Coupled perturbed Hartree-Fock method for non-Hermitian Hamiltonians

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Abstract. In order to investigate conductive properties of the system composed of a channel molecule and electrodes, a coupled perturbed Hartree-Fock method for non-Hermitian perturbation Hamiltonians is derived. A non-Hermitian perturbation Hamiltonian which describes interactions between the channel molecule and an electrode is given to represent inflow and outflow at the interface. The effects of electrodes includes the states of the density of state of the channel molecule and the statistical distribution of electrons in electrodes. Benzenedithiol and dihydro-phenylenedithiol are studied in this paper, and the first order perturbations of molecular orbital energies of them are obtained.

1. Introduction
Conductive properties of single molecules have been discussed in many articles [1, 2, 3, 4, 5, 6, 7, 8]. The conductive properties of the molecules are often analyzed by using methods based on Green’s functions [9, 10, 11, 12, 13, 14]. For these methods, the effects of electrodes are often described as non-Hermitian self-energy matrices [15]. This method has succeeded to estimate currents and conductances through the molecules. Previously, Shimazaki et al. calculated the transmission probabilities of benzenedithiol (BDT) and its derivatives based on the Hartree-Fock (HF) method with the self-energy matrices [16]. In their paper, an approximate Green’s function for a channel molecule is calculated by using the first order perturbation energies of molecular orbitals (MOs), \( \varepsilon_p^{(1)} \), where the subscript \( p \) indicates the \( p \)th MO. \( \varepsilon_p^{(1)} \) is calculated as,

\[
\varepsilon_p^{(1)} = \langle \psi_p^{(0)} | \Sigma_L + \Sigma_R | \psi_p^{(0)} \rangle,
\]

where \( \Sigma_L, R \) are the self-energies of the left and right electrodes, respectively. The obtained predictions of currents and conductances based on Green’s function show similar patterns to another theoretical calculation based on density functional theory and a non-equilibrium Green’s function [12]. In the above equation, however, the shift of Coulomb and exchange interactions between electrons induced by the perturbation are not considered. In other words, perturbed MOs are not consistent with themselves. As shown by Langhoff et al. in 1960’s [17], the interactions between electrons are important to obtain physical properties which are qualitatively and quantitatively comparable to experimental results or real values. Hence, these interactions should be considered in calculations of perturbed MO energies.

In this work, we study the calculation method of electronic structures perturbed by non-Hermitian Hamiltonians. Our method is based on coupled perturbed HF (CPHF)
equations [17, 18], and we apply them to the case with a non-Hermitian perturbation. MOs obtained by the CPHF method are consistent with Coulomb and exchange interactions between electrons at the HF level.

In order to investigate conductive properties of a molecule based on its electronic structure, the perturbation Hamiltonian inducing the electronic structure with an electric current must be considered. The self-energies of electrodes do not directly correspond to appropriate perturbation Hamiltonians, since they do not include effects of the passing through a channel molecule. In this study, we consider the density of states (DOS) for the molecule and Fermi-Dirac (FD) distributions of electrons in the electrodes in order to include the passing effects. By combining the DOS and the FD distributions with the self-energies, the perturbation Hamiltonian is constructed. It is noted that the DOS for the molecule is calculated by using perturbed orbital energies, and hence the perturbation Hamiltonian must be determined by a self-consistent field method.

In this work, we focus on BDT and dihydro-benzenedithiol (DHBDT). Perturbed MO energies of these molecules are computed.

2. Theory

In this section, CPHF equations for a non-Hermitian perturbation Hamiltonian are introduced. By using our method, perturbation effects of the Coulomb and exchange interactions between electrons can be included at the HF level. It is emphasized that our method shown in this section can be applied not only to the perturbation Hamiltonian introduced in this paper but also to other general non-Hermitian perturbation Hamiltonians. Although equations only for the first order perturbation are shown, equations for higher order perturbation are probably derived by using conventional CPHF schemes with appropriate conditions. Furthermore, it is considered that the CPHF equations for a non-Hermitian perturbation Hamiltonian can be applied to post-HF computations as well as the conventional ones can be done.

The indices \(i\) and \(j\) represent those of occupied spin-orbitals. The indices \(a\) and \(b\) are those of virtual (unoccupied) spin-orbitals. The indices \(p, q, r, \ldots\) are used for both occupied and unoccupied ones. Unperturbed canonical MOs, \(|p^{(0)}\rangle\), are used as basis. They satisfy the following HF equations without perturbation,

\[
F^{(0)}|p^{(0)}\rangle = \varepsilon_p^{(0)}|p^{(0)}\rangle, \quad (2)
\]

\[
\langle p^{(0)}|F^{(0)} = \langle p^{(0)}|\varepsilon_p^{(0)}, \quad (3)
\]

where \(F^{(0)}\) is the Fock matrix without perturbation and \(\varepsilon_p^{(0)}\) is the energy of \(|p^{(0)}\rangle\). Provided that \(F^{(0)}\) is Hermitian, (2) and (3) are equal to each other. Next, the change by the addition of perturbation Hamiltonian, \(H^{(1)}\), is discussed. In this study, \(H^{(1)}\) is not assumed to be Hermitian. For a non-Hermitian matrix, its right and left eigenvectors are different from each other. In this section, the superscripts \(L\) and \(R\) are used for the left and right eigenvectors, respectively. Perturbed MOs \(|p^R\rangle\) and \(|p^L\rangle\) satisfy the following HF equations with perturbation, respectively,

\[
F|p^R\rangle = \varepsilon_p|p^R\rangle, \quad (4)
\]

\[
\langle p^L|F = \langle p^L|\varepsilon_p, \quad (5)
\]

where \(F\) is the Fock matrix with perturbation and \(\varepsilon_p\) is the energy of \(|p^R\rangle\) and \(|p^L\rangle\). It is noted that \(F\) cannot be assumed to be Hermitian because of \(H^{(1)}\), and hence the right and left eigenvectors are generally different from each other. The zeroth and first order Fock matrices,
\( F^{(0)} \) and \( F^{(1)} \), respectively, can be written as,

\[
F^{(0)} = H^{(0)} + G(P^{(0)}),
\]

\[
F^{(1)} = H^{(1)} + G(P^{(1)}),
\]

where \( H^{(0)} \) is one-electron interactions without perturbation. The matrix \( G(P) \) represents two-electron interactions and is written as,

\[
G_{pq}(P) = \sum_{r,s} P_{sr} \langle pr | qs \rangle,
\]

where \( P \) is a density matrix and \( \langle pq | rs \rangle \) is a two electron integral. The zeroth and the first order density matrices, \( P^{(0)} \) and \( P^{(1)} \), respectively, can be obtained as,

\[
P^{(0)} = \sum_i |i^{(0)}\rangle \langle i^{(0)}|,
\]

\[
P^{(1)} = \sum_i \left( |i^{(0)}\rangle \langle i^{L(1)}| + |i^{R(1)}\rangle \langle i^{(0)}| \right).
\]

It is emphasized that \( P^{(1)} \) consists of both the left and right eigenvectors. \( |p^R\rangle \) is written by using a matrix \( \kappa \) as,

\[
|p^R\rangle = \sum_q \exp(\kappa_{qp}) |q^{(0)}\rangle.
\]

Specifically, the first order perturbed MOs, \( |p^{R(1)}\rangle \), can be written as,

\[
|p^{R(1)}\rangle = \sum_q \kappa_{qp} |q^{(0)}\rangle.
\]

Due to properties of determinants, occupied-occupied and virtual-virtual elements of \( \kappa \) can be neglected in the rest of this section, since these elements do not contribute to the Slater determinant of the ground state. The left and right eigenvectors satisfy the following biorthonormal condition,

\[
\langle p^L | q^R \rangle = \delta_{pq}.
\]

In order to satisfy (13), \( \langle p^L | \) should take a simple form with \( \kappa \),

\[
\langle p^L | = \sum_q \langle q^{(0)} | \exp(-\kappa)_{pq},
\]

and the first order perturbed \( \langle p^{L(1)} | \) can be written as,

\[
\langle p^{L(1)} | = \sum_q \langle q^{(0)} | (-\kappa_{pq}).
\]

The following equation is obtained by multiplying (4) \( \langle p^L | \) from the left,

\[
\langle p^L | F | q^R \rangle = \varepsilon_p \delta_{pq}.
\]
In order to satisfy (16) at the first order level, the virtual-occupied elements of \( \kappa \) are required to satisfy the following equation,

\[
\langle a^{(1)} | F^{(0)} | \psi^{(0)} \rangle + \langle a^{(0)} | F^{(1)} | \psi^{(0)} \rangle + \langle a^{(0)} | F^{(0)} | \psi^{(1)} \rangle = 0.
\]  

(17)

By substituting (7), (12), and (15) in (17), the following CPHF equation for a non-Hermitian Hamiltonian is derived,

\[
\varepsilon_a^{(0)} - \varepsilon_i^{(0)} \kappa_{ai} = -H_{ai}^{(1)} - \sum_{b,j} \left( -\kappa_{jb} \langle ab | ij \rangle + \kappa_{bj} \langle aj | ib \rangle \right).
\]  

(18)

By the same manner, we can obtain the following equation for occupied-virtual elements of \( \kappa \),

\[
\varepsilon_a^{(0)} - \varepsilon_i^{(0)} \kappa_{ia} = H_{ia}^{(1)} + \sum_{b,j} \left( -\kappa_{jb} \langle ib | aj \rangle + \kappa_{bj} \langle ij | ab \rangle \right).
\]  

(19)

Actually, we can simplify the calculation of (18) and (19) by dividing \( H^{(1)} \) into the Hermitian and anti-Hermitian parts, \( H^{(1) \dagger} \) and \( H^{(1)} \dagger \), respectively. For \( H^{(1) \dagger} \), (18) and (19) give the same equation, and anti-Hermitian \( \kappa \) is obtained. Hence the number of simultaneous equations to be solved decreases by half. In a similar way, Hermitian \( \kappa \) can be obtained for \( H^{(1)} \dagger \). Due to the linearity of the first order perturbation, \( \kappa \) for the original \( H^{(1)} \) can be obtained as the sum of the ones for \( H^{(1) \dagger} \) and \( H^{(1)} \dagger \).

By using (16) and \( \kappa \) calculated from (18) or (19), \( \varepsilon_p^{(1)} \) can be obtained as,

\[
\varepsilon_p^{(1)} = \langle p^{L(1)} | F^{(0)} | p^{(0)} \rangle + \langle p^{(0)} | F^{(1)} | p^{(0)} \rangle + \langle p^{(0)} | F^{(0)} | p^{R(1)} \rangle = H_{pp}^{(1)} + \sum_{a,i} \left( -\kappa_{ia} \langle pa | pi \rangle + \kappa_{ai} \langle pi | pa \rangle \right).
\]  

(20)

The improvement on (1) exists in the second term. The first order perturbation for the expectation value of an one body operator, \( \hat{O} \), can be calculated as,

\[
\langle \hat{O} \rangle^{(1)} = \sum_i \left( \langle \hat{i}^{L(1)} | \hat{O} | \psi^{(0)} \rangle + \langle \hat{i}^{(0)} | \hat{O} | \psi^{(1)} \rangle \right)
\]

\[
= \sum_{a,i} \left( -\kappa_{ia} \langle a^{(0)} | \hat{O} | a^{(0)} \rangle + \kappa_{ai} \langle a^{(0)} | \hat{O} | a^{(0)} \rangle \right).
\]  

(21)

Due to the Hermitian part of \( \kappa \) derived from \( H^{(1)} \dagger \), the value of \( \langle \hat{O} \rangle^{(1)} \) is generally a complex number. It should be noted that even if non-Hermitian perturbation is applied, the total number of electrons \( n_e \) does not change up to the first order level. This can easily be seen by the following equation,

\[
n_e^{(1)} = \sum_i \left( \langle \hat{i}^{L(1)} | \psi^{(0)} \rangle + \langle \hat{i}^{(0)} | \psi^{(1)} \rangle \right)
\]

\[
= \sum_{a,i} \left( -\kappa_{ia} \langle a^{(0)} | \hat{O} | a^{(0)} \rangle + \kappa_{ai} \langle a^{(0)} | \hat{O} | a^{(0)} \rangle \right)
\]

\[
= 0.
\]  

(22)
In terms of $\kappa$ and $\varepsilon_p^{(1)}$, several approximate Green’s functions are reported. One of them is proposed by Shimazaki et al. [13], which is given as,

$$G_1(E) = \sum_p \frac{|p^{(0)}\rangle\langle p^{(0)}|}{E - (\varepsilon_p^{(0)} + \varepsilon_p^{(1)})}. \quad (23)$$

While (1) is used in [13] for obtaining $\varepsilon_p^{(1)}$, we can use (20) instead. $\varepsilon_p^{(1)}$ of (20) adds the effects of $\kappa$ to the Green’s function. Another improvement is given as,

$$G_2(E) = G_1(E) + \sum_p \frac{|p^{(0)}\rangle\langle p^{L(1)}| + |p^{R(1)}\rangle\langle p^{(0)}|}{E - (\varepsilon_p^{(0)} + \varepsilon_p^{(1)})}$$

$$= G_1(E) + \sum_{p,q} \frac{-\kappa_{pq}|p^{(0)}\rangle\langle q^{(0)}| + \kappa_{qp}|q^{(0)}\rangle\langle p^{(0)}|}{E - (\varepsilon_p^{(0)} + \varepsilon_p^{(1)})}. \quad (24)$$

In this improvement, perturbation effects on MOs through $\kappa$ are added. If the self-energies of electrodes are given as perturbation Hamiltonian, transmission probabilities can be calculated by the conventional method based on these Green’s functions.

3. Calculation Methods
3.1. Perturbation Hamiltonian inducing electronic structures with electric currents

In this subsection, we show how we construct a perturbation Hamiltonian giving electronic structures with electric currents. We focus on a channel molecule between two electrodes (see Fig. 1). The Hamiltonian of the whole system, $H_{\text{whole}}$, can be written as,

$$H_{\text{whole}} = \begin{pmatrix} H_{LL} & H_{LM} & H_{LR} \\ H_{ML} & H_{MM} & H_{MR} \\ H_{RL} & H_{RM} & H_{RR} \end{pmatrix}, \quad (25)$$

where the indices $L$, $R$, and $M$ represent the left electrode, the right electrode, and the channel molecule, respectively. Since interactions between the two electrodes are negligibly small, $H_{LR} = H_{RL} = 0$. $H_{MM}$ is regarded as $F^{(0)}$ in (6). The self-energy of the left electrode, $\Sigma_L(E)$, can be calculated by using the following equation [15],

$$\Sigma_L(E) = H_{ML} g_L(E) H_{LM}, \quad (26)$$
where $E$ is the energy of electrons passing through the channel molecule, and $g_L(E)$ is the surface Green’s function of the left electrode. $\Sigma_R(E)$ for the right electrode can be obtained as the same form. The derivation of $g_{L,R}(E)$ is discussed in the later part of this subsection. $\Sigma_{L,R}(E)$ generates the outflow of electrons from the channel molecule, while $\Sigma_{L,R}^\dagger(E)$ represents the inflow. We define the matrix $\Sigma(E)$ as,

$$\Sigma(E) = \left( \Sigma_L(E) + \Sigma_R^\dagger(E) \right) \left( 1 - f_L(E) \right) f_R(E)$$

$$+ \left( \Sigma_L^\dagger(E) + \Sigma_R(E) \right) f_L(E) \left( 1 - f_R(E) \right),$$  \hspace{1cm} \text{(27)}$$

where $f_L(E)$ and $f_R(E)$ are FD distribution functions for the left and right electrodes, respectively. The first term induces electrons which pass from the right electrode to the left one, while the second term induces the opposite flow. Both terms are weighted by $f_L(E)$ and $f_R(E)$. In this study, zero Kelvin is assumed in $f_L(E)$ and $f_R(E)$. The perturbation Hamiltonian inducing electronic currents is given by the following equation,

$$H^{(1)} = \int_{-\infty}^{\infty} \Sigma(E) w(E) dE,$$  \hspace{1cm} \text{(28)}$$

where $w(E)$ is the DOS for the channel molecule. $H^{(1)}$ includes transmission effects through $f_{L,R}(E)$ and $w(E)$. $w(E)$ is given by using the orbital energy, $\varepsilon_p$, and its width, $\gamma_p$, as,

$$w(E) = \frac{1}{\pi} \sum_p \frac{\gamma_p}{(E - \varepsilon_p)^2 + \gamma_p^2}.$$  \hspace{1cm} \text{(29)}$$

$\varepsilon_p$ and $\gamma_p$ are determined as,

$$\varepsilon_p = \varepsilon_p^{(0)} + \text{Re}(\varepsilon_p^{(1)}),$$

$$\gamma_p = \text{Im}(\varepsilon_p^{(1)}),$$  \hspace{1cm} \text{(30)}$$

(31)

and hence $H^{(1)}$ depends on itself. Therefore, perturbation calculations are repeated iteratively until $H^{(1)}$ becomes self-consistent.

There are various calculation methods for $g_{L,R}$. In this study, we adopt the method proposed by Shimazaki et al. [13] due to its simplicity. In this method, a one-dimensional electrode is assumed. Then $g_L$ is given as,

$$g_L = \exp(ikc)/\beta_L,$$  \hspace{1cm} \text{(32)}$$

$$E = \alpha_L + 2\beta_L \cos(kc),$$  \hspace{1cm} \text{(33)}$$

where $\alpha_L$ is the Fermi energy of the left electrode, and $\beta_L$ is the nearest-neighbor electronic coupling element [15, 19]. The sign of $k$ is determined so that it represents the outflow of electrons. $g_R$ is given in the same form. In this study, $\beta_{L,R}$ is fixed as $\beta_{L,R} = -3.00$ eV [13]. $\alpha_L$ is given by the following equation,

$$\alpha_L = E_F - \frac{eV_D}{2},$$  \hspace{1cm} \text{(34)}$$

where $E_F$ is the Fermi energy of the channel molecule, $e$ is the elementary charge, and $V_D$ is the bias voltage. In this study, $E_F$ is fixed as $E_F = -4.77$ eV [13]. Similarly, $\alpha_R$ is given as,

$$\alpha_R = E_F + \frac{eV_D}{2}.$$  \hspace{1cm} \text{(35)}$$
3.2. Computational models
In this work, the method explained above is applied to BDT and DHBDT. Optimized structures of them are shown in Fig. 2. DHBDT is composed of BDT and two additional hydrogen atoms. This molecule is used for the comparison between the effects of \( \pi \) and \( \sigma \) electrons. The sulfur atoms at the ends of the molecules are implicitly assumed to be connected to one-dimensional gold nanowire electrodes with coupling constants, \(-2.0\) eV, through \(3p_x\) and \(3p_y\) atomic orbitals. The STO-6G basis set [20, 21] is used for all the atoms. Optimized structures are obtained by using Gaussian 09 [22] at the HF level, and CPHF computations are performed by using our original code.

4. Results and Discussion
Computed energies of the lowest unoccupied MO (LUMO), the highest occupied MO (HOMO), HOMO-1, and HOMO-2 for BDT and DHBDT are summarized in Table 1. As for occupied MOs, HOMO-1 and HOMO-2 of BDT have larger absolute values of Im(\(\varepsilon^{(1)}\)) than that of HOMO. For DHBDT, on the other hand, HOMO-1 has a larger value, followed by HOMO and HOMO-2. This is investigated in relation to electronic structures of MOs shown in Fig. 3. HOMO of BDT and HOMO-2 of DHBDT, which have smaller values of Im(\(\varepsilon^{(1)}\)), have similar structures. Hence, it can be speculated that the MOs consisting of \(\pi\) bonds have small Im(\(\varepsilon^{(1)}\)). It is noted that the smaller values of Im(\(\varepsilon^{(1)}\)) of DHBDT than those of BDT are mainly due to wider HOMO-LUMO gap. The wide HOMO-LUMO gap induces small \( w(E) \) in (29) around \( E_F \), and the perturbation effects are smaller.

In order to improve the results in this study, a larger basis set should be used. Actually, the STO-6G basis set provides poor results for orbital energies of BDT. Results from our method strongly depend on orbital energies of the channel molecule through (29), and hence a larger basis set probably improves the results. In addition, several theoretical reports show the importance of electron correlation [14, 23]. Therefore, our method should be extended to
post-HF computations. This is our future task.

Previously, we have reported the local currents and conductivities of nanomaterials [24, 25, 26, 27]. These local quantities are defined in rigged quantum electrodynamics [28, 29] and useful for understanding effects of defects, impurities, or interfaces on conductive properties. In our future study, our method will be applied in order to obtain these local quantities.

5. Conclusion
In this study, we report on a method for investigating conductive properties of a system composed of a channel molecule and electrodes. Our method is based on CPHF equations for non-Hermitian perturbation Hamiltonians. In our method, perturbed MOs can be determined so as to be consistent with perturbed Coulomb and exchange interactions between electrons at the HF level. A non-Hermitian perturbation Hamiltonian which describes interactions with electrodes is also introduced. For this Hamiltonian, the effects of electrodes are included through the statistical distributions of electrons. The Hamiltonian also includes the effect of the DOS of a channel molecule. The BDT and DHBDT are analyzed by our method, and the first order perturbations of MO energies of them are computed.

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