

# Polarization Propagator and Equation of Motion Methods

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## 1 Derivation of general propagator methods

We have derived earlier a response function, or frequency dependent polarizability,

$$\Pi(BA|\omega) = \lim_{\eta \rightarrow 0} \left( \frac{1}{\hbar} \right) \sum_{n \neq 0} \left\{ \frac{\langle 0|B|n\rangle\langle n|A|0\rangle}{\omega + i\eta - \omega_{0n}} - \frac{\langle 0|A|n\rangle\langle n|B|0\rangle}{\omega + i\eta + \omega_{0n}} \right\} \quad (1)$$

where  $A$  is the applied perturbation, and  $B$  is the observable, and both are assumed to be Hermitian.  $\omega_{0n}$  is the excitation energy for the change between states 0 and  $n$ . It should be clear that the response function has poles when  $\omega$  — the applied field frequency — equals to the excitation energy  $\omega_{0n}$ . Finding these poles is precisely the goal of polarization propagator methods. In the polarization propagator approach, the above equation has  $\eta$  set to 0, and the response function (the ‘propagator’), defined as:

$$\langle\langle B; A \rangle\rangle_{\omega} \equiv \sum_{n \neq 0} \left\{ \frac{\langle 0|B|n\rangle\langle n|A|0\rangle}{\hbar\omega - \hbar\omega_{0n}} + \frac{\langle 0|A|n\rangle\langle n|B|0\rangle}{-\hbar\omega - \hbar\omega_{0n}} \right\} \quad (2)$$

Now we want to describe the propagator in terms of commutators between  $A$  and  $B$ . Make the observation that  $\frac{ab}{c+d} = \frac{ab}{c} - \frac{d}{c} \left( \frac{ab}{c+d} \right)$ , and applying to the first term of eq. (2) yields:

$$\sum_{n \neq 0} \frac{\langle 0|B|n\rangle\langle n|A|0\rangle}{\hbar\omega - \hbar\omega_{0n}} = \sum_{n \neq 0} \frac{\langle 0|B|n\rangle\langle n|A|0\rangle}{\hbar\omega} - \sum_{n \neq 0} \frac{-\hbar\omega_{0n}\langle 0|B|n\rangle\langle n|A|0\rangle}{\hbar\omega(\hbar\omega - \hbar\omega_{0n})} \quad (3)$$

Do the same for the second term of eq. (2) and combine, recognizing that the  $n = 0$  term vanishes in the first part (thus we get a sum over all  $n$ ):

$$\begin{aligned} \langle\langle B; A \rangle\rangle_{\omega} &= \frac{1}{\hbar\omega} \sum_n \{ \langle 0|B|n\rangle\langle n|A|0\rangle - \langle 0|A|n\rangle\langle n|B|0\rangle \} \\ &\quad - \frac{1}{\hbar\omega} \sum_{n \neq 0} \left\{ \frac{-\hbar\omega_{0n}\langle 0|B|n\rangle\langle n|A|0\rangle}{\hbar\omega - \hbar\omega_{0n}} - \frac{-\hbar\omega_{0n}\langle 0|A|n\rangle\langle n|B|0\rangle}{-\hbar\omega - \hbar\omega_{0n}} \right\} \end{aligned} \quad (4)$$

Making use of the fact that  $1 = \sum_n |n\rangle\langle n|$  and  $H|n\rangle = E_n|n\rangle$  and  $\hbar\omega_{0n} = E_n - E_0$ :

$$\langle\langle B; A \rangle\rangle_{\omega} = \frac{1}{\hbar\omega} \langle 0|[B, A]|0\rangle + \frac{1}{\hbar\omega} \sum_{n \neq 0} \left\{ \frac{\langle 0|B|n\rangle\langle n|[H, A]|0\rangle}{\hbar\omega - \hbar\omega_{0n}} + \frac{\langle 0|[H, A]|n\rangle\langle n|B|0\rangle}{-\hbar\omega - \hbar\omega_{0n}} \right\} \quad (5)$$

Which is to say that

$$\langle\langle B; A \rangle\rangle_{\omega} = \frac{1}{\hbar\omega} \langle 0|[B, A]|0\rangle + \frac{1}{\hbar\omega} \langle\langle B; [H, A] \rangle\rangle_{\omega} \quad (6)$$

Or, as we will use it:

$$\hbar\omega\langle\langle B; A \rangle\rangle_\omega = \langle 0 | [B, A] | 0 \rangle - \langle\langle [H, B]; A \rangle\rangle_\omega \quad (7)$$

As you may have started to see, we can define the propagator iteratively in terms of commutator expectation values of ever-increasing complexity. This is what is known as the so-called “moment expansion” of the propagator. Thus by iteration:

$$\langle\langle B; A \rangle\rangle_\omega = \frac{1}{\hbar\omega} \left\{ \langle 0 | [B, A] | 0 \rangle + \left( \frac{-1}{\hbar\omega} \right) \langle 0 | [[H, B], A] | 0 \rangle + \left( \frac{-1}{\hbar\omega} \right)^2 \langle 0 | [[H, [H, B]], A] | 0 \rangle + \dots \right\} \quad (8)$$

We introduce the “superoperator” (analogous to the Liouville operator in Statistical Mechanics), which acts on operators to give their commutator:

$$\hat{H}B = [H, B], \quad \hat{H}^2B = [H, [H, B]], \quad \hat{H}^3B = [H, [H, [H, B]]], \quad \dots \quad (9)$$

With this definition, we have the power series

$$\langle\langle B; A \rangle\rangle_\omega = \frac{1}{\hbar\omega} \sum_{n=0}^{\infty} \left( \frac{-1}{\hbar\omega} \right)^n \langle 0 | [\hat{H}^n B, A] | 0 \rangle \quad (10)$$

At this point we make two useful observations. First, recognize that

$$\langle 0 | [\hat{H}B, A] | 0 \rangle = -\langle 0 | [B, \hat{H}A] | 0 \rangle \quad (11)$$

and so  $\hat{H}$  can be applied to  $A$  instead of  $B$  insofar as we introduce a factor of  $(-1)^n$ . Furthermore, note that the power series is equivalent to

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + \dots \quad (12)$$

Making use of these two observations (and using  $\hat{1}X = X$  and  $\hat{H}^0 = \hat{1}$ , where  $\hat{1}$  is the unit superoperator), we have

$$\langle\langle B; A \rangle\rangle_\omega = \langle 0 | \left[ B, \left( \hbar\omega\hat{1} - \hat{H} \right)^{-1} A \right] | 0 \rangle \quad (13)$$

Which is merely a cosmetic change at this point, as the superoperator resolvent is defined by the series expansion. We need to find a matrix representation of the resolvent, which implies that we find a complete basis set of operators. To do this, we are going to develop an “operator space”, where  $\hat{H}$  is defined by its effect on operators instead of vectors. Introducing the notation

$$(X|Y) = \langle 0 | [X^\dagger, Y] | 0 \rangle \quad (14)$$

and it follows that  $(Y|X) = (X|Y)^*$ . As defined, we now have

$$\langle\langle B; A \rangle\rangle_\omega = \left( B^\dagger | \left( \hbar\omega\hat{1} - \hat{H} \right)^{-1} | A \right) \quad (15)$$

Which is formally exact, albeit useless until we develop approximations. However, the form of the above equation *does* look similar to ordinary vector spaces in Hartree-Fock, *etc.* methods. Truncation of a basis in linear vector space  $V$  to  $n$  elements produces a subspace  $V_n$ , and truncation of a general vector corresponds to finding its projection onto the subspace. It follows, then, that we need to find a projection operator  $\rho$ , associated with the truncated basis. If the basis ( $\mathbf{e}$ , say) is orthonormal we write

$$\rho = \sum_i e_i e_i^* = \mathbf{e} \mathbf{e}^\dagger \quad (16)$$

which in a complete basis gives:

$$\rho = \sum_i |e_i\rangle\langle e_i| = \mathbf{1} \quad (17)$$

If it is not an orthonormal basis, we must include the metric matrix  $\mathbf{S} = \mathbf{e}^\dagger \mathbf{e}$  (or Löwdin basis  $\bar{\mathbf{e}}\mathbf{S}^{-1/2}$ ):

$$\rho = \mathbf{e}\mathbf{S}^{-1}\mathbf{e}^\dagger = \sum_{ij} e_i(S^{-1})_{ij}e_j^* \quad (18)$$

When using a truncated basis in *operator space*, two kinds of projections are useful (Löwdin, 1977, 1982),

$$A' = \rho A \rho, \quad A'' = A^{1/2} \rho A^{1/2} \quad (19)$$

which are the *outer projection* and *inner projection*, respectively, onto space  $V_n$  defined by  $\rho$ . Note that  $AB = C \not\Rightarrow A'B' = C' \not\Rightarrow A''B'' = C''$ . Plugging the metric into  $A''$ :

$$A'' = A^{1/2} \mathbf{e}\mathbf{S}^{-1} \mathbf{e}^\dagger A^{1/2} \quad (20)$$

and we define

$$\mathbf{f} \equiv A^{1/2} \mathbf{e} = \begin{pmatrix} A^{1/2} \mathbf{e}_1 & A^{1/2} \mathbf{e}_1 & \dots \end{pmatrix} \quad (21)$$

We assume that  $A$  is Hermitian and positive-definite, so that  $A^{1/2}$  can be defined. Note that  $\mathbf{S} = \mathbf{e}^\dagger \mathbf{e} = (A^{-1/2} \mathbf{f})^\dagger (A^{-1/2} \mathbf{f}) = \mathbf{f}^\dagger A^{-1} \mathbf{f} \Rightarrow A'' = \mathbf{f} (\mathbf{f}^\dagger A^{-1} \mathbf{f})^{-1} \mathbf{f}^\dagger$ . Because  $A$  is arbitrary, replace it with  $A^{-1}$ , and since  $\mathbf{f}^\dagger \mathbf{A} \mathbf{f} = \mathbf{A}$  with  $A_{ij} = \langle f_i | A | f_j \rangle$ :

$$(\mathbf{A}^{-1})'' = \mathbf{f} (\mathbf{f}^\dagger \mathbf{A} \mathbf{f})^{-1} \mathbf{f}^\dagger = \mathbf{f} \mathbf{A}^{-1} \mathbf{f}^\dagger \quad (22)$$

As the basis  $V_n \rightarrow V$ , the inner projection  $\rightarrow \mathbf{A}^{-1}$ , else it is simply a finite basis approximation to the inverse. This is the operator inverse in terms of a matrix inverse. Since  $\mathbf{e}$  was an arbitrary basis defining  $V_n$ , let  $\mathbf{f}$  define  $n$ -dimensional subspace  $V'_n$ . Thus:

$$\mathbf{A}^{-1} \approx \mathbf{e} \mathbf{A}^{-1} \mathbf{e}^\dagger = \sum_{ij} e_i (\mathbf{e}^\dagger \mathbf{A} \mathbf{e})_{ij}^{-1} e_j^* \quad (23)$$

Thus the inner projection leads to an approximation for the projector. Let us define the (as of yet undefined) operator basis:

$$\mathbf{n} = (\mathbf{n}_1 \quad \mathbf{n}_2 \quad \mathbf{n}_3 \quad \dots) \quad (24)$$

Given that the binary product (compare with  $\langle x|y\rangle = x^*y$  for vectors)

$$X^\dagger \cdot Y = (X|Y) = \langle 0| [X^\dagger, Y] |0\rangle \quad (25)$$

then for our resolvent superoperator we have

$$\hat{R}(\omega) = (\hbar\omega\hat{1} - \hat{H})^{-1} = \mathbf{n}R(\omega)\mathbf{n}^\dagger = \sum_{r,s} \mathbf{n}_r [R(\omega)]_{rs} \mathbf{n}_s^\dagger \quad (26)$$

where  $\mathbf{n}_r$  and  $\mathbf{n}_s^\dagger$  are the analogues of  $\mathbf{e}$  and  $\mathbf{e}^*$  in operator space. Finally, if

$$R(\omega) = M(\omega)^{-1}, \quad M(\omega) = \mathbf{n}^\dagger (\hbar\omega\hat{1} - \hat{H}) \mathbf{n} \quad (27)$$

then we have

$$\langle\langle B; A \rangle\rangle_\omega = B \cdot R(\omega) \cdot A = B \cdot \mathbf{n}R(\omega)\mathbf{n}^\dagger \cdot A \quad (28)$$

which is the key to calculating approximations to response properties. The matrix  $M$  is determined once we have chosen an operator basis. This approximation depends on two things: 1) the basis  $\mathbf{n}$  (and its truncations), and 2) the reference function, that is not the exact ground state. Any approximations to these two things are where we get out various response methods.

## 2 Polarization propagator derivation of RPA

When  $A$  and  $B$  are one-electron number conserving, e.g. creation/annihilation operators are in pairs, we have

$$A = \sum_{rs} A_{rs} a_r^\dagger a_s, \quad B = \sum_{rs} B_{rs} a_r^\dagger a_s \quad (29)$$

which allow us to define the general polarization propagator. If the elements did not conserve the number of electrons, we could use the same formalism to get the electron propagator, which can describe the attachment/detachment of electrons from a system, thus describing processes such as ionization. In general, it is sufficient to consider the typical elements  $A \rightarrow a_r^\dagger a_s$  and  $B \rightarrow a_i^\dagger a_u$ . If spin-orbitals of reference are  $\psi_i, \psi_j, \dots$ , then a ‘‘particle-hole’’ basis includes only ‘‘excitation’’ and ‘‘de-excitation’’ operators  $a_a^\dagger a_i$  and  $a_i^\dagger a_a$ , respectively. Thus the basis and its dual:

$$\mathbf{n} = (\mathbf{e} \ \mathbf{d}), \quad \mathbf{n}^\dagger = \begin{pmatrix} \mathbf{e}^\dagger \\ \mathbf{d}^\dagger \end{pmatrix}, \quad e_{ia} = a_a^\dagger a_i = E_{ia}, \quad d_{ai} = a_i^\dagger a_a = E_{ia}^\dagger \quad (30)$$

This gives, for our resolvent,

$$R(\omega) = [\mathbf{n}^\dagger(\hbar\omega\hat{1} - \hat{H})\mathbf{n}]^{-1} = \begin{bmatrix} \mathbf{e}^\dagger(\hbar\omega\hat{1} - \hat{H})\mathbf{e} & \mathbf{e}^\dagger(\hbar\omega\hat{1} - \hat{H})\mathbf{d} \\ \mathbf{d}^\dagger(\hbar\omega\hat{1} - \hat{H})\mathbf{e} & \mathbf{d}^\dagger(\hbar\omega\hat{1} - \hat{H})\mathbf{d} \end{bmatrix}^{-1} \quad (31)$$

As an example, we give the elements of the first block:

$$E_{ia}^\dagger(\hbar\omega\hat{1} - \hat{H})E_{jb} = \hbar\omega E_{ia}^\dagger E_{jb} - E_{ia}^\dagger [H, E_{jb}] \quad (32)$$

with scalar products

$$E_{ia}^\dagger E_{jb} = \langle \psi_0 | [E_{ia}^\dagger, E_{jb}] | \psi_0 \rangle, \quad E_{ia}^\dagger [H, E_{jb}] = \langle \psi_0 | [E_{ia}^\dagger, [H, E_{jb}]] | \psi_0 \rangle \quad (33)$$

Evaluating these products gives

$$E_{ia}^\dagger E_{jb} = \langle \psi_0 | [E_{ia}^\dagger, E_{jb}] | \psi_0 \rangle = \langle \psi_0 | E_{ia}^\dagger E_{jb} | \psi_0 \rangle - \langle \psi_0 | E_{jb} E_{ia}^\dagger | \psi_0 \rangle = \langle \psi_0 | E_{ia}^\dagger E_{jb} | \psi_0 \rangle = \delta_{ia,jb} \quad (34)$$

and

$$\begin{aligned} E_{ia}^\dagger [H, E_{jb}] &= \langle \psi_0 | [E_{ia}^\dagger, [H, E_{jb}]] | \psi_0 \rangle \\ &= \langle \psi_0 | E_{ia}^\dagger H E_{jb} | \psi_0 \rangle - \langle \psi_0 | E_{ia}^\dagger E_{jb} H | \psi_0 \rangle - \langle \psi_0 | H E_{jb} E_{ia}^\dagger | \psi_0 \rangle + \langle \psi_0 | E_{jb} H E_{ia}^\dagger | \psi_0 \rangle \\ &= \langle \psi_i^a | H | \psi_j^b \rangle - \delta_{ia} \delta_{jb} \langle \psi_0 | H | \psi_0 \rangle \quad * \text{ see (11) of Maurice \& Head-Gordon IJQC (1995)} \\ &= E_0 \delta_{ij} \delta_{ab} + F_{ab} \delta_{ij} - F_{ij} \delta_{ab} + \langle a j | i b \rangle - \delta_{ia} \delta_{jb} E_0 \\ &= (\epsilon_a - \epsilon_i) \delta_{ia} \delta_{ab} + \langle a j | i b \rangle = \mathbf{A} \end{aligned} \quad (35)$$

Which is precisely the same elements as we have derived earlier for TDHF. Completing the rest, we have:

$$R(\omega) = M(\omega)^{-1} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} - \hbar\omega \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{bmatrix} \quad (36)$$

With  $\mathbf{B} = \langle ab || ij \rangle$ . Now, we saw from the definition of the resolvent that  $R(\omega) \rightarrow \infty$  at  $\omega \rightarrow \omega_{0n}$ , which are the poles of  $R(\omega)$ . Therefore,  $R(\omega)^{-1} \rightarrow 0$  and

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} = \hbar\omega \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} \quad (37)$$

which are the RPA/TDHF equations. The eigencolumns determine the linear combinations of excitation and de-excitation operators that produce corresponding approximate excited states when working on the reference state  $|\psi_0\rangle$ .

### 3 Equation of Motion (EOM) derivation of RPA

Given an *exact* ground state, we can say that

$$H|n\rangle = E_n|n\rangle \quad (38)$$

Define operator  $Q_n^\dagger$  and  $Q_n$ :

$$|n\rangle = Q_n^\dagger|0\rangle, \quad Q_n|0\rangle = 0 \implies Q_n^\dagger = |n\rangle\langle 0| \quad (39)$$

These operators generate excited states from the ground state (*not* excited determinants, as in the case of post-HF correlation methods). So it is clear that, when acting on an exact ground state:

$$[H, Q_n^\dagger]|0\rangle = (E_n - E_0)Q_n^\dagger|0\rangle = \hbar\omega_{0n}Q_n^\dagger|0\rangle \quad (40)$$

Multiply on left by arbitrary state of form  $\langle 0|\delta Q$ , giving

$$\langle 0|[\delta Q, [H, Q_n^\dagger]]|0\rangle = \hbar\omega_{0n}\langle 0|[\delta Q, Q_n^\dagger]|0\rangle \quad (41)$$

Where we have made use of the fact that  $\langle 0|Q_n^\dagger = \langle 0|HQ_n^\dagger = 0$ . Note that if we express  $Q$  by particle-hole operators  $a_p^\dagger a_q$ ,  $a_p^\dagger a_q^\dagger a_r a_s$  with coefficients  $C_{pq}$  and  $C_{pqrs}$ , then  $\delta Q$  is given by  $\frac{\partial Q}{\partial C}\delta C$  for arbitrary variations  $\delta C$ . These are in principle exact, since  $\delta Q|0\rangle$  exhausts the whole Hilbert space, such that the above equation corresponds to the full Schrödinger equation. Tamm-Dancoff (or Configuration Interaction Singles) can be obtained by approximating  $|0\rangle \rightarrow |\text{HF}\rangle$  and the operator  $Q_n^\dagger = \sum_{ia} C_{ia} a_a^\dagger a_i$ , restricting ourselves to 1p-1h excitations. Thus  $\delta Q|0\rangle = \sum_{ia} a_a^\dagger a_i |\text{HF}\rangle \delta C_{ai}$ , ( $\delta C_{ai}$  cancels), and

$$\sum_{bj} \langle \text{HF} | [a_i^\dagger a_a, [H, a_b^\dagger a_j]] | \text{HF} \rangle C_{jb} = \hbar\omega \langle \text{HF} | [a_i^\dagger a_a, a_a^\dagger a_i] | \text{HF} \rangle C_{ia} \quad (42)$$

These are the CIS equations. Put another way:

$$\sum_{bj} \{(\epsilon_a - \epsilon_i)\delta_{ab}\delta_{ij} + \langle aj||ib\rangle\} C_{bj} = E^{CIS} C_{ai} \quad (43)$$

Similarly, for RPA/TDHF, if we consider a ground state containing 2p-2h correlations, we can not only create a p-h pair, but also destroy one. Thus (choosing the minus sign for convenience):

$$Q_n^\dagger = \sum_{ia} X_{ia} a_a^\dagger a_i - \sum_{ia} Y_{ia} a_i^\dagger a_a, \quad \text{and } Q_n|RPA\rangle = 0 \quad (44)$$

So instead of the basis of only single excitations, and therefore one matrix  $C_{ia}$ , we work in a basis of single excitations and single de-excitations, and have two matrices  $X_{ia}$  and  $Y_{ia}$ . We also have two kinds of variations  $\delta Q|0\rangle$ , namely  $a_a^\dagger a_i|0\rangle$  and  $a_i^\dagger a_a|0\rangle$ . This gives us two sets of equations:

$$\begin{aligned} \langle \text{RPA} | [a_i^\dagger a_a, [H, Q_n^\dagger]] | \text{RPA} \rangle &= \hbar\omega \langle \text{RPA} | [a_i^\dagger a_a, Q_n^\dagger] | \text{RPA} \rangle \\ \langle \text{RPA} | [a_a^\dagger a_i, [H, Q_n^\dagger]] | \text{RPA} \rangle &= \hbar\omega \langle \text{RPA} | [a_a^\dagger a_i, Q_n^\dagger] | \text{RPA} \rangle \end{aligned} \quad (45)$$

These contain only expectation values of our four Fermion operators, which cannot be calculated since we still do not know  $|\text{RPA}\rangle$ . Thus we assume  $|\text{RPA}\rangle \rightarrow |\text{HF}\rangle$ . This gives

$$\langle \text{RPA} | [a_i^\dagger a_a, a_b^\dagger a_j] | \text{RPA} \rangle = \langle \text{HF} | [a_i^\dagger a_a, a_b^\dagger a_j] | \text{HF} \rangle = \delta_{ij}\delta_{ab} \quad (46)$$

The probability of finding states  $a_a^\dagger a_i|0\rangle$  and  $a_i^\dagger a_a|0\rangle$  in excited state  $|n\rangle$ , that is, the p-h and h-p matrix elements of transition density matrix  $\rho^{(1)}$  are:

$$\rho_{ai}^{(1)} = \langle 0 | a_i^\dagger a_a | n \rangle \simeq \langle \text{HF} | [a_i^\dagger a_a, Q_n^\dagger] | \text{HF} \rangle = X_{ia} \quad (47)$$

$$\rho_{ia}^{(1)} = \langle 0 | a_a^\dagger a_i | n \rangle \simeq \langle \text{HF} | [a_a^\dagger a_i, Q_n^\dagger] | \text{HF} \rangle = Y_{ia} \quad (48)$$

Thus altogether

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} = \hbar\omega \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} \quad (49)$$

with

$$A_{ia,jb} = \langle \text{HF} | [a_i^\dagger a_a, [H, a_b^\dagger a_j]] | \text{HF} \rangle \quad (50)$$

and

$$B_{ia,jb} = -\langle \text{HF} | [a_i^\dagger a_a, [H, a_j^\dagger a_b]] | \text{HF} \rangle \quad (51)$$

which are the TDHF/RPA equations.