

# Green function methods for the large scale electronic structure calculations.

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## abstract

In order to calculate physical quantities of a system, it is necessary to obtain either eigen states or density matrix of the system. The calculation of eigen states is reduced to a matrix diagonalization procedure. However, this procedure results in a severe computational cost for a large scale system. The essential methodology for large scale calculations is how to obtain the density matrix  $\hat{\rho}$  without calculating eigen states[1,2]. The density matrix can be obtained by means of energy integration of the Green function,  $G_{i,j}$  ;

$$\rho_{ij} = -\frac{1}{\pi} \text{Im} \int G_{ij}(\varepsilon + i0^+) f\left(\frac{\varepsilon - \mu}{k_B T}\right) d\varepsilon. \quad (1)$$

Here,  $i, j$  represent atom or orbital index, and  $f$  is the Fermi distribution function. We have developed Green function methods, such as (1) recursion method [3] and (2) conjugate gradient (CG) method [4].

For the recursion method, we adopt the following method to achieve computational efficiency in calculation of its off-diagonal elements  $G_{ij}$ . As usual procedure of the recursion method, we obtain tridiagonalized Hamiltonian of finite size,  $H^L$ , by means of transformation matrix from atomic basis  $|i\rangle$  into Lanczos basis  $|n\rangle$ ,  $u_{nj}$ . By diagonalizing  $H^L$ , Green function within Lanczos basis,  $G_{in}^L$ , is constructed, and is combined with  $u$  to form the target Green function;  $G_{ij} = \sum_n G_{in}^L u_{nj}$ . This procedure reduces computation time of off-diagonal part to almost that of diagonal part. For the CG method, to obtain Green function, the procedure to solve linear equation  $(z - H) |x_i\rangle = |i\rangle$ , is adopted. Once the linear equation is solved, one can obtain both diagonal and off-diagonal part of the Green function simultaneously as  $\langle j | x_i \rangle = \langle j | (z - H)^{-1} | i \rangle = G_{ji}$ . These Green function methods are easy to modify to suit parallel code because of its independent nature with respect to basis  $|i\rangle$ .

The presentation will be devoted to short review of these methods and their application to large scale system. We also apply hybrid method[5] and parallel computation to simulate large scale systems[6].

[1] T. Hoshi and T. Fujiwara, JPSJ **69**, 3773 (2000). [2] T. Hoshi and T. Fujiwara, cond-mat/0210366, to appear in JPSJ **72**, Vol. 10 (2003). [3] R. Haydock, Solid State Phys., **35**, 215 (1980). [4] T. Sogabe and S.-L. Zhang, private communication. [5] T. Hoshi, R. Takayama, and T. Fujiwara, present workshop. [6] R. Takayama, T. Hoshi, and T. Fujiwara, Abstract 23aWD-6 in the Autumn Meeting 2003 of The Physical Society of Japan.