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::ERNewtonLocalizer

- + ERNewtonLocalizer()
- + calculateGradientMatrix()
- + calculateHessianTensor()
- + calculateNewFullOrbitalGenerators()
- + prepareOrbitalDerivatives Calculation()
- + calculateGradientMatrixElement()
- + calculateHessianTensorElement()

GOCP::QCMethodNewtonOrbital Optimizer

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- + ~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()