GQCP::BaseOrbitalOptimizer

is_converged
convergence_threshold
maximum_number_of_iterations
number_of_iterations

+ BaseOrbitalOptimizer()
+ ~BaseOrbitalOptimizer()
+ calculateNewRotationMatrix()
+ checkForConvergence()
+ prepareConvergenceChecking()
+ numberOfIterations()
+ optimize()

GQCP::NewtonOrbitalOptimizer

hessian_modifier
gradient
hessian

+ NewtonOrbitalOptimizer()
+ ~NewtonOrbitalOptimizer()
+ calculateGradientMatrix()
+ calculateHessianTensor()
+ calculateNewFullOrbitalGenerators()
+ prepareOrbitalDerivatives
Calculation()
+ calculateNewRotationMatrix()
+ checkForConvergence()
+ prepareConvergenceChecking()
+ calculateGradientVector()
+ calculateHessianMatrix()
+ calculateNewFreeOrbitalGenerators()
+ directionFromIndefiniteHessian()
+ newtonStepIsWellDefined()

GQCP::QCMethodNewtonOrbital
Optimizer

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+ ~QCMethodNewtonOrbitalOptimizer()
+ calculate1DM()
+ calculate2DM()
+ prepareDMCalculation()
+ calculateGradientMatrix()
+ calculateHessianTensor()
+ prepareOrbitalDerivatives
Calculation()
+ oneDM()
+ twoDM()
+ NewtonOrbitalOptimizer()

GQCP::DOCINewtonOrbitalOptimizer
< _EigenproblemSolver >

+ DOCINewtonOrbitalOptimizer()
+ calculate1DM()
+ calculate2DM()
+ calculateNewFullOrbitalGenerators()
+ prepareDMCalculation()
+ eigenpair()
+ eigenpairs()
+ makeLinearExpansion()