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()

+ prepareOrbitalDerivatives

Calculation()

+ calculateNewFullOrbitalGenerators()

+ calculateGradientMatrixElement() + calculateHessianTensorElement()

GOCP::BaseOrbitalOptimizer