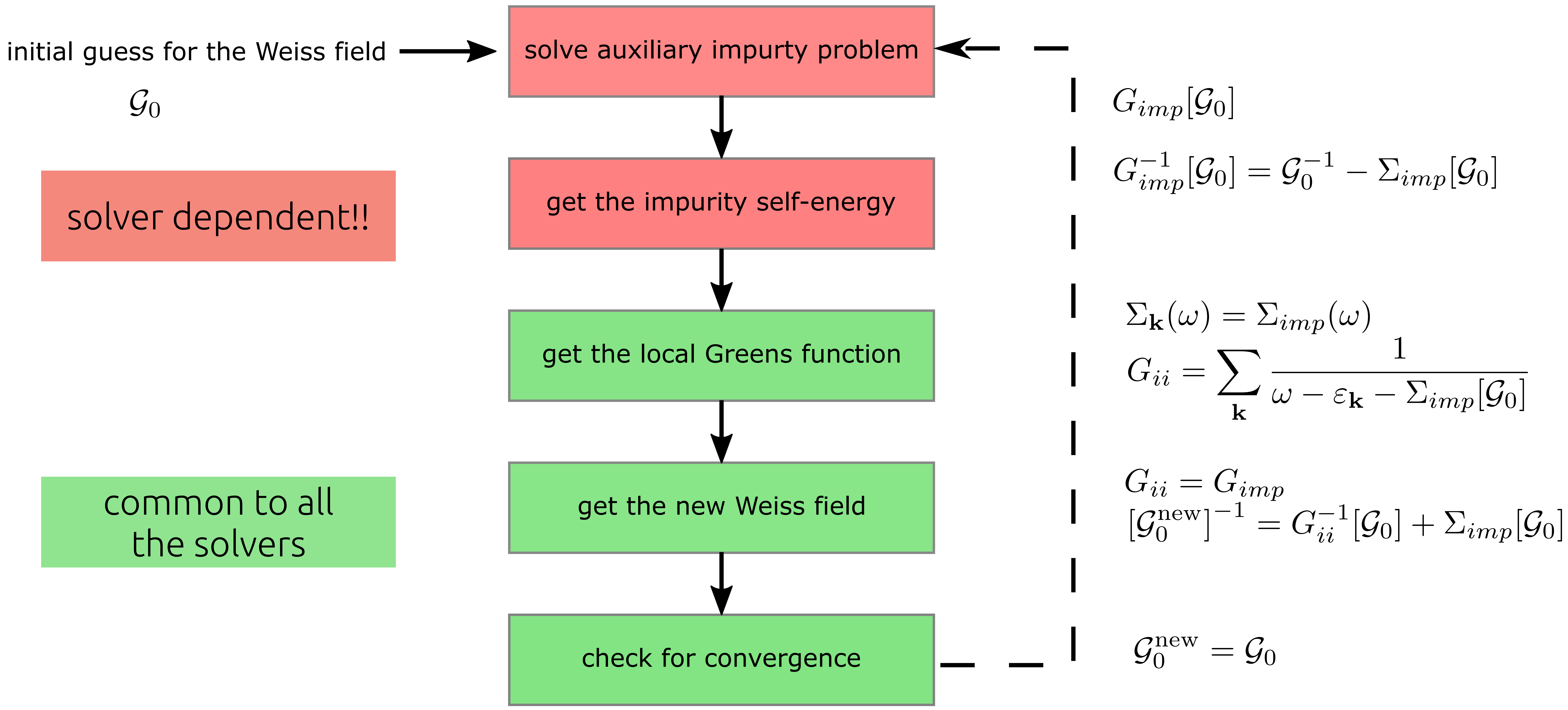

initial guess for the Weiss field
$\mathcal{G}_0$
solver dependent!!
common to all the solvers
solve auxiliary impurty problem
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General Hamiltonian with local interactions

$$H = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\alpha\beta} \sum_{\sigma} t^{\alpha\beta}_{\mathbf{R}\mathbf{R}'} c^{\dagger}_{\mathbf{R}\alpha\sigma} c_{\mathbf{R}'\beta\sigma} + \sum_{\mathbf{R}} H_{int}(\mathbf{R}).$$

$$\begin{aligned} H_{int}(\mathbf{R}) =& U \sum_{\alpha} n_{\mathbf{R}\alpha\uparrow} n_{\mathbf{R}\alpha\downarrow} + U' \sum_{\alpha\neq\beta} n_{\mathbf{R}\alpha\uparrow} n_{\mathbf{R}\beta\downarrow} + (U' - J_H) \sum_{\alpha<\beta} \sum_{\sigma} n_{\mathbf{R}\alpha\sigma} n_{\mathbf{R}\beta\sigma} \\ &+ J_X \sum_{\alpha\neq\beta} c^{\dagger}_{\alpha\uparrow} c^{\dagger}_{\beta\downarrow} c_{\alpha\downarrow} c_{\beta\uparrow} + J_P \sum_{\alpha\neq\beta} c^{\dagger}_{\alpha\uparrow} c^{\dagger}_{\alpha\downarrow} c_{\beta\downarrow} c_{\beta\uparrow}. \end{aligned}$$

U intra-orbital repulsion

U' inter-orbital repulsion

J_H Hund's coupling

J_X Spin-flip

J_P Pair-hoppings

- Model Hamiltonians
- ab-initio Hamiltonian