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()
- + calculate/acobiCoefficients()
- + calculateOptimalRotation Angle()
- + calculateScalarFunctionChange()
- + prepareJacobiSpecificConvergence Checking()
- + calculateNewRotationMatrix()
- + checkForConvergence()
- + prepareConvergenceChecking()
- + calculateOptimalJacobiParameters()
- + comparer()