# KELBG-MATRIX WITH LONG INTERACTIONS PACKAGE FOR PATH INTEGRAL MONTE CARLO AND QUASICLASSICAL DYNAMICS SIMULATIONS

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The KelbgLIP code [1] is a set of three subroutines necessary for simulation of hydrogen plasma with path integrals using Monte Carlo or molecular dynamics methods. It allows the calculation of the Coulomb matrix, the Kelbg pseudopotential, and the potential energy and action, taking into account the Coulomb long-range interaction. This long-range interaction is taken into account by solving the Bloch equation for the angular-averaged Ewald potential [2,3].

The Kelbg pseudopotential for quasi-classical molecular dynamics has also been corrected at small distances using an improved Kelbg pseudopotential [4]. This improvement allows the simulation of an non-degenerated hydrogen plasma over a wide range of temperatures.

In summary, KelbgLIP allows the calculation of diagonal and non-diagonal elements of the density matrix, as well as associated pseudopotentials that remain finite at small distances, preventing the collapse of the system. This makes it possible to use the program both in classical simulation methods, such as molecular dynamics, and in quantum methods, such as path integral Monte Carlo, including exchange effects for fermions. The program supports atomic units.

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