GQCP::BaseOrbitalOptimizer # is converged # convergence threshold # maximum_number_of_iterations # number of iterations + BaseOrbitalOptimizer() + ~BaseOrbitalOptimizer() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + numberOfIterations() + optimize() Д GQCP::NewtonOrbitalOptimizer # hessian_modifier # gradient # hessian + NewtonOrbitalOptimizer() + ~NewtonOrbitalOptimizer() + calculateGradientMatrix() + calculateHessianTensor() + calculateNewFullOrbitalGenerators() + prepareOrbitalDerivatives Calculation() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + calculateGradientVector() + calculateHessianMatrix() + calculateNewFreeOrbitalGenerators() + directionFromIndefiniteHessian() + newtonStepIsWellDefined() GQCP::QCMethodNewtonOrbital Optimizer GQCP::ERNewtonLocalizer # D # d + ~QCMethodNewtonOrbitalOptimizer() + ERNewtonLocalizer() + calculate1DM() + calculateGradientMatrix() + calculate2DM() + calculateHessianTensor() + prepareDMCalculation() + calculateNewFullOrbitalGenerators() + calculateGradientMatrix() + prepareOrbitalDerivatives + calculateHessianTensor() Calculation() + prepareOrbitalDerivatives + calculateGradientMatrixElement() Calculation() + calculateHessianTensorElement() + oneDM() + twoDM() + NewtonOrbitalOptimizer() GQCP::AP1roGLagrangianNewton OrbitalOptimizer GQCP::DOCINewtonOrbitalOptimizer < _EigenproblemSolver > + AP1roGLagrangianNewtonOrbital Optimizer() + DOCINewtonOrbitalOptimizer() + AP1roGLagrangianNewtonOrbital + calculate1DM() Optimizer() + calculate2DM() + prepareDMCalculation() + calculateNewFullOrbitalGenerators() + calculate1DM() + prepareDMCalculation() + calculate2DM() + eigenpair() + calculateNewFullOrbitalGenerators() + eigenpairs() + electronicEnergy() + makeLinearExpansion() + geminalCoefficients() + multipliers()