Several Numerical Methods of DOS Calculation

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1. Definition of DOS

Let’s start with the Green’s function in energy representations .

Here gives the definition of DOS operators and DOS .

So,

1. Diagonalization of Hamiltonian

In periodic system, quantum numbers of eigenstate are .

1. Inverse to calculate Green’s function

In periodic system,

1. Kernel Polynomial Method (KPM)

Chebyshev polynomials expansion

To be more efficient, redefine :

To eliminate the Gibbs oscillation in finite series of expansion,

DOS

Scale the energy from to ,

In periodic system,