Random Green's function method: probing the density matrix of large scale systems

We report a random (nonequilibrium) Green's function (rGF) method for simulating the large-scale materials and devices. In this method, the rGF is defined on a set of random states and is efficiently calculated by solving a set of linear equations. With the rGF method, the Fermi-Dirac operator for equilibrium materials and the nonequilibrium density matrix of nanoelectornic device can be obtained directly. We demonstrate the applicability of rGF by accurately calculating the charge, total energy of H_2O, Si, and quantum transport properties of large-scale disordered junctions. The rGF method provides an effective stochastic method for large-scale materials and devices simulation, replacing the truncation error with statistical error in computational physics.