Brief explanation

October 3, 2024

1 Current-current correlation function

Current operator $\hat{J}$: see below of Eq.3 of https://arxiv.org/abs/1807.01625. Current-current correlation function C_J is defined as below

$$C_J = \langle\Psi|\hat{J}\hat{J}|\Psi\rangle \tag{1}$$

(where $|\Psi\rangle$ is a wavefunction of system) In this program, C_J is limited to a case with same time and same position (i.e. JJ has only two AO indices)

2 Spin-spin correlation function

The z component of the spin operator is given below, ignoring the constant multiple terms.

$$S^z = \sum_i (a^\dagger_{i\alpha} a_{i\alpha} - a^\dagger_{i\beta} a_{i\beta}) \tag{2}$$

Spin-spin correlation function is given below:

$$C_s = \langle\Psi|\hat{S}^z\hat{S}^z|\Psi\rangle \tag{3}$$

3 Charge-charge correlation function

Occupation number operator at site i is given below:

$$\hat{n}_i = \hat{a}^\dagger_{i\alpha}\hat{a}_{i\alpha} + \hat{a}^\dagger_{i\beta}\hat{a}_{i\beta} \tag{4}$$

Charge-charge correlation function is given below:

$$C_n^{ij} = \langle\Psi|\hat{n}_i\hat{n}_j|\Psi\rangle - \langle\Psi|\hat{n}_i|\Psi\rangle\langle\Psi|\hat{n}_j|\Psi\rangle \tag{5}$$

4 Exciton correlation

The equation for random phase approximation (RPA) is below:

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} \tag{6}$$

The RPA wavefunction is below:

$$|\Phi\rangle = \sum_{mi} (X_{mi}|mi\rangle - Y_{mi}|im\rangle) \tag{7}$$

Note that m is the index of the occupied moleculart orbital, i is the index of the virtual molecular orbital, and $|mi\rangle$ は $\hat{a}_i^\dagger \hat{a}_m|\mathrm{HF}\rangle$ Convert X_{mi} to AO basis with molecular orbital coefficients to obtain exciton correlation.

5 Green's function for a mean-field calculation

See Eq.7 of https://arxiv.org/abs/2002.05875. Note in this program, real space not reciprocal space is treated.