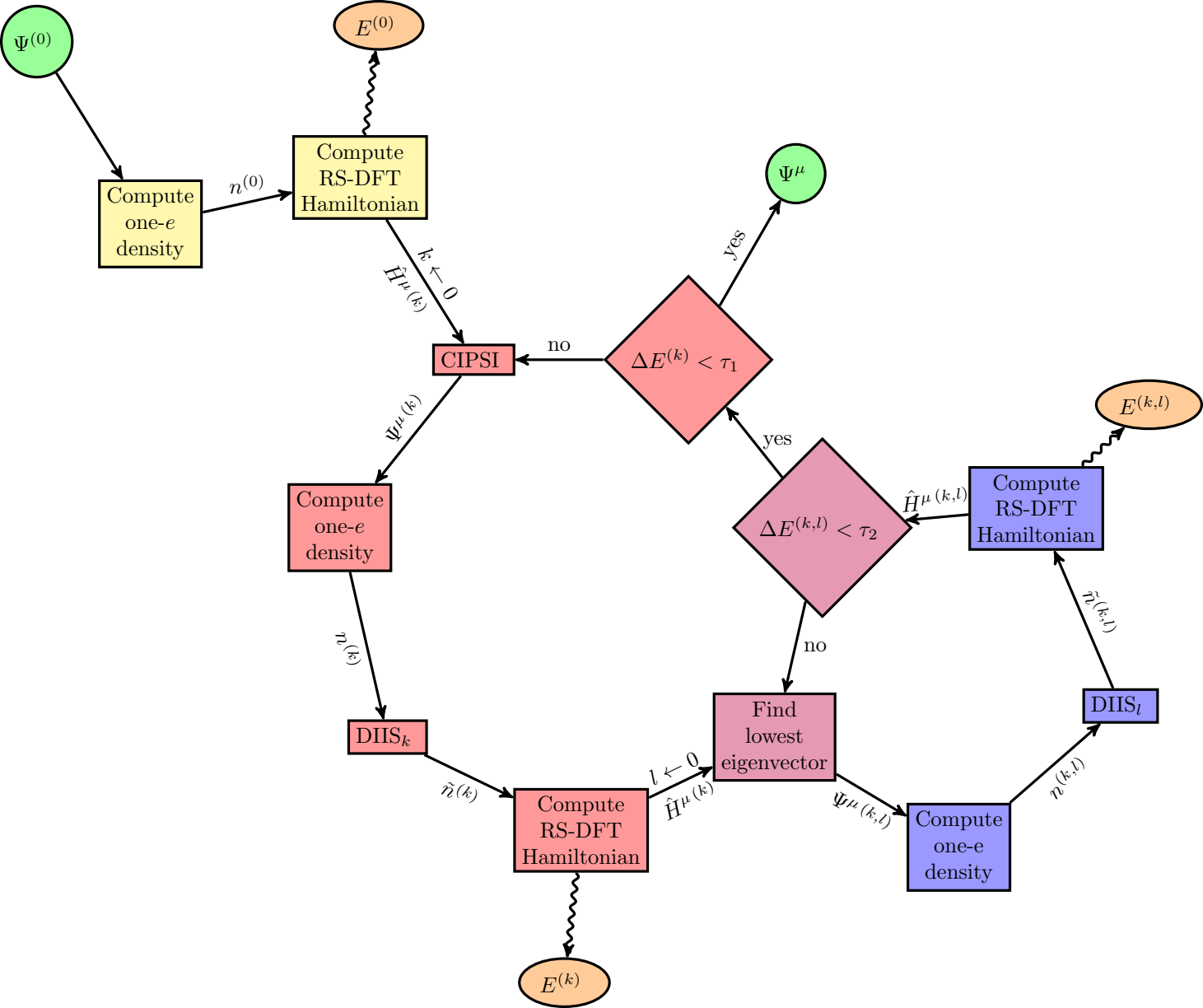
$\Psi^{(0)}$
$E^{(0)}$
Compute one-e density
$n^{(0)}$
Compute RS-DFT Hamiltonian
$\hat{H}^{\mu\,(k)}$
$k \leftarrow 0$
CIPSI
no
$\Delta E^{(k)} < \tau_1$
yes
Ψ^{μ}
$\Psi^{\mu\,(k)}$
Compute one-e density
$n^{(k)}$
DIIS$_k$
$\tilde{n}^{(k)}$
Compute RS-DFT Hamiltonian
$E^{(k)}$
$l \leftarrow 0$
$\hat{H}^{\mu\,(k)}$
Find lowest eigenvector
$\Psi^{\mu\,(k,l)}$
Compute one-e density
$n^{(k,l)}$
DIIS$_l$
$\tilde{n}^{(k,l)}$
Compute RS-DFT Hamiltonian
$E^{(k,l)}$
$\hat{H}^{\mu\,(k,l)}$
$\Delta E^{(k,l)} < \tau_2$
yes
no