

# Brief explanation

October 3, 2024

## 1 Current-current correlation function

Current operator  $\hat{J}$  is formulated in the literatures. For example, see below of Eq.3 of <https://arxiv.org/abs/1807.01625>. Then, current-current correlation function  $C_J$  is defined as below

$$C_J = \langle \Psi | \hat{J} \hat{J} | \Psi \rangle \quad (1)$$

(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.  $C_J$  has only two AO indices)

## 2 Spin-spin correlation function

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

$$S^z = \sum_i (a_{i\alpha}^\dagger a_{i\alpha} - a_{i\beta}^\dagger a_{i\beta}) \quad (2)$$

Then, spin-spin correlation function is given below:

$$C_s = \langle \Psi | \hat{S}^z \hat{S}^z | \Psi \rangle \quad (3)$$

## 3 Charge-charge correlation function

Occupation number operator at site  $i$  is given below:

$$\hat{n}_i = \hat{a}_{i\alpha}^\dagger \hat{a}_{i\alpha} + \hat{a}_{i\beta}^\dagger \hat{a}_{i\beta} \quad (4)$$

Then, charge-charge correlation function is given below:

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

## 4 Exciton correlation

The equation for random phase approximation (RPA) which is used in the TDDFT method is below:

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

The solution of the RPA equation (RPA wavefunction) for the  $\nu$ th excited state is expressed as below:

$$|\Phi\rangle = \sum_{mi} (X_{mi}^\nu |mi\rangle + (Y\text{term})) \quad (7)$$

Note that  $m$  is the index of the occupied molecular orbital,  $i$  is the index of the virtual molecular orbital, and  $|mi\rangle \equiv \hat{a}_i^\dagger \hat{a}_m |\text{HF}\rangle$ . Convert  $X_{mi}$  to AO basis by multiplying molecular orbital coefficient to obtain exciton correlation. Note in the Tamm-Dancoff approximation which is simplification of RPA, only  $X$  appears in the working equation.

## 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.