Quantum finite many-body system

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Contents

Chapter 1

Linear response theory

1.1 Time-dependent Hartree-Fock equation

The time-dependent Hartree-Fock equation can be written in the small amplitude limit,

$$i\hbar\frac{\partial}{\partial t}\delta\psi_h(\boldsymbol{r}t) = \left(h(\boldsymbol{r})-\epsilon_h^0\right)\delta\psi_h(\boldsymbol{r}t)+\left[\int d\boldsymbol{r}'\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r}')}\delta\rho(\boldsymbol{r}'t)+f(\boldsymbol{r}t)\right]\phi_h(\boldsymbol{r}) \tag{1.1}$$

under following small amplitude conditions,

$$h(\boldsymbol{r})\phi_h(\boldsymbol{r}) = \epsilon_h^0\phi_h(\boldsymbol{r}) \tag{1.2}$$
$$h(\boldsymbol{r})\phi_p(\boldsymbol{r}) = \epsilon_p^0\phi_p(\boldsymbol{r}) \tag{1.3}$$
$$\psi_h(\boldsymbol{r}t) = \left(\phi_h(\boldsymbol{r})+\delta\psi_h(\boldsymbol{r}t)\right)e^{-i\epsilon_h t/\hbar} \tag{1.4}$$
$$\rho(\boldsymbol{r}t) = \sum_h \psi_h^*(\boldsymbol{r}t)\psi_h(\boldsymbol{r}t) \tag{1.5}$$
$$\simeq \rho_0(\boldsymbol{r})+\delta\rho(\boldsymbol{r}t) \tag{1.6}$$

where

$$\rho_0(\boldsymbol{r}) = \sum_h \phi_h^*(\boldsymbol{r})\phi_h(\boldsymbol{r}) \tag{1.7}$$
$$\delta\rho(\boldsymbol{r}t) = \sum_h \left\{\phi_h^*(\boldsymbol{r})\delta\psi_h(\boldsymbol{r}t)+\phi_h(\boldsymbol{r})\delta\psi_h^*(\boldsymbol{r}t)\right\} \tag{1.8}$$

where $h(\boldsymbol{r})$ is the meanfield Hamiltonian. Note that "h" denotes hole states. In this chapter, we use the notation for the single particle states, "p" for particle statees, "k" for all states.

And also note that "ϵ^0" means unperturbed single particle levels defined by Eq.(1.2) and Eq.(1.3).

1.2 RPA equation

By inserting Eq.(1.8) and multiplying $\int d\boldsymbol{r}\phi_p^*(\boldsymbol{r})$ to Eq.(1.1), then we get

$$\begin{aligned}
& i\hbar\frac{\partial}{\partial t}\int d\boldsymbol{r}\phi_p^*(\boldsymbol{r})\delta\psi_h(\boldsymbol{r}t) \\
&= (\epsilon_p^0-\epsilon_h^0)\int d\boldsymbol{r}\phi_p^*(\boldsymbol{r})\delta\psi_h(\boldsymbol{r}t)+\sum_{h'}\iint d\boldsymbol{r}d\boldsymbol{r}'\phi_p^*(\boldsymbol{r})\phi_{h'}^*(\boldsymbol{r}')\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r}')}\phi_h(\boldsymbol{r})\delta\psi_{h'}(\boldsymbol{r}'t) \\
&\quad +\sum_{h'}\iint d\boldsymbol{r}d\boldsymbol{r}'\phi_p^*(\boldsymbol{r})\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r}')}\phi_{h'}(\boldsymbol{r}')\phi_h(\boldsymbol{r})\delta\psi_{h'}^*(\boldsymbol{r}'t)+\int d\boldsymbol{r}\phi_p^*(\boldsymbol{r})f(\boldsymbol{r}t)\phi_h(\boldsymbol{r})
\end{aligned} \tag{1.9}$$

By taking the complex conjugate of Eq.(1.9), we get the equation for $\delta\psi_h^*(\boldsymbol{r}t)$,

$$
\begin{aligned}
&-i\hbar\frac{\partial}{\partial t}\int d\boldsymbol{r}\phi_p(\boldsymbol{r})\delta\psi_h^*(\boldsymbol{r}t) \\
&= (\epsilon_p^0-\epsilon_h^0)\int d\boldsymbol{r}\phi_p(\boldsymbol{r})\delta\psi_h^*(\boldsymbol{r}t)+\sum_{h'}\iint d\boldsymbol{r}d\boldsymbol{r'}\phi_p(\boldsymbol{r})\phi_{h'}(\boldsymbol{r'})\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r'})}\phi_h^*(\boldsymbol{r})\delta\psi_{h'}^*(\boldsymbol{r'}t) \\
&\quad+\sum_{h'}\iint d\boldsymbol{r}d\boldsymbol{r'}\phi_p(\boldsymbol{r})\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r'})}\phi_{h'}^*(\boldsymbol{r'})\phi_h^*(\boldsymbol{r})\delta\psi_{h'}^*(\boldsymbol{r'}t)+\int d\boldsymbol{r}\phi_p(\boldsymbol{r})f(\boldsymbol{r}t)\phi_h^*(\boldsymbol{r})
\end{aligned}
\tag{1.10}
$$

Here we suppose

$$\delta\psi_h(\boldsymbol{r}t)=\sum_p\phi_p(\boldsymbol{r})\delta\psi_{ph}(t) \tag{1.11}$$

and insert this into Eq.(1.9) and Eq.(1.10), then we get

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\delta\psi_{ph}(t)\\ -\delta\psi_{ph}^*(t)\end{pmatrix}=\sum_{p'h'}\begin{pmatrix}A_{ph,p'h'} & B_{ph,p'h'}\\ B_{ph,p'h'}^* & A_{ph,p'h'}^*\end{pmatrix}\begin{pmatrix}\delta\psi_{p'h'}(t)\\ \delta\psi_{p'h'}^*(t)\end{pmatrix}+\begin{pmatrix}f_{ph}(t)\\ f_{ph}^*(t)\end{pmatrix} \tag{1.12}$$

where

$$
\begin{aligned}
A_{ph,p'h'} &= (\epsilon_p^0-\epsilon_h^0)\delta_{pp'}\delta_{hh'}+\iint d\boldsymbol{r}d\boldsymbol{r'}\phi_p^*(\boldsymbol{r})\phi_{h'}^*(\boldsymbol{r'})\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r'})}\phi_h(\boldsymbol{r})\phi_{p'}(\boldsymbol{r'}) && (1.13)\\
B_{ph,p'h'} &= \iint d\boldsymbol{r}d\boldsymbol{r'}\phi_p^*(\boldsymbol{r})\phi_{p'}^*(\boldsymbol{r'})\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r'})}\phi_h(\boldsymbol{r})\phi_{h'}(\boldsymbol{r'}) && (1.14)\\
f_{ph}(t) &= \int d\boldsymbol{r}\phi_p^*(\boldsymbol{r})f(\boldsymbol{r}t)\phi_h(\boldsymbol{r}) && (1.15)
\end{aligned}
$$

If we suppose in Eq.(1.12),

$$
\begin{aligned}
\delta\psi_{ph}(t) &= \rho_{ph}^{(1)}(\omega)e^{-i\omega t}+\rho_{hp}^{(1)*}(\omega)e^{+i\omega t} && (1.16)\\
f(\boldsymbol{r}t) &= f(\boldsymbol{r})e^{-i\omega t}+f^*(\boldsymbol{r})e^{+i\omega t} && (1.17)
\end{aligned}
$$

Then finally we get

$$\sum_{p'h'}\left[\begin{pmatrix}A_{ph,p'h'} & B_{ph,p'h'}\\ B_{ph,p'h'}^* & A_{ph,p'h'}^*\end{pmatrix}-\hbar\omega\begin{pmatrix}\delta_{pp'}\delta_{hh'} & 0\\ 0 & -\delta_{pp'}\delta_{hh'}\end{pmatrix}\right]\begin{pmatrix}\rho_{p'h'}^{(1)}(\omega)\\ \rho_{h'p'}^{(1)}(\omega)\end{pmatrix}=-\begin{pmatrix}f_{ph}\\ f_{hp}\end{pmatrix} \tag{1.18}$$

where $f_{ph}=\langle p|f|h\rangle$.
By using Eq.(A.27) and Eq.(A.30), we can derive

$$
\begin{aligned}
&\left[\begin{pmatrix}A_{ph,p'h'} & B_{ph,p'h'}\\ B_{ph,p'h'}^* & A_{ph,p'h'}^*\end{pmatrix}-\hbar\omega\begin{pmatrix}\delta_{pp'}\delta_{hh'} & 0\\ 0 & -\delta_{pp'}\delta_{hh'}\end{pmatrix}\right] \\
&=\sum_\nu\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}X_{ph}^\nu & Y_{ph}^{\nu*}\\ Y_{ph}^\nu & X_{ph}^{\nu*}\end{pmatrix}\left[\hbar\omega_\nu\begin{pmatrix}1&0\\0&-1\end{pmatrix}-\hbar\omega_\nu\begin{pmatrix}1&0\\0&1\end{pmatrix}\right]\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}X_{p'h'}^\nu & Y_{p'h'}^{\nu*}\\ Y_{p'h'}^\nu & X_{p'h'}^{\nu*}\end{pmatrix}^\dagger\begin{pmatrix}1&0\\0&-1\end{pmatrix}
\end{aligned}
\tag{1.19}
$$

The inverse matrix, therefore, can be found very easily,

$$
\begin{aligned}
&\left[\begin{pmatrix} A_{ph,p'h'} & B_{ph,p'h'} \\ B^*_{ph,p'h'} & A^*_{ph,p'h'} \end{pmatrix} - \hbar\omega \begin{pmatrix} \delta_{pp'}\delta_{hh'} & 0 \\ 0 & -\delta_{pp'}\delta_{hh'} \end{pmatrix}\right]^{-1} \\
&= \frac{1}{\hbar}\sum_{\nu} \begin{pmatrix} X^{\nu}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu *}_{ph} \end{pmatrix} \begin{pmatrix} \frac{1}{\omega_\nu-\omega} & 0 \\ 0 & \frac{1}{\omega_\nu+\omega} \end{pmatrix} \begin{pmatrix} X^{\nu *}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu}_{ph} \end{pmatrix} \\
&= \frac{1}{\hbar}\sum_{\nu} \begin{pmatrix} \frac{X^{\nu}_{ph}X^{\nu *}_{p'h'}}{\omega_\nu-\omega} + \frac{Y^{\nu *}_{ph}Y^{\nu}_{p'h'}}{\omega_\nu+\omega} & \frac{X^{\nu}_{ph}Y^{\nu *}_{p'h'}}{\omega_\nu-\omega} + \frac{Y^{\nu *}_{ph}X^{\nu}_{p'h'}}{\omega_\nu+\omega} \\ \frac{Y^{\nu}_{ph}X^{\nu *}_{p'h'}}{\omega_\nu-\omega} + \frac{X^{\nu *}_{ph}Y^{\nu}_{p'h'}}{\omega_\nu+\omega} & \frac{Y^{\nu}_{ph}Y^{\nu *}_{p'h'}}{\omega_\nu-\omega} + \frac{X^{\nu *}_{ph}X^{\nu}_{p'h'}}{\omega_\nu+\omega} \end{pmatrix} &(1.20)\\
&= \frac{1}{\hbar}\sum_{\nu} \begin{pmatrix} \frac{\langle 0|b_h a_p|\nu\rangle\langle\nu|a^\dagger_{p'}b^\dagger_{h'}|0\rangle}{\omega_\nu-\omega} + \frac{\langle 0|a^\dagger_{p'}b^\dagger_{h'}|\nu\rangle\langle\nu|b_h a_p|0\rangle}{\omega_\nu+\omega} & \frac{\langle 0|b_h a_p|\nu\rangle\langle\nu|b_{h'} a_{p'}|0\rangle}{\omega_\nu-\omega} + \frac{\langle 0|b_{h'} a_{p'}|\nu\rangle\langle\nu|b_h a_p|0\rangle}{\omega_\nu+\omega} \\ \frac{\langle 0|a^\dagger_p b^\dagger_h|\nu\rangle\langle\nu|a^\dagger_{p'}b^\dagger_{h'}|0\rangle}{\omega_\nu-\omega} + \frac{\langle 0|a^\dagger_{p'}b^\dagger_{h'}|\nu\rangle\langle\nu|a^\dagger_p b^\dagger_h|0\rangle}{\omega_\nu+\omega} & \frac{\langle 0|a^\dagger_p b^\dagger_h|\nu\rangle\langle\nu|b_{h'} a_{p'}|0\rangle}{\omega_\nu-\omega} + \frac{\langle 0|b_{h'} a_{p'}|\nu\rangle\langle\nu|a^\dagger_p b^\dagger_h|0\rangle}{\omega_\nu+\omega} \end{pmatrix} &(1.21)
\end{aligned}
$$

The response function is defined by

$$
\begin{pmatrix} \rho^{(1)}_{p'h'}(\omega) \\ \rho^{(1)}_{h'p'}(\omega) \end{pmatrix} = \sum_{p'h'} \begin{pmatrix} R_{ph,p'h'}(\omega) & R_{ph,h'p'}(\omega) \\ R_{hp,p'h'}(\omega) & R_{hp,h'p'}(\omega) \end{pmatrix} \begin{pmatrix} f_{p'h'} \\ f_{h'p'} \end{pmatrix} \tag{1.22}
$$

therefore

$$
\begin{aligned}
&\begin{pmatrix} R_{ph,p'h'}(\omega) & R_{ph,h'p'}(\omega) \\ R_{hp,p'h'}(\omega) & R_{hp,h'p'}(\omega) \end{pmatrix} \\
&= \frac{1}{\hbar}\sum_{\nu} \begin{pmatrix} \frac{\langle 0|b_h a_p|\nu\rangle\langle\nu|a^\dagger_{p'}b^\dagger_{h'}|0\rangle}{\omega-\omega_\nu} - \frac{\langle 0|a^\dagger_{p'}b^\dagger_{h'}|\nu\rangle\langle\nu|b_h a_p|0\rangle}{\omega+\omega_\nu} & \frac{\langle 0|b_h a_p|\nu\rangle\langle\nu|b_{h'} a_{p'}|0\rangle}{\omega-\omega_\nu} + \frac{\langle 0|b_{h'} a_{p'}|\nu\rangle\langle\nu|b_h a_p|0\rangle}{\omega+\omega_\nu} \\ \frac{\langle 0|a^\dagger_p b^\dagger_h|\nu\rangle\langle\nu|a^\dagger_{p'}b^\dagger_{h'}|0\rangle}{\omega-\omega_\nu} + \frac{\langle 0|a^\dagger_{p'}b^\dagger_{h'}|\nu\rangle\langle\nu|a^\dagger_p b^\dagger_h|0\rangle}{\omega+\omega_\nu} & \frac{\langle 0|a^\dagger_p b^\dagger_h|\nu\rangle\langle\nu|b_{h'} a_{p'}|0\rangle}{\omega-\omega_\nu} + \frac{\langle 0|b_{h'} a_{p'}|\nu\rangle\langle\nu|a^\dagger_p b^\dagger_h|0\rangle}{\omega+\omega_\nu} \end{pmatrix} &(1.23)
\end{aligned}
$$

Then we find

$$
R_{kq,k'q'}(\omega) = \frac{1}{\hbar}\sum_{\nu}\left\{\frac{\langle 0|c^\dagger_q c_k|\nu\rangle\langle\nu|c^\dagger_{k'}c_{q'}|0\rangle}{\omega-\omega_\nu} - \frac{\langle 0|c^\dagger_{k'}c_{q'}|\nu\rangle\langle\nu|c^\dagger_q c_k|0\rangle}{\omega+\omega_\nu}\right\} \tag{1.24}
$$

1.3 Bethe-Salpeter equation

Here combinning Eq.(1.11) and Eq.(1.16), we defined as,

$$
\begin{aligned}
\delta\psi_h(\boldsymbol{r}t) &= \sum_p \phi_p(\boldsymbol{r})\delta\psi_{ph}(t) \\
&= \sum_p \phi_p(\boldsymbol{r})\left(\rho^{(1)}_{ph}(\omega)e^{-i\omega t} + \rho^{(1)*}_{hp}(\omega)e^{+i\omega t}\right) \\
&\equiv X_h(\boldsymbol{r}\omega)e^{-i\omega t} + Y_h(\boldsymbol{r}\omega)e^{+i\omega t} &(1.25)
\end{aligned}
$$

and instead of using Eq.(1.8), we suppose

$$
\delta\rho(\boldsymbol{r}t) = \delta\rho(\boldsymbol{r}\omega)e^{-i\omega t} + \delta\rho^*(\boldsymbol{r}\omega)e^{+i\omega t} \tag{1.26}
$$

and also use Eq.(1.17) in Eq.(1.1), then we obtain

$$
\begin{aligned}
\left[\hbar\omega - h(\boldsymbol{r}) + \epsilon^0_h\right] X_h(\boldsymbol{r}) &= \left[\int d\boldsymbol{r}'\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r}')}\delta\rho(\boldsymbol{r}'\omega) + f(\boldsymbol{r})\right]\phi_h(\boldsymbol{r}) &(1.27)\\
Y^*_h(\boldsymbol{r})\left[-\hbar\omega - h(\boldsymbol{r}) + \epsilon^0_h\right] &= \phi^*_h(\boldsymbol{r})\left[\int d\boldsymbol{r}'\frac{\partial h(\boldsymbol{r})}{\partial\rho(\boldsymbol{r}')}\delta\rho(\boldsymbol{r}'\omega) + f(\boldsymbol{r})\right] &(1.28)
\end{aligned}
$$

These equations are so-called "Sturm-Liouville equation", therefore the solution is expressed by the Green's function as,

$$X_h(\boldsymbol{r}) = \int d\boldsymbol{r}' G_0(\boldsymbol{r}\boldsymbol{r}';\hbar\omega + \epsilon_h^0) \left[\int d\boldsymbol{r}'' \frac{\partial h(\boldsymbol{r}')}{\partial \rho(\boldsymbol{r}'')} \delta\rho(\boldsymbol{r}''\omega) + f(\boldsymbol{r}')\right] \phi_h(\boldsymbol{r}') \tag{1.29}$$

$$Y_h^*(\boldsymbol{r}) = \int d\boldsymbol{r}' \phi_h^*(\boldsymbol{r}') \left[\int d\boldsymbol{r}'' \frac{\partial h(\boldsymbol{r}')}{\partial \rho(\boldsymbol{r}'')} \delta\rho(\boldsymbol{r}''\omega) + f(\boldsymbol{r}')\right] G_0(\boldsymbol{r}'\boldsymbol{r};-\hbar\omega + \epsilon_h^0) \tag{1.30}$$

where the Green's function defined by

$$[\hbar\omega - h(\boldsymbol{r})]G_0(\boldsymbol{r}\boldsymbol{r}';\omega) = \delta(\boldsymbol{r}-\boldsymbol{r}') \tag{1.31}$$

Note that, we used the property of the Green's function $G_0^*(\boldsymbol{r}\boldsymbol{r}') = G_0(\boldsymbol{r}'\boldsymbol{r})$ to derive the equation fot Y_h.

By the way, by inserting Eq.(1.25) into Eq.(1.8), we get

$$\delta\rho(\boldsymbol{r}\omega) = \sum_h \{\phi_h^*(\boldsymbol{r})X_h(\boldsymbol{r}\omega) + Y_h^*(\boldsymbol{r}\omega)\phi_h(\boldsymbol{r})\} \tag{1.32}$$

We insert Eq.(1.29) and Eq.(1.30) into Eq.(1.32), then we get

$$\delta\rho(\boldsymbol{r}\omega) = \int d\boldsymbol{r}' R_0(\boldsymbol{r}\boldsymbol{r}';\omega) \left[\int d\boldsymbol{r}'' \frac{\partial h(\boldsymbol{r}')}{\partial \rho(\boldsymbol{r}'')} \delta\rho(\boldsymbol{r}''\omega) + f(\boldsymbol{r}')\right] \tag{1.33}$$

where

$$R_0(\boldsymbol{r}\boldsymbol{r}';\omega) = \sum_h \left[\phi_h^*(\boldsymbol{r})G_0(\boldsymbol{r}\boldsymbol{r}';\hbar\omega + \epsilon_h^0)\phi_h(\boldsymbol{r}') + \phi_h^*(\boldsymbol{r}')G_0(\boldsymbol{r}'\boldsymbol{r};-\hbar\omega + \epsilon_h^0)\phi_h(\boldsymbol{r})\right] \tag{1.34}$$

If one defines the perturbed response function as

$$\delta\rho(\boldsymbol{r}\omega) = \int d\boldsymbol{r}' R(\boldsymbol{r},\boldsymbol{r}';\omega)\delta\rho(\boldsymbol{r}'\omega) \tag{1.35}$$

then Eq.(1.33) can be rewritten as

$$R(\boldsymbol{r},\boldsymbol{r}';\omega) = R_0(\boldsymbol{r},\boldsymbol{r}';\omega) + \int d\boldsymbol{r}'' R_0(\boldsymbol{r},\boldsymbol{r}'';\omega) \int d\boldsymbol{r}''' \frac{\partial h(\boldsymbol{r}'')}{\partial \rho(\boldsymbol{r}''')} R(\boldsymbol{r}''',\boldsymbol{r}';\omega) \tag{1.36}$$

1.4 Spurious mode

The RPA equation and the transition density are expressed as following,

$$\sum_{p'h'}\left[\begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^*_{php'h'} & A^*_{php'h'}\end{pmatrix} - \hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}\right]\begin{pmatrix}\rho^{(1)}_{p'h'}(\omega) \\ \rho^{(1)}_{h'p'}(\omega)\end{pmatrix} = -\begin{pmatrix} f_{ph} \\ f_{hp}\end{pmatrix} \tag{1.37}$$

$$\delta\rho(\boldsymbol{r}\boldsymbol{r'};\omega) = \sum_{ph}\left[\phi^*_h(\boldsymbol{r'})\phi_p(\boldsymbol{r})\rho^{(1)}_{ph}(\omega) + \rho^{(1)}_{hp}(\omega)\phi^*_p(\boldsymbol{r'})\phi_h(\boldsymbol{r})\right] \tag{1.38}$$

$$= \sum_{h}\left[\phi^*_h(\boldsymbol{r'})X_h(\boldsymbol{r};\omega) + Y^*_h(\boldsymbol{r'};\omega)\phi_h(\boldsymbol{r})\right] \tag{1.39}$$

Note that $\delta\rho(\boldsymbol{r};\omega) = \delta\rho(\boldsymbol{r}\boldsymbol{r};\omega)$.

The bound HF solution breaks translational invariance, *i.e.*, $[P,\rho_0] \neq 0$. Then the RPA equation has a spurious solution. It is so-called Nambu-Goldstone (NG) modes.

$$\sum_{p'h'}\begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^*_{php'h'} & A^*_{php'h'}\end{pmatrix}\begin{pmatrix} P_{p'h'} \\ -P_{h'p'}\end{pmatrix} = 0 \tag{1.40}$$

$$\delta\rho_P(\boldsymbol{r}\boldsymbol{r'}) = \sum_{ph}\left[\phi^*_h(\boldsymbol{r'})\phi_p(\boldsymbol{r})P_{ph} - P_{hp}\phi^*_p(\boldsymbol{r'})\phi_h(\boldsymbol{r})\right] \tag{1.41}$$

where

$$\begin{aligned} P_{ph} &= \langle p|P|h\rangle && (1.42)\\ &= \int d\boldsymbol{r}\phi^*_p(\boldsymbol{r})\left(-i\hbar\overrightarrow{\nabla}_z\right)\phi_h(\boldsymbol{r}) && (1.43)\\ &= \int d\boldsymbol{r}\phi^*_p(\boldsymbol{r})\frac{i\hbar}{2}\left(\overleftarrow{\nabla}_z - \overrightarrow{\nabla}_z\right)\phi_h(\boldsymbol{r}) && (1.44)\\ &= \int d\boldsymbol{r}\phi^*_p(\boldsymbol{r})\frac{i\hbar}{2}\left(\overleftarrow{\nabla}_z - \overrightarrow{\nabla}'_z\right)\phi_h(\boldsymbol{r'})|_{\boldsymbol{r'}=\boldsymbol{r}} \equiv \int d\boldsymbol{r}\phi^*_p(\boldsymbol{r})P(\boldsymbol{r},\boldsymbol{r'})\phi_h(\boldsymbol{r'})|_{\boldsymbol{r'}=\boldsymbol{r}} && (1.45)\end{aligned}$$

There is also another equation for another operator Q which satisfies the canonical commutation relation, $[Q,P] = i\hbar$ as following. The following equation descrives the boost motion of the center Mass of the system which is derived from $[h-\alpha P,\rho] = 0$.

$$\sum_{p'h'}\begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^*_{php'h'} & A^*_{php'h'}\end{pmatrix}\begin{pmatrix} Q_{p'h'} \\ -Q_{h'p'}\end{pmatrix} = -\frac{i\hbar}{M_0}\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}\begin{pmatrix} P_{ph} \\ -P_{hp}\end{pmatrix} \tag{1.46}$$

$$\delta\rho_Q(\boldsymbol{r}\boldsymbol{r'}) = \sum_{ph}\left[\phi^*_h(\boldsymbol{r'})\phi_p(\boldsymbol{r})Q_{ph} - Q_{hp}\phi^*_p(\boldsymbol{r'})\phi_h(\boldsymbol{r})\right] \tag{1.47}$$

where

$$\begin{aligned} Q_{ph} &= \langle p|Q|h\rangle && (1.48)\\ &= \int d\boldsymbol{r}\phi^*_p(\boldsymbol{r})Z\phi_h(\boldsymbol{r}) && (1.49)\end{aligned}$$

By following [1], we assume that there is a mixture of NG modes in a calculated transition density, $\delta\rho_{\text{cal}}(\omega)$, but here we apply the assumption to the transition density in the coordinate space representation.

$$\delta\rho_{\text{cal}}(\boldsymbol{r};\omega) = \delta\rho_{\text{phy}}(\boldsymbol{r};\omega) + \lambda_P(\omega)\delta\rho_P(\boldsymbol{r}) + \lambda_Q(\omega)\delta\rho_Q(\boldsymbol{r}) \tag{1.50}$$

where "physical" transition density $\delta\rho_{\rm phy}$ is free from the NG modes. As the same discussion with [1], since the $\delta\rho_{\rm phy}$ should be orthogonal to the NG modes, then we have

$$\int d\boldsymbol{r} P(\boldsymbol{r})\delta\rho_{\rm phy}(\boldsymbol{r};\omega)(= i\mathrm{Tr}\{[\delta\rho_P, \delta\rho_{phy}(\omega)]\}) \tag{1.51}$$

$$= \int d\boldsymbol{r} Q(\boldsymbol{r})\delta\rho_{\rm phy}(\boldsymbol{r};\omega)(= i\mathrm{Tr}\{[\delta\rho_Q, \delta\rho_{phy}(\omega)]\}) = 0 \tag{1.52}$$

Using Eq.(1.50), therefore we obtain

$$\int d\boldsymbol{r} P(\boldsymbol{r})\delta\rho_{\rm phy}(\boldsymbol{r};\omega) = \int d\boldsymbol{r} P(\boldsymbol{r})\delta\rho_{\rm cal}(\boldsymbol{r};\omega) - \lambda_Q(\omega)\int d\boldsymbol{r} P(\boldsymbol{r})\delta\rho_{\rm Q}(\boldsymbol{r}) = 0 \tag{1.53}$$

$$\int d\boldsymbol{r} Q(\boldsymbol{r})\delta\rho_{\rm phy}(\boldsymbol{r};\omega) = \int d\boldsymbol{r} Q(\boldsymbol{r})\delta\rho_{\rm cal}(\boldsymbol{r};\omega) - \lambda_P(\omega)\int d\boldsymbol{r} Q(\boldsymbol{r})\delta\rho_{\rm P}(\boldsymbol{r}) = 0 \tag{1.54}$$

By the way, using the canonicity condition $[Q, P] = i\hbar$, then we get,

$$\int d\boldsymbol{r} Q(\boldsymbol{r})\delta\rho_{\rm P}(\boldsymbol{r}) = -\int d\boldsymbol{r} P(\boldsymbol{r})\delta\rho_{\rm Q}(\boldsymbol{r}) \left(= -\int d\boldsymbol{r} P(\boldsymbol{r}'\boldsymbol{r})\delta\rho_{\rm Q}(\boldsymbol{r}\boldsymbol{r}')|_{\boldsymbol{r}'=\boldsymbol{r}}\right) \tag{1.55}$$

$$= \sum_{ph}[P_{ph}Q_{hp} - P_{hp}Q_{ph}] = i\hbar \tag{1.56}$$

Then we can get the expression for λ_Q and λ_P as,

$$\lambda_Q(\omega) = -\frac{1}{i\hbar}\int d\boldsymbol{r} P(\boldsymbol{r}'\boldsymbol{r})\delta\rho_{\rm cal}(\boldsymbol{r}\boldsymbol{r}';\omega)|_{\boldsymbol{r}'=\boldsymbol{r}} \tag{1.57}$$

$$= -\frac{1}{2}\int d\boldsymbol{r}\sum_h\left[\phi_h^*(\boldsymbol{r})\left(\overleftarrow{\nabla}_z - \overrightarrow{\nabla}_z\right)X_h(\boldsymbol{r};\omega) + Y_h^*(\boldsymbol{r};\omega)\left(\overleftarrow{\nabla}_z - \overrightarrow{\nabla}_z\right)\phi_h(\boldsymbol{r})\right] \tag{1.58}$$

$$\lambda_P(\omega) = \frac{1}{i\hbar}\int d\boldsymbol{r} Q(\boldsymbol{r})\delta\rho_{\rm cal}(\boldsymbol{r};\omega) \tag{1.59}$$

$$= \frac{1}{i\hbar}\int d\boldsymbol{r}\sum_h[\phi_h^*(\boldsymbol{r})ZX_h(\boldsymbol{r};\omega) + Y_h^*(\boldsymbol{r};\omega)Z\phi_h(\boldsymbol{r})] \tag{1.60}$$

Appendix A

A.1 Hartree-Fock approximation

The total exact Hamiltonian is given by

$$\hat{H} = \hat{T} + \hat{V} \tag{A.1}$$

where

$$\hat{T} = \sum_{kk'} t_{kk'} c_k^\dagger c_{k'} \tag{A.2}$$

$$\hat{V} = \frac{1}{2} \sum_{k_1,k_2,k_3,k_4} v_{k_1k_2k_3k_4} c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} \tag{A.3}$$

When one thinks the Hartree-Fock approximation, one can define the Hartree-Fock(HF) vacuum by using the particle and hole annihilation operator (a, b).

$$\left.\begin{array}{ll} a_k|0\rangle_{HF} & (k > k_F) \\ b_k|0\rangle_{HF} & (k \leq k_F) \end{array}\right\} = 0 \tag{A.4}$$

The relationship between the creation-annihilation operator for the real vacuum $(c, c^\dagger)$ and the particle-hole operators for HF vacuum is given by

$$c_k = \theta(k - k_F)a_k + \theta(k_F - k)b_k^\dagger \tag{A.5}$$

$$c_k^\dagger = \theta(k - k_F)a_k^\dagger + \theta(k_F - k)b_k \tag{A.6}$$

Then by applying the Wick's theorem, the total Hamiltonian can be rewritten as

$$\hat{H} = E_0^{HF} + \hat{h}_{HF} + \hat{H}_{res} \tag{A.7}$$

where

$$E_0^{HF} = \langle 0|\hat{H}|0\rangle_{HF} \tag{A.8}$$

$$\hat{h}_{HF} = \sum_m \epsilon_m^0 : a_m^\dagger a_m : - \sum_i \epsilon_i^0 : b_i^\dagger b_i : \tag{A.9}$$

$$\hat{H}_{res} = \frac{1}{2} \sum_{k_1,k_2,k_3,k_4} v_{k_1k_2k_3k_4} : c_{k_1}^\dagger c_{k_2}^\dagger c_{k_4} c_{k_3} : \tag{A.10}$$

A.2 RPA –Equation and Hamiltonian–

A.2.1 Derivation of RPA equation

First of all, we think the time-dependent state by using the time-evolution from the Hartree-Fock ground state.

$$|\Phi(t)\rangle = e^{-i\frac{E_0}{\hbar}t} e^{\hat{G}}(t)|0_{HF}\rangle \tag{A.11}$$

This expression is justified by Thouless's theprem, and expresses the fluctuation of the state around the stationally point(HF ground state) depending the time evolution.

According to the Thouless theorem, $\hat{G}(t)$ is given by

$$\hat{G}(t) = \sum_{ph} \left(g_{ph}(t)\Gamma^{\dagger}_{ph} - g^{*}_{ph}(t)\Gamma_{ph} \right) \tag{A.12}$$

where $\Gamma^{\dagger}_{ph} = a^{\dagger}_{p} b^{\dagger}_{h}$.

In order $|\Phi(t)\rangle$ satisfies the time-dependent Hartree-Fock equation $i\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle = H|\Phi(t)\rangle$, $\hat{G}(t)$ must satisfy

$$i\hbar\frac{\partial \hat{G}(t)}{\partial t} = [H, \hat{G}(t)] \tag{A.13}$$

We define the Lagrangian $\mathcal{L}$ by

$$\mathcal{L} = i\hbar\frac{\partial}{\partial t} - H \tag{A.14}$$

and consider the variational principle

$$\delta \int dt \langle\Phi(t)|\mathcal{L}|\Phi(t)\rangle = 0 \tag{A.15}$$

for g and g^{*}. But before to do that, we extend the expectation value of the Hamiltonian by using the Baker-Hausedorff formula upto 2nd order of g and g^{*}, and then take the variational proncipl.

Then we get

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} g_{ph}(t) \\ g^{*}_{ph}(t) \end{pmatrix} = \sum_{p'h'} \begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^{*}_{php'h'} & A^{*}_{php'h'} \end{pmatrix} \begin{pmatrix} g_{p'h'}(t) \\ g^{*}_{p'h'}(t) \end{pmatrix} \tag{A.16}$$

Here if we suppose,

$$g_{ph}(t) = \sum_{\nu} C_{\nu} \left(X^{\nu}_{ph} e^{-i\omega_{\nu}t} + Y^{\nu *}_{ph} e^{+i\omega_{\nu}t} \right) \tag{A.17}$$

then the equation becomes,

$$\sum_{p'h'} \begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^{*}_{php'h'} & A^{*}_{php'h'} \end{pmatrix} \begin{pmatrix} X^{\nu}_{p'h'} \\ Y^{\nu}_{p'h'} \end{pmatrix} = \hbar\omega_{\nu} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^{\nu}_{ph} \\ Y^{\nu}_{ph} \end{pmatrix} \tag{A.18}$$

This is so-called RPA equation.

A.2.2 RPA Hamiltonian

Definition of the RPA states

If we define the RPA vacuum and the excited states as,

$$\hat{\mathcal{O}}_\nu|0) = 0, \qquad |\nu) = \hat{\mathcal{O}}^\dagger_\nu|0) \tag{A.19}$$

where

$$\begin{pmatrix} \hat{\mathcal{O}}_\nu \\ \hat{\mathcal{O}}^\dagger_\nu \end{pmatrix} = \sum_{ph} \begin{pmatrix} X^{\nu *}_{ph} & -Y^{\nu *}_{ph} \\ -Y^{\nu}_{ph} & X^{\nu}_{ph} \end{pmatrix} \begin{pmatrix} \Gamma_{ph} \\ \Gamma^\dagger_{ph} \end{pmatrix} \tag{A.20}$$

From Eq.(A.12), Eq.(A.17) and Eq.(A.20), $\hat{G}(t)$ can be rewritten as

$$\begin{aligned} \hat{G}(t) &= \sum_\nu C_\nu \left\{ \sum_{ph} \left(X^\nu_{ph}\Gamma^\dagger_{ph} - Y^\nu_{ph}\Gamma_{ph} \right) e^{-i\omega_\nu t} - \sum_{ph} \left(X^{\nu *}_{ph}\Gamma_{ph} - Y^{\nu *}_{ph}\Gamma^\dagger_{ph} \right) e^{+i\omega_\nu t} \right\} && \text{(A.21)} \\ &= \sum_\nu C_\nu \left\{ \hat{\mathcal{O}}^\dagger_\nu e^{-i\omega_\nu t} - \hat{\mathcal{O}}_\nu e^{+i\omega_\nu t} \right\} && \text{(A.22)} \end{aligned}$$

and Eq.(A.13) gives

$$i\hbar \frac{\partial \hat{G}(t)}{\partial t} = \sum_\nu \hbar\omega_\nu C_\nu \left\{ \hat{\mathcal{O}}^\dagger_\nu e^{-i\omega_\nu t} + \hat{\mathcal{O}}_\nu e^{+i\omega_\nu t} \right\} \tag{A.23}$$

$$[H, \hat{G}(t)] = \sum_\nu C_\nu \left\{ [H, \hat{\mathcal{O}}^\dagger_\nu] e^{-i\omega_\nu t} - [H, \hat{\mathcal{O}}_\nu] e^{+i\omega_\nu t} \right\} \tag{A.24}$$

So Eq.(A.13) requires

$$[H, \hat{\mathcal{O}}^\dagger_\nu] = \hbar\omega_\nu \hat{\mathcal{O}}^\dagger_\nu, \quad \text{and} \quad [H, \hat{\mathcal{O}}_\nu] = -\hbar\omega_\nu \hat{\mathcal{O}}_\nu \tag{A.25}$$

This implies the RPA Hamiltonian takes the form as

$$H_{RPA} = \sum_\nu \hbar\omega_\nu \hat{\mathcal{O}}^\dagger_\nu \hat{\mathcal{O}}_\nu \tag{A.26}$$

RPA equation and RPA Hamiltonian

From Eq.(A.18), simple matrix algebra shows

$$\sum_{p'h'} \begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^*_{php'h'} & A^*_{php'h'} \end{pmatrix} \begin{pmatrix} X^\nu_{p'h'} & Y^{\nu *}_{p'h'} \\ Y^\nu_{p'h'} & X^{\nu *}_{p'h'} \end{pmatrix} = \hbar\omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^\nu_{ph} & Y^{\nu *}_{ph} \\ Y^\nu_{ph} & X^{\nu *}_{ph} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.27}$$

and also we show the well-known formula.

$$\sum_{ph} \begin{pmatrix} X^\nu_{ph} & Y^{\nu *}_{ph} \\ Y^\nu_{ph} & X^{\nu *}_{ph} \end{pmatrix}^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^{\nu'}_{ph} & Y^{\nu' *}_{ph} \\ Y^{\nu'}_{ph} & X^{\nu' *}_{ph} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.28}$$

$$\sum_{\nu} \begin{pmatrix} X^\nu_{ph} & Y^{\nu *}_{ph} \\ Y^\nu_{ph} & X^{\nu *}_{ph} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^{\nu}_{p'h'} & Y^{\nu *}_{p'h'} \\ Y^{\nu}_{p'h'} & X^{\nu *}_{p'h'} \end{pmatrix}^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.29}$$

Eq.(A.28) and Eq.(A.29) are equivalent with the orthogonality of X and Y amplitudes. And also, from Eq.(A.28) and Eq.(A.29), we can find

$$\begin{pmatrix} X^{\nu}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu *}_{ph} \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^{\nu}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu *}_{ph} \end{pmatrix}^{\dagger} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} X^{\nu *}_{ph} & -Y^{\nu *}_{ph} \\ -Y^{\nu}_{ph} & X^{\nu}_{ph} \end{pmatrix} \tag{A.30}$$

Therefore we find Eq.(A.20) is

$$\begin{pmatrix} \hat{\mathcal{O}}_{\nu} \\ \hat{\mathcal{O}}^{\dagger}_{\nu} \end{pmatrix} = \sum_{ph} \begin{pmatrix} X^{\nu}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu *}_{ph} \end{pmatrix}^{-1} \begin{pmatrix} \Gamma_{ph} \\ \Gamma^{\dagger}_{ph} \end{pmatrix} \tag{A.31}$$

and also

$$\begin{pmatrix} \Gamma_{ph} \\ \Gamma^{\dagger}_{ph} \end{pmatrix} = \sum_{\nu} \begin{pmatrix} X^{\nu}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu *}_{ph} \end{pmatrix} \begin{pmatrix} \hat{\mathcal{O}}_{\nu} \\ \hat{\mathcal{O}}^{\dagger}_{\nu} \end{pmatrix} \tag{A.32}$$

It is well known that, in the quasiboson approximation, the Hamiltonian can be written by

$$H = E_{HF} - \frac{1}{2}\mathrm{Tr}A + \frac{1}{2} \sum_{ph,p'h'} \left(\Gamma^{\dagger}_{ph}, \Gamma_{ph} \right) \begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^{*}_{php'h'} & A^{*}_{php'h'} \end{pmatrix} \begin{pmatrix} \Gamma_{p'h'} \\ \Gamma^{\dagger}_{p'h'} \end{pmatrix} \tag{A.33}$$

Using Eq.(A.32) and Eq.(A.18), the Hamiltonian can is rewritten as

$$\begin{aligned} H &= E_{HF} - \frac{1}{2}\mathrm{Tr}A \\ &\quad + \frac{1}{2} \sum_{ph,p'h',\nu\nu'} \left(\hat{\mathcal{O}}^{\dagger}_{\nu} \quad \hat{\mathcal{O}}_{\nu} \right) \begin{pmatrix} X^{\nu}_{ph} & Y^{\nu *}_{ph} \\ Y^{\nu}_{ph} & X^{\nu *}_{ph} \end{pmatrix}^{\dagger} \begin{pmatrix} A_{php'h'} & B_{php'h'} \\ B^{*}_{php'h'} & A^{*}_{php'h'} \end{pmatrix} \begin{pmatrix} X^{\nu'}_{p'h'} & Y^{\nu' *}_{p'h'} \\ Y^{\nu'}_{p'h'} & X^{\nu' *}_{p'h'} \end{pmatrix} \begin{pmatrix} \hat{\mathcal{O}}_{\nu'} \\ \hat{\mathcal{O}}^{\dagger}_{\nu'} \end{pmatrix} \qquad \text{(A.34)} \\ &= E_{HF} - \frac{1}{2}\mathrm{Tr}A + \frac{1}{2} \sum_{\nu} \hbar\omega_{\nu} \left(\hat{\mathcal{O}}^{\dagger}_{\nu} \quad \hat{\mathcal{O}}_{\nu} \right) \begin{pmatrix} \hat{\mathcal{O}}_{\nu} \\ \hat{\mathcal{O}}^{\dagger}_{\nu} \end{pmatrix} \\ &= E_{HF} - \frac{1}{2}\mathrm{Tr}A + \sum_{\nu} \hbar\omega_{\nu} \left(\hat{\mathcal{O}}^{\dagger}_{\nu} \hat{\mathcal{O}}_{\nu} + \frac{1}{2} \right) \qquad \text{(A.35)} \end{aligned}$$

Appendix B

Key formula and theorem

B.1 Complex analysys

B.1.1 Useful formula

$$\lim_{\epsilon\to 0}\frac{1}{z\pm i\epsilon} = P\frac{1}{z}\mp i\pi\delta(z) \tag{B.1}$$

$$\int_{-\infty}^{\infty} dte^{i\omega t} = 2\pi\delta(\omega) \tag{B.2}$$

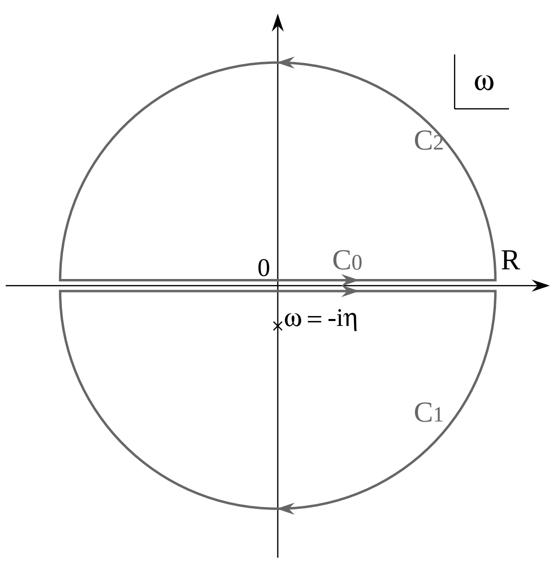
$$\int_{0}^{\pm\infty} dte^{i\omega t} = \lim_{\epsilon\to 0}\frac{-1}{i\omega\mp\epsilon} = i\left(\frac{1}{\omega}\mp i\pi\delta(\omega)\right) \tag{B.3}$$

B.1.2 Unit step function

$$\theta(t-t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} d\tilde{\omega}\frac{e^{i\tilde{\omega}(t-t')}}{\tilde{\omega}-i\eta}\left(=\frac{-1}{2\pi i}\int_{-\infty}^{\infty} d\tilde{\omega}\frac{e^{-i\tilde{\omega}(t-t')}}{\tilde{\omega}+i\eta}\right) \tag{B.4}$$

The proof of (B.4)

$$\theta(t-t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} d\omega\frac{e^{-i\omega(t-t')}}{\omega+i\eta}$$



To show the proof of this relation for the step function, we think the contour integration(left figure). When $t-t'>0(t-t'<0)$ one takes a path $C_0+C_1(C_0+C_2)$, because $e^{-i\omega(t-t')}$ converges on $C_1(C_2)$ plane at the limit $\omega\to\infty$, and also

$$\int_{C_1(C_2)}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}\bigg|_{R\to\infty}\to 0.$$

Then one can calculate by using the residue theorem,

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta} = \int_{C_0}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}$$
$$= \begin{cases} (t-t'>0) & \displaystyle\int_{C_0+C_1}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}\bigg|_{\eta\to 0}\to -1 \\ (t-t'<0) & \displaystyle\int_{C_0+C_2}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta} = 0 \end{cases}$$

B.1.3 Cauchy's theorem for the Green' function

If the single (quasi)particle HF(B) Green's function is defined by

$$
\begin{aligned}
\mathcal{G}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &= \sum_{\mu} \left\{ \frac{\phi_\mu(\boldsymbol{r}\sigma)\phi_\mu^\dagger(\boldsymbol{r}'\sigma')}{E - E_\mu} + \frac{\bar{\phi}_{\tilde{\mu}}(\boldsymbol{r}\sigma)\bar{\phi}_{\tilde{\mu}}^\dagger(\boldsymbol{r}'\sigma')}{E + E_\mu} \right\} &\text{(B.5)}\\
&= \sum_{\mu} \mathcal{G}_\mu(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.6)}
\end{aligned}
$$

This Green's function has the poles at $E = E_\mu$ and $E = -E_\mu$. According to the Cauchy's theorem, the following formula is satisfied as

$$
\begin{aligned}
\sum_{\mu} f(-E_\mu)\bar{\phi}_{\tilde{\mu}}(\boldsymbol{r}\sigma)\bar{\phi}_{\tilde{\mu}}^\dagger(\boldsymbol{r}'\sigma') &= \sum_{\mu} f(-E_\mu) \lim_{E\to -E_\mu} (E + E_\mu)\mathcal{G}_\mu(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.7)}\\
&= \lim_{E\to -E_\mu} f(E) \sum_{\mu} (E + E_\mu)\mathcal{G}_\mu(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.8)}\\
&= \lim_{E\to -E_\mu} f(E) \sum_{\mu} (E + E_\mu) \sum_{\nu} \mathcal{G}_\nu(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.9)}\\
&= \lim_{E\to -E_\mu} f(E) \sum_{\mu} (E + E_\mu)\mathcal{G}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.10)}\\
&= \lim_{E\to -E_\mu} \sum_{\mu} (E + E_\mu) f(E)\mathcal{G}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.11)}\\
&= \frac{1}{2\pi i} \int_C dE f(E)\mathcal{G}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) &\text{(B.12)}
\end{aligned}
$$

because the Green's function has the poles of the 1st rank.

$f(E)$ is an arbitraly function, but on the right hand side, $f(E)$ **must not have any poles in the contour integration area.**

The contour path C is shown by Fig.B.1.

So finally one can get the most general relatioship,

$$
\lim_{E\to -E_\mu} \sum_{\mu} (E + E_\mu) f(E)\mathcal{G}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) = \frac{1}{2\pi i} \int_C dE f(E)\mathcal{G}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma', E) \qquad \text{(B.13)}
$$

Of course, the left hand side of Eq.(B.13) is available only for the spectral representation of the Green's function. The right hand side does not depend on the representation.

B.2 Matrix and Operator

B.2.1 Useful formula

$$
\frac{1}{\boldsymbol{A}} = \frac{1}{\boldsymbol{B}} + \frac{1}{\boldsymbol{B}}(\boldsymbol{B} - \boldsymbol{A})\frac{1}{\boldsymbol{A}} \qquad \text{(B.14)}
$$

B.2.2 *Baker-Hausdorff formula*

$$
\begin{aligned}
e^{iG}He^{-iG} &= H + [iG, H] + \frac{1}{2}[iG, [iG, H]] + \cdots &\text{(B.15)}\\
e^{A}e^{B} &= e^{A+B+\frac{1}{2}[A,B]} &\text{(B.16)}
\end{aligned}
$$

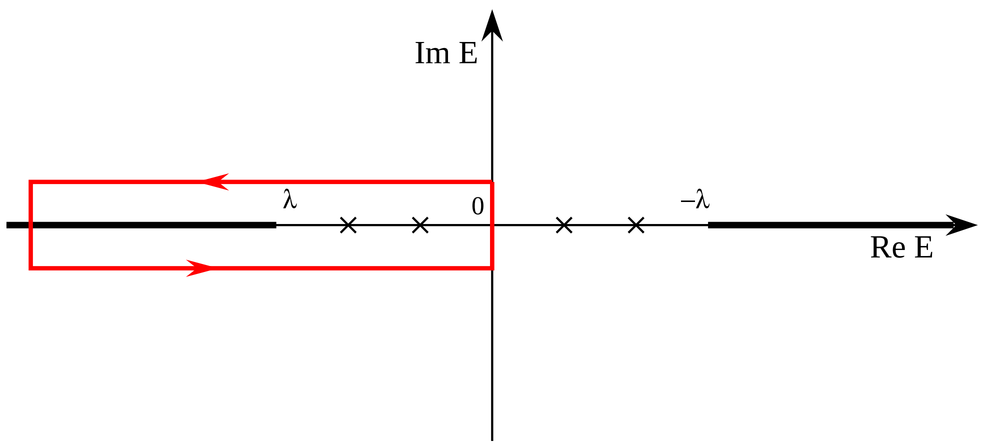


Figure B.1: The contour path C for the integration of B.12. λ is the Fermi energy.

Bibliography

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