GQCP::BaseOrbitalOptimizer # is converged # convergence threshold # maximum_number_of_iterations # number of iterations + BaseOrbitalOptimizer() + ~BaseOrbitalOptimizer() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + numberOfIterations() + optimize() GQCP::NewtonOrbitalOptimizer GQCP:: Jacobi Orbital Optimizer # hessian modifier # gradient # optimal jacobi with # hessian + NewtonOrbitalOptimizer() + JacobiOrbitalOptimizer() + ~NewtonOrbitalOptimizer() + ~JacobiOrbitalOptimizer() + calculateGradientMatrix() + calculateJacobiCoefficients() + calculateHessianTensor() + calculateOptimalRotation + calculateNewFullOrbitalGenerators() + prepareOrbitalDerivatives + calculateScalarFunctionChange() Calculation() + preparelacobiSpecificConvergence + calculateNewRotationMatrix() + checkForConvergence() + calculateNewRotationMatrix() + prepareConvergenceChecking() + checkForConvergence() + calculateGradientVector() + prepareConvergenceChecking() + calculateHessianMatrix() + calculateOptimalJacobiParameters() + calculateNewFreeOrbitalGenerators() + directionFromIndefiniteHessian() + newtonStepIsWellDefined() GOCP::QCMethodNewtonOrbital Optimizer GQCP::ERNewtonLocalizer # D GQCP::ERJacobiLocalizer # d + ~QCMethodNewtonOrbitalOptimizer() + ERNewtonLocalizer() + calculateJacobiCoefficients() + calculate1DM() + calculateGradientMatrix() + calculateOptimalRotation + calculate2DM() + calculateHessianTensor() + prepareDMCalculation() + calculateNewFullOrbitalGenerators() + calculateScalarFunctionChange() + calculateGradientMatrix() + prepareOrbitalDerivatives + prepareJacobiSpecificConvergence + calculateHessianTensor() Calculation() + prepareOrbitalDerivatives + calculateGradientMatrixElement() + JacobiOrbitalOptimizer() Calculation() + calculateHessianTensorElement() + oneDM() + twoDM() + NewtonOrbitalOptimizer() GQCP::AP1roGLagrangianNewton OrbitalOptimizer GQCP::DOCINewtonOrbitalOptimizer < _EigenproblemSolver > + AP1roGLagrangianNewtonOrbital Optimizer() + DOCINewtonOrbitalOptimizer() + AP1roGLagrangianNewtonOrbital + calculate1DM() Optimizer()

+ prepareDMCalculation()

+ calculateNewFullOrbitalGenerators()

+ calculate1DM()

+ calculate2DM()

+ multipliers()

+ electronicEnergy()

+ geminalCoefficients()

+ calculate2DM()

+ eigenpair()

+ eigenpairs()

+ prepareDMCalculation()

+ makeLinearExpansion()

+ calculateNewFullOrbitalGenerators()

dim

scalar

Angle()

Checking()

+ comparer()

Angle()

GQCP::AP1roGJacobiOrbital

Optimizer

+ AP1roGJacobiOrbitalOptimizer()

+ AP1roGlacobiOrbitalOptimizer()

+ calculateScalarFunctionChange()

+ prepareJacobiSpecificConvergence

+ calculateJacobiCoefficients()

+ calculateOptimalRotation

Angle()

Checking()

+ electronicEnergy()