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The Hartree potential is defined as the electrostatic potential from the electron charge density and must be calculated from the Poisson equation:

$$\nabla^2 V_H[n](r) = -4\pi n(r).$$

The Poisson equation is a second-order differential equation and a boundary condition is required in order to fix the solution. Molecular systems have the boundary condition that the potential goes asymptotically to zero. In bulk systems, the boundary condition is that the potential is periodic.

**Note**

Periodic boundary conditions only determine the Hartree potential up to an additive constant, which reflects the physics that the bulk electrostatic potential does not have a fixed value relative to the vacuum level. Experimentally, this can be measured through the different work functions of different facets of a crystal.

**Solving the Poisson equation using a Fourier transform**

For systems with periodic boundary conditions and no dielectric and metallic regions, the Poisson equation can be solved using the `FastFourierSolver`, which is the most efficient FFT solver in the QuantumATK package.

**Solving the Poisson equation with a real-space solver**

For general systems, the Poisson equation is solved using an algebraic `MultigridSolver` or `DirectSolver`. The system is enclosed in a bounding box, and the Hartree potential is defined on a regular grid inside the bounding box. Different boundary conditions can be imposed on the solution at the bounding box surface by using the keyword `boundary_conditions`:

```python
poisson_solver = MultigridSolver(  
    boundary_conditions=[[PeriodicBoundaryCondition(), PeriodicBoundaryCondition()],  
                        [DirichletBoundaryCondition(), DirichletBoundaryCondition()],  
                        [PeriodicBoundaryCondition(), PeriodicBoundaryCondition()])
```

**DirichletBoundaryCondition:**
The Hartree potential is zero at the boundary.

**NeumannBoundaryCondition:**

The negative gradient of the Hartree potential, e.g., the electric field, is zero at the boundary.

**PeriodicBoundaryCondition:**

The potential has identical values on opposite faced boundaries.

**MultipoleBoundaryCondition:**

The potential at the boundary is determined by calculating the monopole, dipole and quadrupole moments of the charge distribution inside the box, and using these moments to extrapolate the value of the electrostatic potential at the boundary of the box.

It is possible to include an electrostatic interaction with a continuum of metallic or dielectric material inside the bounding box. The continuum metals are handled by constraining the Hartree potential within the metallic region to a fixed value. Dielectric materials are handled by introducing a spatially dependent dielectric constant, 

\[ \epsilon(r) = \epsilon_K \text { inside the dielectric material with dielectric constant } \epsilon_K, \text { and } \]

\[ \epsilon(r) = \epsilon_0 \text { outside the dielectric material. } \]

It is possible to perform calculations of solvents. In this case, the volume of the configuration is defined by inscribing each atom in a sphere with a size given by the van der Waals radius of the element. Inside the volume of the configuration, the dielectric constant is 1, and outside the volume of the configuration, the dielectric constant is equal to the value of `solvent_dielectric_constant`.