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()

GOCP::QCMethodNewtonOrbital Optimizer

- # D
- # d
- + ~QCMethodNewtonOrbitalOptimizer()
- + calculate1DM()
- + calculate2DM()
- + prepareDMCalculation()
- + calculateGradientMatrix()
- + calculateHessianTensor()
- + prepareOrbitalDerivatives
- Calculation()
- + oneDM()
- + twoDM()
- + NewtonOrbitalOptimizer()

GQCP::AP1roGLagrangianNewton **OrbitalOptimizer**

- + AP1roGLagrangianNewtonOrbital Optimizer()
- + AP1roGLagrangianNewtonOrbital Optimizer()
- + prepareDMCalculation()
- + calculate1DM()
- + calculate2DM()
- + calculateNewFullOrbitalGenerators()
- + electronicEnergy()
- + geminalCoefficients()
- + multipliers()

GQCP::DOCINewtonOrbitalOptimizer < _EigenproblemSolver >

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