GQCP::BaseOrbitalOptimizer # is converged # convergence threshold # maximum_number_of_iterations # number of iterations + BaseOrbitalOptimizer() + ~BaseOrbitalOptimizer() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + numberOfIterations() + optimize() GQCP:: Jacobi Orbital Optimizer # dim # optimal jacobi with scalar + JacobiOrbitalOptimizer() + ~ [acobiOrbitalOptimizer() + calculatelacobiCoefficients() + calculateOptimalRotation Angle() + calculateScalarFunctionChange() + prepareJacobiSpecificConvergence Checking() + calculateNewRotationMatrix() + checkForConvergence() + prepareConvergenceChecking() + calculateOptimalJacobiParameters() + comparer() GQCP::AP1roGlacobiOrbital Optimizer GQCP::ERJacobiLocalizer + AP1roGlacobiOrbitalOptimizer() + calculate/acobiCoefficients() + AP1roGlacobiOrbitalOptimizer() + calculateOptimalRotation + calculateJacobiCoefficients() Anale() + calculateOptimalRotation + calculateScalarFunctionChange() + prepareJacobiSpecificConvergence + calculateScalarFunctionChange() Checking() + preparelacobiSpecificConvergence + lacobiOrbitalOptimizer() + electronicEnergy()

Anale()

Checking()