Wave and Second Quantization

$$E(x,t)=\sum_k E_k e^{-i(kx+\omega t)} \quad ; \quad E^+(x,t)=\sum_k E_k e^{i(kx+\omega t)}$$

$$E(x,t)=E^F(x,t)+E^B(x,t)=\sum_k E_k e^{-i(kx-\omega t)}+\sum_k E_k e^{i(kx-\omega t)}$$

$$=\sum_k E_k\left(e^{-i(kx+\omega t)}+e^{i(kx+\omega t)}\right)$$

The amplitude of EM field (or the photon number density)

$$A=\left|E(x,t)\right|^2=\sum_k \left|E_k\right|^2$$

For the matter wave

Def ine the field operator

$$\varphi(x)=\sum_k c_k a_k(x) \quad ; \quad \varphi^+(x)=\sum_k a_k^+(x)c_k^+$$

$$[c_k,c_{k'}]=\delta_{kk'} \text{ for fermion ; } \{c_k,c_{k'}\}=\delta_{kk'} \text{ for boson}$$

Hamiltonain

the particle number:

$$n = \langle \varphi | \varphi \rangle = \int d^3x \varphi^+(x)\varphi(x) = \sum_k a_k^+ a_k c_k^+ c_k$$

Let $a_k^+ a_k = 1$ $\quad n = \sum_k n_k = \sum_k c_k^+ c_k$

the Kinetic Hamiltonian

$$H_K = \langle \varphi | \hat{T} | \varphi \rangle = \int d^3x \varphi^+(x)\hat{T}\varphi(x)$$

$\hat{T}(x) \equiv -\frac{\hbar^2}{2m}\nabla_x^2$ is any one-body kinetic operator

the interaction Hamiltonian for two praticle interaction:

$$H_{\text{int}} = \frac{1}{2}\int d^3x \int d^3x' \varphi^+(x)\varphi^+(x')V(x,x')\varphi(x')\varphi(x)$$

$V(x,x')$ is the interaction potential between particles

Coulomb interaction : $V(x,x') = \frac{e^2}{|x-x'|} \Rightarrow V(k) = \frac{e^2}{k}$

if the variation of $V(k)$ is small i.e. $V(k) = U = \text{constant}$

$$H_{\text{int}} = \frac{U}{2}\int d^3x \int d^3x' \varphi^+(x)\varphi^+(x')\varphi(x')\varphi(x) = \sum_{kk'} \frac{U}{2} c_k^+ c_{k'}^+ c_{k'} c_k = \sum_{kk'} \frac{U}{2} \hat{n}_k \hat{n}_{k'}$$

The Green Function

$$G(x,x') \equiv \frac{-i}{\hbar}\frac{\langle \Psi_0 | T\{\varphi_H(x)\varphi_H^+(x')\} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$= \frac{-i}{\hbar}\frac{\theta(t-t')\langle \Psi_0 | \varphi_H(x)\varphi_H^+(x') | \Psi_0 \rangle \mp \theta(t'-t)\langle \Psi_0 | \varphi_H^+(x')\varphi_H(x) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$T\{....\}$: time ordering operator

$|\Psi_0\rangle$: the ground state of system $\Rightarrow\ H|\Psi_0\rangle = E_0|\Psi_0\rangle$

$\varphi_H(x), \varphi_H^+(x')$: the annihilate and create operator in Heisenberg picture.

$\langle \Psi_0 | \Psi_0 \rangle$ is the renormalization factor

The Pictures

1.the Schordinger picture: wave functions are time dependent and operators are time independent

$$i\frac{\partial}{\partial t}\varphi(t) = H\varphi(t)$$

2.the Heisenberg picture: wave functions are time independent and operators are time dependent

$$\hat{O}_H(t) = e^{iHt}\hat{O}_H(0)e^{-iHt}$$

3.the interaction picture

$$H = H_0 + V \;\; ; \;\; \varphi(t) = e^{iH_0 t}e^{-iHt}\varphi(0) \;\; ; \;\; \hat{O}_I(t) = e^{iH_0 t}\hat{O}_I(0)e^{-iH_0 t}$$

The Green Function in Interaction Picture

1.S matrix:

$$S(t,t')=Te^{-i\int_{t'}^{t}dt_1\hat{V}(t_1)}\ ;\ S^+(t,t')=S(t',t)\ ;\ S^+S=1$$

2.The ground state:

Heisenberg Ground state $|\Psi_0\rangle$; Interacting picture Ground state $|\Phi_0\rangle$

$$|\Psi_0\rangle=S(0,-\infty)|\Phi_0\rangle\Leftrightarrow|\Phi_0\rangle=S(-\infty,0)|\Psi_0\rangle$$

(Gell-Mann and Low theorem, adiabatic switch on approximation)

3. the operator

$$\hat{O}_H(t)=e^{iHt}\hat{O}_H(0)e^{-iHt}\quad;\quad\hat{O}_I(t)=e^{iH_0t}\hat{O}_I(0)e^{-iH_0t}$$

$$\hat{O}_H(t)=e^{iVt}e^{iH_0t}\hat{O}_H(0)e^{-iH_0t}e^{-iVt}=e^{iVt}\hat{O}_I(t)e^{-iVt}$$

4.the Green function in interaction picture

$$G(t,t')\equiv\frac{-i}{\hbar}\frac{\langle\Psi_0|T\{\varphi_H(t)\varphi_H^+(t')\}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}=\frac{-i}{\hbar}\frac{\langle\Phi_0|T\{S(\infty,0)S(0,t)\varphi(t)S(t,t')\varphi^+(t')S(t',0)S(0,-\infty)\}|\Phi_0\rangle}{\langle\Phi_0|(\infty,-\infty)|\Phi_0\rangle}$$

$$=\frac{-i}{\hbar}\frac{\langle\Phi_0|T\{S(\infty,t)\varphi(t)S(t,t')\varphi^+(t')S(t',-\infty)\}|\Phi_0\rangle}{\langle\Phi_0|(\infty,-\infty)|\Phi_0\rangle}=\frac{-i}{\hbar}\frac{\langle\Phi_0|T\{S(\infty,-\infty)\varphi(t)\varphi^+(t')\}|\Phi_0\rangle}{\langle\Phi_0|(\infty,-\infty)|\Phi_0\rangle}$$

The Wick's theorem

$$\left\langle T\left\{S(\infty,-\infty)\varphi(t)\varphi^{+}(t')\right\}\right\rangle$$

$$\propto \left\langle T\left\{\varphi(t)\varphi^{+}(t')\right\}\right\rangle$$

$$+(-i)\int dt_1 V_0 \left\langle T\left\{\varphi(t)\varphi^{+}(t')\phi^{+}(t_1)\varphi(t_1)\right\}\right\rangle$$

$$+(-i)^2\int dt_1\int dt_2 \left|V_0\right|^2 \left\langle T\left\{\varphi(t)\varphi^{+}(t')\phi^{+}(t_1)\varphi(t_1)\varphi^{+}(t_2)\phi(t_2)\right\}\right\rangle$$

$$\times(1+(-i)\int dt_1 V_0 \left\langle T\left\{\varphi(t)\varphi^{+}(t')\phi^{+}(t_1)\varphi(t_1)\right\}\right\rangle\cdots)$$

$$\left\langle T\left\{\varphi(t)\varphi^{+}(t')\phi^{+}(t_1)\varphi(t_1)\varphi^{+}(t_2)\phi(t_2)\right\}\right\rangle$$

$$=\left\langle T\left\{\varphi(t)\varphi^{+}(t')\right\}\right\rangle\bullet\left[\left\langle T\left\{\varphi(t_1)\phi^{+}(t_1)\right\}\right\rangle\left\langle T\left\{\phi(t_2)\varphi^{+}(t_2)\right\}\right\rangle-\left\langle T\left\{\varphi(t_1)\varphi^{+}(t_2)\right\}\right\rangle\left\langle T\left\{\phi(t_2)\phi^{+}(t_1)\right\}\right\rangle\right]$$

0 non-connecteed

$$-\left\langle T\left\{\varphi(t)\phi^{+}(t_1)\right\}\right\rangle\bullet\left[\left\langle T\left\{\varphi(t_1)\varphi^{+}(t')\right\}\right\rangle\left\langle T\left\{\phi(t_2)\varphi^{+}(t_2)\right\}\right\rangle-\left\langle T\left\{\varphi(t_1)\varphi^{+}(t')\right\}\right\rangle\left\langle T\left\{\phi(t_2)\varphi^{+}(t_2)\right\}\right\rangle\right]$$

0 0

$$-\left\langle T\left\{\varphi(t)\varphi^{+}(t_2)\right\}\right\rangle\bullet\left[\left\langle T\left\{\phi(t_2)\varphi^{+}(t')\right\}\right\rangle\left\langle T\left\{\varphi(t_1)\phi^{+}(t_1)\right\}\right\rangle-\left\langle T\left\{\phi(t_2)\phi^{+}(t_1)\right\}\right\rangle\left\langle T\left\{\varphi(t_1)\varphi^{+}(t')\right\}\right\rangle\right]$$

0 connected

The Wick's theorem says that the result of the product of many field operators is the sum of all pairwise contraction.

Cancel Theorem

$$G(t,t') = \frac{-i}{\hbar} \frac{\left\langle \Phi_0 \left| T\left\{ S(\infty,-\infty)\varphi(t)\varphi^+(t') \right\} \right| \Phi_0 \right\rangle}{\left\langle \Phi_0 \left| \left(\infty,-\infty \right) \right| \Phi_0 \right\rangle}$$

$$= \frac{-i}{\hbar} \frac{\left\langle \Phi_0 \left| T\left\{ S(\infty,-\infty)\varphi(t)\varphi^+(t') \right\} \right| \Phi_0 \right\rangle_{connected} \left\langle \Phi_0 \left| T\left\{ S(\infty,-\infty)\varphi(t)\varphi^+(t') \right\} \right| \Phi_0 \right\rangle_{non-connected}}{\left\langle \Phi_0 \left| \left(\infty,-\infty \right) \right| \Phi_0 \right\rangle_{non-connected}}$$

$$= \frac{-i}{\hbar} \left\langle \Phi_0 \left| T\left\{ S(\infty,-\infty)\varphi(t)\varphi^+(t') \right\} \right| \Phi_0 \right\rangle_{connected}$$

$$= \frac{-i}{\hbar} \left\langle \Phi_0 \left| T\left\{ S(\infty,-\infty)\varphi(t)\varphi^+(t') \right\} \right| \Phi_0 \right\rangle_{connected}$$

The S Matrix and Perturbation Expension

$$S(\infty,-\infty)=Te^{-i\int_{t'}^{t}dt_1\hat{V}(t_1)}=T\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\cdots dt_n\left\{\hat{V}(t_1)\cdots\hat{V}(t_n)\right\}$$

$$=1+(-i)T\left[\int dt_1\hat{V}(t_1)\right]+\frac{(-i)^2}{2}T\int dt_1\int dt_2\hat{V}(t_1)\hat{V}(t_2)\cdots$$

$$+T\int dt_1\cdots\int dt_n\hat{V}(t_1)\cdots\hat{V}(t_n)$$

$$=\sum_{n=0}^{\infty}(-i)^n\int_{-\infty}^{\infty}dt_1\cdots dt_n\left\{T\hat{V}(t_1)\cdots\hat{V}(t_n)\right\}$$

$$G(t,t')=\frac{-i}{\hbar}\sum_{n}(-i)^n\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_n\left\langle T\left\{\varphi(t)\varphi^+(t')\hat{V}(t_1)\cdots\hat{V}(t_n)\right\}\right\rangle_{\text{different connected}}$$

Simple Examples

The resonant-level Model

$$H = \varepsilon_0 d^+ d + \sum_k \varepsilon_k c_k^+ c_k + \sum_k V_k \left(d^+ c_k + h.c. \right)$$

$$= H_0 + H_{res} + H_T$$

$$G(t,t') = -i \left\langle T \left\{ S(t,t') d(t) d^+(t) \right\} \right\rangle$$

$$TS(t,t') = 1 + (-i)^1 \int_{-\infty}^{\infty} dt_1 TH(t_1) + \left[(-i)^2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 T \left[H_T(t_1) H_T(t_2) \right] \right] S(t_2, t')$$

$$G(t,t') = -i \left\langle T \left\{ d^+(t) d(t) \right\} \right\rangle$$

$$+ (-i)(-i) \sum_k V_k \int_{-\infty}^{\infty} dt_1 \left\langle T \left\{ d(t) \left[d^+(t_1) c_k(t_1) + h.c. \right] d^+(t') \right\} \right\rangle$$

$$+ (-i)(-i)^2 \sum_{kk'} V_k V_{k'} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \left\langle T \left\{ d(t) \left[d^+(t_1) c_k(t_1) + h.c. \right] S(t_2, t') d^+(t') \right\} \right\rangle$$

$$= (-i) \left\langle T \left\{ d^+(t) d(t) \right\} \right\rangle + \sum_{kk'} V_k V_{k'} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 (-i) \left\langle T \left\{ d(t) d^+(t_1) \right\} \right\rangle (-i) \left\langle T \left\{ c_k(t_1) c_k^+(t_2) \right\} \right\rangle (-i) \left\langle T \left\{ d(t_2) S(t_2, t') d^+(t') \right\} \right\rangle$$

$$= G^0(t,t') + \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 G^0(t,t_1) \sum_k \left| V_k \right|^2 g_k(t_1, t_2) G(t_2, t')$$

$$G(\omega) = G^0(\omega) + G^0(\omega) \sum_k \left| V_k \right|^2 g_k(\omega) G(\omega) \equiv G^0(\omega) + G^0(\omega) \Sigma_T(\omega) G(\omega)$$

$$G = \frac{1}{(G^0)^{-1} - \Sigma_T}$$

The electron –photon interaction

The electron photon interaction

$$H=\sum_k \varepsilon_k c_k^+ c_k+\sum_q \omega_q b_q^+ b_q+\sum_q M_q c_{k+q}^+ c_k A_q \qquad \text{where } A_q \equiv \left(b_q+b_{-q}^+\right)$$

$$=H_e+H_{ph}+H_{e-ph}$$

$$G(t,t')=-i\left\langle T\left\{S(\infty,-\infty)d(t)d^+(t)\right\}\right\rangle$$

$$TS(t,t')=1+(-i)^1\int_{-\infty}^{\infty} dt_1 TH_{e-ph}(t_1)+\left[(-i)^2\int_{-\infty}^{\infty} dt_1\int_{-\infty}^{\infty} dt_2 T\left[H_{e-ph}(t_1)H_{e-ph}(t_2)\right]\right]S(\infty,-\infty)$$

$$G_k(t,t')=-i\left\langle T\left\{c_k(t)c_k^+(t')\right\}\right\rangle$$

$$+(-i)(-i)\sum_q M_q\int_{-\infty}^{\infty} dt_1\left\langle T\left\{c_k(t)\left[c_{k-q}^+ c_k\ A_q(t_1).\right]c_k^+(t')\right\}\right\rangle$$

$$+(-i)(-i)^2\sum_{qq'} M_q M_{q'}\int_{-\infty}^{\infty} dt_1\int_{-\infty}^{\infty} dt_2\left\langle T\left\{c_k(t)\left[M_q c_k^+ c_{k-q}\ A_q(t_1)+h.c.\right]\left[M_q c_{k-q}^+ c_k\ A_q(t_2)+h.c.\right]S(\infty,-\infty)d^+(t')\right\}\right\rangle$$

$$=(-i)\left\langle T\left\{d^+(t)d(t)\right\}\right\rangle$$

$$+\int_{-\infty}^{\infty} dt_1\int_{-\infty}^{\infty} dt_2(-i)\left\langle T\left\{c_k(t)c_k^+(t_1)\right\}\right\rangle\sum_q\left|M_q\right|^2(-i)\left[\left\langle T\left\{c_{k-q}(t_1)c_{k-q}^+(t_2)\right\}\right\rangle\left\langle T\left\{\ A_q(t_1)\ A_q^+(t_2)\right\}\right\rangle\right](-i)\left\langle T\left\{d(t_2)S(t_2,t')d^+(t')\right\}\right\rangle$$

$$=G_k^0(t,t')+\int_{-\infty}^{\infty} dt_1\int_{-\infty}^{\infty} dt_2 G_k^0(t,t_1)(-i)\sum_q\left|M_q\right|^2 G_{k-q}^0(t_1,t_2)D_q(t_1,t_2)G_k(t_2,t')$$

where the photon Green function $D_q(t_1,t_2)\equiv -i\left\langle T\left\{\ A_q(t_1)\ A_q^+(t_2)\right\}\right\rangle$

$F.T.$

$$G_k(\omega)=G_k^0(\omega)+G_k^0(\omega)\Sigma_{eph}(\omega)G(\omega)$$

the electron-photon interaction self-energy $\Sigma_{eph}(\omega)=(-i)\int\frac{d\varepsilon}{2\pi}\sum_q\left|M_q\right|^2 G_{k-q}^0(\omega-\varepsilon)D_q(\omega)$

Retard, Advanced and Lesser, Greater Green Functions

$$G^r(t,t') = -i\theta(t-t')\left\langle\left\{\varphi(t),\varphi^+(t')\right\}\right\rangle \qquad G^a(t,t') = i\theta(t'-t)\left\langle\left\{\varphi(t),\varphi^+(t')\right\}\right\rangle$$

$$G^<(t,t') = i\left\langle\varphi^+(t')\varphi(t)\right\rangle \qquad G^>(t,t') = -i\left\langle\varphi(t)\varphi^+(t')\right\rangle$$

$$G(t,t') = \theta(t-t')G^>(t,t') + \theta(t'-t)G^<(t,t')$$

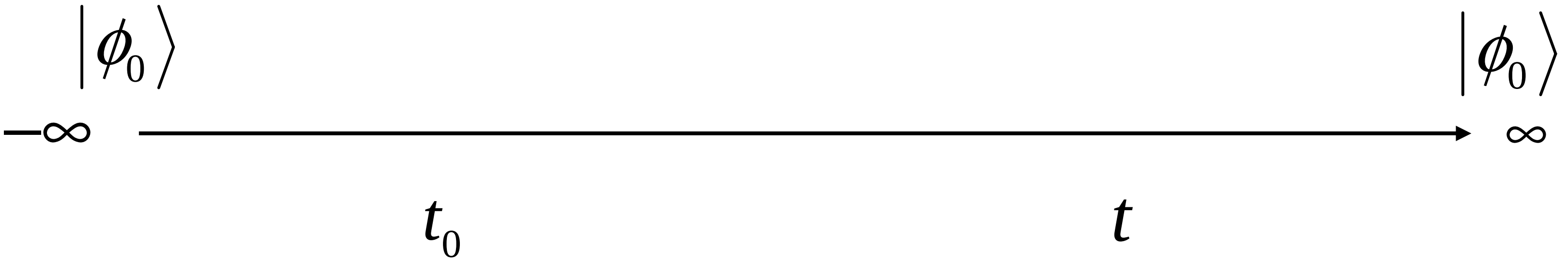
$$G^{r,a} = \pm\theta(\pm t \mp t')\left[G^>(t,t') - G^<(t,t')\right]$$

1. $G(t,t')$ has a systematic perturbation theory
2. $G^{r,a}(t,t')$ have a nice analystic structure and well-suited for calculating a physical response. Information about spectral propertise, densities of states, and scattering rates aer contained in $G^{r,a}(t,t')$
3. $G^{<,>}(t,t')$ aer directly linked to observables and kinteic properties, such as particle densities or current.

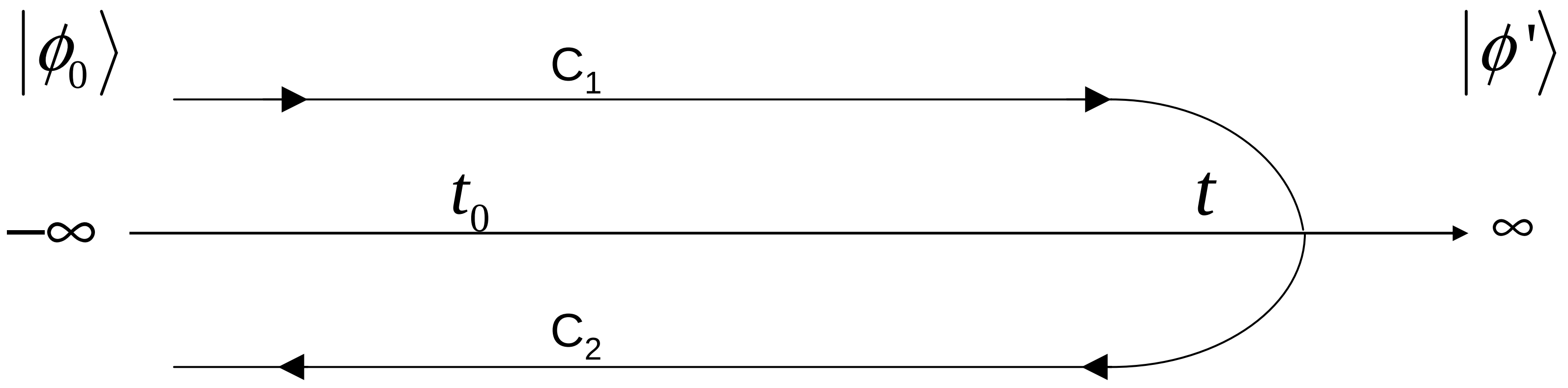
$$A(k,\omega) = i\left[G^r(k,\omega) - G^a(k,\omega)\right] = i\left[G^>(k,\omega) - G^<(k,\omega)\right]$$

$$G^<(k,\omega) = if(\omega)A(k,\omega) \;\; ; \;\; G^<(k,\omega) = -i\left[1 - f(\omega)\right]A(k,\omega)$$

Nonequilibrium System and Contour Ordered



Time ordered



Contour ordered

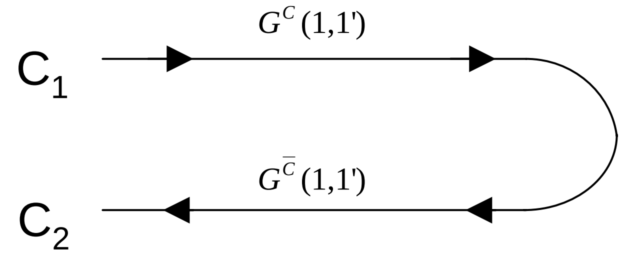
The Equilibrium Green Function

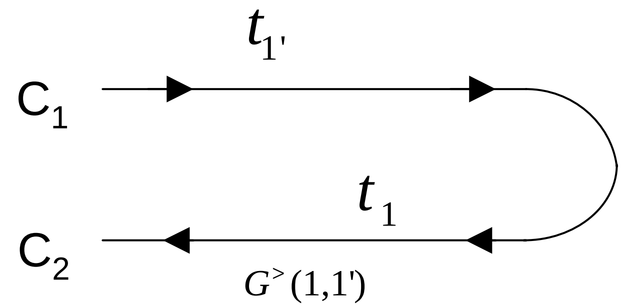
$$G^{C}(1,1') \qquad t_1, t_{1'} \in C_1$$

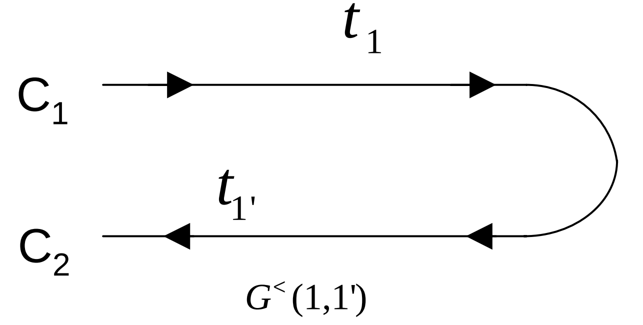
$$G^{>}(1,1') \qquad t_1 \in C_2, t_{1'} \in C_1$$

$$G^{<}(1,1') \qquad t_1 \in C_1, t_{1'} \in C_2$$

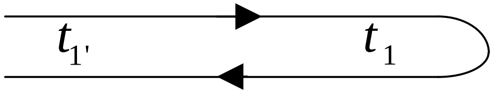
$$G^{\overline{C}}(1,1') \qquad t_1, t_{1'} \in C_2$$

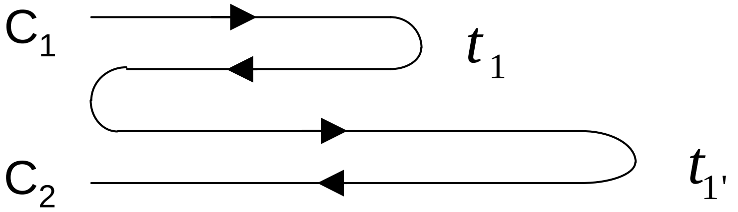






The Langreth Theorem





$$C^C(1,1') = \int_C \mathrm{d}\tau A(t_1,\tau)B(\tau,t_{1'})$$

$$C^<(1,1') = \int_{C_1} \mathrm{d}\tau A(t_1,\tau)B^<(\tau,t_{1'}) + \int_{C_2} \mathrm{d}\tau A^<(t_1,\tau)B(\tau,t_{1'})$$

$$\int_{C_1} \mathrm{d}\tau A(t_1,\tau)B^<(\tau,t_{1'}) = \int_{-\infty}^{t_1} dt A^>(t_1,t)B^<(t,t_{1'}) + \int_{t_1}^{-\infty} dt A^>(t_1,t)B^<(t,t_{1'})$$

$$\equiv \int_{-\infty}^{\infty} dt A^r(t_1,t)B^<(t,t_{1'})$$

A similar analysis can be applied to the second term involving countour $C_{1'}$, the result is

$$C^<(1,1') = \int_{-\infty}^{\infty} dt \left[A^r(t_1,t)B^<(t,t_{1'}) + A^<(t_1,t)B^a(t,t_{1'}) \right]$$

$$\text{if } D^C(t,t') = \int_C d\tau_1 \int_C d\tau_2 A(t_1,\tau_1)B(\tau_1,\tau_2)C(\tau_2,t_{1'})$$

$$\text{Let } E = \int d\tau AB \Rightarrow E^C(t,t') = \int_C d\tau_1 A(t_1,\tau_1)B(\tau_1,\tau_2)$$

$$D^<(t,t')=\int \mathrm{d}\tau_1 \left[E^r(t_1,\tau_2)C^<(\tau_2,t_{1'}) + E^<(t_1,\tau_2)C^a(\tau_2,t_{1'}) \right]$$

$$E^C(t,t')=\int_{\mathrm{C}} \mathrm{d}\tau A(t_1,\tau)B(\tau,t')$$

$$E^r(t,t')=\theta\left(t-t'\right)\left[E^>(t,t')-E^<(t,t')\right] = \theta\left(t-t'\right)\int_{-\infty}^{\infty} dt \left[A^r\left(B^> - B^<\right) + \left(A^> - A^<\right)B^a \right]$$

$$= \theta\left(t-t'\right)\left[\int_{-\infty}^{t} dt\left(A^> - A^<\right)\left(B^> - B^<\right) + \int_{-\infty}^{t'} dt\left(A^> - A^<\right)\left(B^< - B^>\right)\right]$$

$$= \int_{-\infty}^{\infty} d\tau A^r(t,\tau)B^r(\tau,t')$$

$$E^<(t,t')=\int_{-\infty}^{\infty} d\tau \left[A^r(t,\tau)B^<(\tau,t') + A^<(t,\tau)B^a(\tau,t') \right]$$

$$D^<(t,t') = \int_{-\infty}^{\infty} d\tau_1 \int_{-\infty}^{\infty} d\tau_2 \left[A^r(t,\tau_1)B^r(\tau_1,\tau_2)C^<(\tau_2,t_{1'}) + A^r(t,\tau_1)B^<(\tau_1,\tau_2)C^a(\tau_2,t_{1'}) + A^<(t,\tau_1)B^a(\tau_1,\tau_2)C^a(\tau_2,t_{1'}) \right]$$

Table of Langreth Theorem

Contour	Real axis
$C = \int_C AB$	$C^< = \int_t \left[A^r B^< + A^< B^a \right]$ $C^r = \int_t A^r B^r$
$D = \int_C ABC$	$D^< = \int_t \left[A^r B^r C^< + A^r B^< C^a + A^< B^a C^a \right]$ $D^r = \int_t A^r B^r C^r$
$C(\tau,\tau') = A(\tau,\tau')B(\tau,\tau')$	$C^<(t,t') = A^<(t,t')B^<(t,t')$ $C^r(t,t') = A^<(t,t')B^r(t,t') + A^r(t,t')B^<(t,t') + A^r(t,t')B^r(t,t')$
$C(\tau,\tau') = A(\tau,\tau')B(\tau',\tau)$	$C^<(t,t') = A^<(t,t')B^>(t',t)$ $C^r(t,t') = A^<(t,t')B^a(t',t) + A^r(t,t')B^<(t',t)$

The Keldysh Formulation

$$G^< = G_0^< + G_0^r \Sigma^r G^< + G_0^r \Sigma^< G^a + G_0^< \Sigma^a G^a$$

$$= G_0^< \left(1 + \Sigma^a G^a\right) + G_0^r \Sigma^r G^< + G_0^r \Sigma^< G^a$$

$$= G_0^< \left(1 + \Sigma^a G^a\right) + G_0^r \Sigma^r \left[G_0^< \left(1 + \Sigma^a G^a\right) + G_0^r \Sigma^r G^< + G_0^r \Sigma^< G^a \right] + G_0^r \Sigma^< G^a$$

$$= \left(1 + G_0^r \Sigma^r\right) G_0^< \left(1 + \Sigma^a G^a\right) + \left(G_0^r + G_0^r \Sigma^r G_0^r\right) \Sigma^< G^a + G_0^r \Sigma^r G_0^r \Sigma^r G^<$$

$$\Rightarrow$$

$$G^< = \left(1 + G^r \Sigma^r\right) G_0^< \left(1 + \Sigma^a G^a\right) + G^r \Sigma^< G^a$$

A Simple Example

The electron –photon interaction

$$\Sigma_{eph}(\omega) = (i)\int \frac{d\varepsilon}{2\pi}\sum_q \left|M_q\right|^2 G^0_{k-q}(\omega-\varepsilon)D_q(\omega)$$

$$\Sigma^r_{e-ph}(\omega) = (i)\int \frac{d\varepsilon}{2\pi}\sum_q \left|M_q\right|^2 \left[G^{0<}_{k-q}(\omega-\varepsilon)D^r_q(\omega) + G^{0r}_{k-q}(\omega-\varepsilon)D^<_q(\omega) + G^{0r}_{k-q}(\omega-\varepsilon)D^r_q(\omega)\right]$$

$$D^<_q(\omega) = -2\pi i\left[\left(N_q+1\right)\delta\left(\omega+\omega_q\right) + N_q\delta\left(\omega-\omega_q\right)\right]$$

$$D^r_q(\omega) = \frac{1}{\omega-\omega_q+i\delta} - \frac{1}{\omega+\omega_q+i\delta}$$

$$G^{0<}_k(\omega) = 2\pi i n_F(\omega)\delta(\omega-\varepsilon_k)$$

$$G^{0r}_k(\omega) = \frac{1}{\omega-\varepsilon_k+i\delta}$$

$$\Sigma^r_{e-ph}(\omega) = \sum_q \left|M_q\right|^2 \left[\frac{N_q - n_F(\varepsilon_{k-q})+1}{\omega-\omega_q-\varepsilon_{k-q}+i\delta} + \frac{N_q - n_F(\varepsilon_{k-q})}{\omega+\omega_q-\varepsilon_{k-q}+i\delta}\right]$$

The electron transport through the interacting region (PRB 50, 5528)

The system and Hamiltonians

the contact :

$$H_c = \sum_{k\alpha} \varepsilon_{k\alpha} c_{k\alpha}^{+} c_k$$

$$g_{k\alpha}^{<}(t,t') = i\left\langle c_{k\alpha}^{+}(t') c_{k\alpha}(t)\right\rangle = if\left(\varepsilon_{k\alpha}^{0}\right)\exp\left[-\int_{t'}^{t} d\tau \varepsilon_{k\alpha}(\tau)\right]$$

$$g_{k\alpha}^{r,a}(t,t') = \mp i\theta\left(\pm t \mp t'\right)\left\langle\left\{c_{k\alpha}(t), c_{k\alpha}^{+}(t')\right\}\right\rangle = \mp i\theta\left(\pm t \mp t'\right)\exp\left[-\int_{t'}^{t} d\tau \varepsilon_{k\alpha}(\tau)\right]$$

the coupling between leads and central (interacting) region

$$H_T = \sum_{k\alpha,m} V_{k\alpha,m}(t) c_{k\alpha}^{+} d_m + h.c$$

the Hamiltonian of central region

$$H_{cen} = \sum_{m} \varepsilon_m d_m^{+} d_m$$

the interacting Hamiltonian

$$H = U n_m n_{\bar{m}}$$

The current formula

$$J_L = -e\left\langle \dot{N}_L \right\rangle = -\frac{ie}{\hbar}\left\langle \left[H, N_L\right]\right\rangle$$

$H = H_c + H_{cen} + H_T$. Since H_c and H_{cen} commute with N_L,

$$J_L = \frac{ie}{\hbar}\sum_{\substack{k,\alpha\in L\\ n}}\left[V_{k\alpha,n}\left\langle c_{k\alpha}^{+} d_n\right\rangle - V_{k\alpha,n}^{*}\left\langle d_n^{+} c_{k\alpha}\right\rangle\right]$$

remind that :

$$G_{n,k\alpha}^{<}(t-t') \equiv i\left\langle c_{k\alpha}^{+}(t')d_n(t)\right\rangle \text{ and } G_{k\alpha,n}^{<}(t-t') \equiv i\left\langle d_n^{+}(t')c_{k\alpha}(t)\right\rangle$$

$$G_{n,k\alpha}^{<}(t,t) = -\left[G_{k\alpha,n}^{<}(t,t)\right]^{*}$$

$$\therefore J_L = \frac{2e}{\hbar}\mathrm{Re}\left\{\sum_{\substack{k,\alpha\in L\\ n}} V_{k\alpha,n}G_{n,k\alpha}^{<}(t,t)\right\}$$

solving the lesser Green function $G_{n,k\alpha}^{<}$ is the goal for getting the formula of current

The current formula in terms of Nonequilibrium Green function

In order to get the lesser Green function $G^{<}_{n,k\alpha}(t,t)$, the contour Green function must be solved first.

$$G^{t}_{n,k\alpha}(t-t')=\sum_m \int dt_1 G^{t}_{nm}(t-\tau_1)V^{*}_{k\alpha,m} g_{k\alpha}(\tau_1,t')$$

$$G^{<}_{n,k\alpha}(t-t')=\sum_m \int dt_1 V^{*}_{k\alpha,m}\left[G^{r}_{nm}(t-\tau_1)g^{<}_{k\alpha}(\tau_1-t')+G^{<}_{nm}(t-t_1)g^{a}_{k\alpha}(\tau_1-t')\right]$$

$$J_L=-\frac{2e}{\hbar}\mathrm{Re}\left\{\sum_{\substack{k,\alpha\in L\\ n}} V_{k\alpha,n}G^{<}_{n,k\alpha}(t,t)\right\}$$

$$=-\frac{2e}{\hbar}\mathrm{Im}\left\{\sum_{\substack{k,\alpha\in L\\ n}} V_{k\alpha,n}(t)\int_{-\infty}^{t} dt_1 e^{i\int_{t_1}^{t} dt_2 \varepsilon_{k\alpha}(t_2)} V^{*}_{k\alpha,m}(t_1)\left[G^{r}_{nm}(t,t_1)f_L(\varepsilon_{ka})+G^{<}_{nm}(t,t_1)\right]\right\}$$

Def: $$\left[\Gamma^L(\varepsilon,t_1,t)\right]_{mn}=2\pi\sum_{\alpha\in L}\rho_\alpha(\varepsilon)V_{k\alpha,n}(t)V^{*}_{k\alpha,m}(t_1)\exp\left[i\int_{t_1}^{t}dt_2\Delta_\alpha(t_2)\right]$$

$$J_L=-\frac{2e}{\hbar}\int_{-\infty}^{t}dt_1\int\frac{d\varepsilon}{2\pi}\mathrm{Im}\,Tr\left\{e^{-i\varepsilon(t_1-t)}\mathbf{\Gamma}^L(\varepsilon,t_1,t)\left[\mathbf{G}^{<}(t,t_1)+f_L(\varepsilon)\mathbf{G}^{r}(t,t_1)\right]\right\}$$

$$J_L=J_L^{out}+J_L^{in}$$

$$J_L^{out}=-\frac{e}{\hbar}\int_{-\infty}^{t}dt_1\int\frac{d\varepsilon}{\pi}Tr\left\{e^{-i\varepsilon(t_1-t)}\mathbf{\Gamma}^L(\varepsilon,t_1,t)\,\mathrm{Im}\,\mathbf{G}^{<}(t,t_1)\right\}=-\frac{e}{\hbar}\Gamma^L(t)N(t)$$

$$J_L^{in}=-\frac{e}{\hbar}\int_{-\infty}^{t}dt_1\int\frac{d\varepsilon}{\pi}\mathrm{Im}\,Tr\left\{e^{-i\varepsilon(t_1-t)}\mathbf{\Gamma}^L(\varepsilon,t_1,t)f_L(\varepsilon)\mathbf{G}^{r}(t,t_1)\right\}$$

Wideband Approximation

$$\mathbf{G}^r(t,t') = \mathbf{g}^r(t,t') + \iint d\tau_1 d\tau_2 \mathbf{g}^r(t,\tau_1)\mathbf{\Sigma}_T^r(\tau_1,\tau_2)\mathbf{G}^r(\tau_2,t')$$

$F.T.$

$$\mathbf{G}^r(\omega) = \mathbf{g}^r(\omega) + \mathbf{g}^r(\omega)\mathbf{\Sigma}_T^r(\omega)\mathbf{G}^r(\omega)$$

$$\mathbf{G}^r(\omega) = \frac{1}{\left[\mathbf{g}^r(\omega)\right]^{-1} - \mathbf{\Sigma}_T^r(\omega)}$$

$$\Sigma_{m,T}^r(\omega) = \sum_{k\alpha,m} \frac{\left|V_{k\alpha,m}\right|}{\omega - \varepsilon_{k\alpha} + i\delta} = \Lambda(\omega) + i\frac{\Gamma_m^L(\omega) + \Gamma_m^R(\omega)}{2}$$

WBL(wideband limit):

1.neglecting the energy shift $\Lambda(\omega)$

2.assuming that the linewidths are energy independent $\Gamma_m^\alpha(\omega) = \Gamma_m^\alpha$

3.allowing a single time dependence, $\Delta_\alpha(t)$ for the energies in each lead.

The retarded Green function

$$\mathbf{G}^r(t,t') = \mathbf{g}^r(t,t') + \int\int dt_1 dt_2 \mathbf{g}^r(t,t_1)\mathbf{\Sigma}^r(t_1,t_2)\mathbf{G}^r(t_2,t')$$

$$\Sigma^r_{nm}(t_1,t_2) = \sum_{k\alpha\in R,L} V^*_{k\alpha,n}(t_1)\, g^r_{k\alpha}(t_1,t_2) V_{k\alpha,m}(t_2)$$

assume : $V_{k\alpha,m}(t) = u^*_\alpha(t) V_{k\alpha,m}(\varepsilon_k)$

Under the WBL, the retard self-energy becomes

$$\Sigma^r(t_1,t_2) = \sum_{\alpha\in L,R} u^*_\alpha(t_1) u_\alpha(t_2) e^{-i\int_{t_2}^{t_1} d\tau \Delta_\alpha(\tau)} \times \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1-t_2)} \theta(t_1-t_2)[-i\Gamma_\alpha]$$

$$= -\frac{i}{2}\left[\Gamma^L(t_1) + \Gamma^R(t_1)\right]\delta(t_1-t_2)$$

where $\Gamma^\alpha(t_1) \equiv \Gamma^\alpha(t_1,t_1) = \Gamma^\alpha \left|u_\alpha(t_2)\right|^2$

with this self-energy, the retarded Green function becomes:

$$G^r(t,t') = g^r(t,t') \exp\left\{-\int_{t'}^{t} dt_1 \frac{1}{2}\left[\Gamma^L(t_1) + \Gamma^R(t_1)\right]\right\}$$

$$g^r(t,t') = -i\theta(t-t') \exp\left[-i\int_{t'}^{t} dt_1 \varepsilon_0(t_1)\right]$$

The lesser Green function

$$G^< = \left(1 + G^r \Sigma^r\right) G_0^< \left(1 + \Sigma^a G^a\right) + G^r \Sigma^< G^a$$

$G_0^< = 0$ for the considered system

$$\mathbf{G}^<(t,t') = \int dt_1 \int dt_2 \mathbf{G}^r(t,t_1) \mathbf{\Sigma}^<(t_1,t_2) \mathbf{G}^a(t_2,t')$$

where

$$\Sigma^<(t_1,t_2) = i \sum_{L,R} \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1-t_2)} f_\alpha(\varepsilon) \mathbf{\Gamma}^\alpha(\varepsilon,t_1,t_2)$$

Hence

$$\mathbf{G}^<(t,t') = \int dt_1 \int dt_2 \mathbf{G}^r(t,t_1) i \sum_{L,R} \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1-t_2)} f_\alpha(\varepsilon) \mathbf{\Gamma}^\alpha(\varepsilon,t_1,t_2) \mathbf{G}^a(t_2,t')$$

$$= \int dt_1 \int dt_2 u_\alpha(t_1) u_\alpha^*(t_2) \mathbf{G}^r(t,t_1) i \sum_{L,R} \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1-t_2)} f_\alpha(\varepsilon) \mathbf{\Gamma}^\alpha(\varepsilon) \mathbf{G}^a(t_2,t')$$

The generalized spectral function

$$A_\alpha(\varepsilon,t) \equiv \int dt_1 u_\alpha(t_1) G^r(t,t_1) \exp\left[i\varepsilon(t-t_1) - i\int_t^{t_1} dt_2 \Delta_\alpha(t_2) \right]$$

For the time independent case, $\Delta_\alpha = 0$ and the generalized spectrum function $A_\alpha(\varepsilon)$ is just the F.T. of the retarded Green function $G^r(\varepsilon)$

$$N(t) = -iG^<(t,t)$$

$$= \int dt_1 \int dt_2 u_\alpha(t_1) u_\alpha^*(t_2) G^r(t,t_1) G^a(t_2,t)$$

$$\times \sum_{L,R} \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1-t_2)} f_\alpha(\varepsilon) \Gamma^\alpha$$

$$= \sum_{L,R} \Gamma^\alpha \int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon) \left| A_\alpha(\varepsilon) \right|^2$$

$$J_\alpha^{out} = -\frac{e}{\hbar} \Gamma^\alpha N(t)$$

$$J_\alpha^{in} = -\frac{e}{\hbar} \int_{-\infty}^{t} dt_1 \int \frac{d\varepsilon}{\pi} \mathrm{Im}\left\{ e^{-i\varepsilon(t_1-t)} \Gamma^\alpha(t_1,t) f_\alpha(\varepsilon) G^r(t,t_1) \right\}$$

$$= -\frac{e}{\hbar} \int_{-\infty}^{t} dt_1 \int \frac{d\varepsilon}{\pi} \Gamma^\alpha u_a(t) \mathrm{Im}\left\{ A_\alpha(\varepsilon) \right\}$$

Time independent case

$$A_\alpha(\varepsilon,t) \equiv \int dt_1 u_\alpha(t_1) G^r(t,t_1) \exp\left[i\varepsilon(t-t_1) - i\int_t^{t_1} dt_2 \Delta_\alpha(t_2) \right]$$

For the time independent case, $\Delta_\alpha = 0$ and the generalized spectrum function $A_\alpha(\varepsilon)$ is just the F.T. of the retarded Green function $G^r(\varepsilon)$

$$A_\alpha(\varepsilon) = G^r(\omega)$$

$$J_\alpha^{in} = \frac{e}{\hbar}\int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon) \Gamma^\alpha (-2) \operatorname{Im}\left\{G^r(\omega)\right\} \Leftrightarrow J_\alpha^{in} = \frac{e}{\hbar}\int \frac{d\varepsilon}{2\pi} Tr\left\{ \mathbf{\Gamma}^\alpha (-2) \operatorname{Im}\left\{\mathbf{G}^r(\omega)\right\}\right\}$$

$$J_\alpha^{out} = -\frac{e}{\hbar}\Gamma^\alpha N \Leftrightarrow J_\alpha^{out} = -\frac{e}{\hbar} Tr\left\{\mathbf{\Gamma}^\alpha \mathbf{N}\right\}$$

In the steady state

$$J = J_L = -J_R = \left(J_L - J_R\right)/2$$

$$J = \frac{e}{2\hbar}\int \frac{d\varepsilon}{2\pi} Tr\left\{\left(f_L(\varepsilon)\mathbf{\Gamma}^L - f_R(\varepsilon)\mathbf{\Gamma}^R \right)(-2)\operatorname{Im}\mathbf{G}^r(\omega)\right\} - \frac{e}{\hbar} Tr\left[\left(\mathbf{\Gamma}^L - \mathbf{\Gamma}^R\right)\mathbf{N}\right]$$

if $\mathbf{\Gamma}^L = \mathbf{\Gamma}^R = \Gamma$

$$J = \frac{e}{2\hbar}\int \frac{d\varepsilon}{2\pi} Tr\Gamma\left\{\left(f_L(\varepsilon) - f_R(\varepsilon)\right)(-2)\operatorname{Im}\mathbf{G}^r(\omega)\right\}$$

The transport through the QD with phonon bath interaction

$$\Sigma_{ep}^{r}=\sum_{q}\left|M_{q}\right|^{2}\left[\frac{\left(N_{q}+1\right)-n_{e}}{\omega-\varepsilon_{0}-\upsilon_{q}+i\delta}+\frac{N_{q}+n_{e}}{\omega-\varepsilon_{0}+\upsilon_{q}+i\delta}\right]$$

the phonon bath spectrum density

$$J(\upsilon_{q})=J_{0}\left(\frac{\upsilon_{q}}{\upsilon_{C}}\right)^{s}e^{-\upsilon_{q}/\upsilon_{C}}\Theta\left(\upsilon_{q}\right)$$

$$\sum_{q}\left|M_{q}\right|^{2}\Rightarrow\int\frac{d\upsilon_{q}}{2\pi}J_{0}\left(\frac{\upsilon_{q}}{\upsilon_{C}}\right)^{s}e^{-\upsilon_{q}/\upsilon_{C}}\Theta\left(\upsilon_{q}\right)$$

$$\Sigma_{ep}^{r}=\frac{J_{0}}{c}\int_{0}^{\infty}\frac{d\upsilon_{q}}{2\pi}\left(\frac{\upsilon_{q}}{\upsilon_{C}}\right)^{s}e^{-\upsilon_{q}/\upsilon_{C}}\left[\frac{\left(N_{q}+1\right)-n_{e}}{\omega-\varepsilon_{0}-\upsilon_{q}+i\delta}+\frac{N_{q}+n_{e}}{\omega-\varepsilon_{0}+\upsilon_{q}+i\delta}\right]$$

ignored the real part

$$\Sigma_{ep}^{r}\propto\int_{0}^{\infty}\frac{d\upsilon_{q}}{2\pi}\left(\frac{\upsilon_{q}}{\upsilon_{C}}\right)^{s}\Theta\left(\upsilon_{q}\right)e^{-\upsilon_{q}/\upsilon_{C}}(-i\pi)\left[\left(N_{q}+1-n_{e}\right)\delta\left(\omega-\varepsilon_{0}-\upsilon_{q}\right)+\left(N_{q}+n_{e}\right)\delta\left(\omega-\varepsilon_{0}+\upsilon_{q}\right)\right]$$

For the case of zero temperature, $N_{q}=0$

$$\Sigma_{ep}^{r}\propto\int_{0}^{\infty}\frac{d\upsilon_{q}}{2\pi}\left(\frac{\upsilon_{q}}{\upsilon_{C}}\right)^{s}e^{-\upsilon_{q}/\upsilon_{C}}\Theta\left(\upsilon_{q}\right)(-i\pi)\left[(1-n_{e})\delta\left(\omega-\varepsilon_{0}-\upsilon_{q}\right)+(+n_{e})\delta\left(\omega-\varepsilon_{0}+\upsilon_{q}\right)\right]$$

$$\Sigma_{ep}^{r}=\begin{cases}\dfrac{(-i)}{2}(1-n_{e})\left(\dfrac{\omega-\varepsilon_{0}}{\upsilon_{C}}\right)^{s}\exp\left(-\dfrac{\omega-\varepsilon_{0}}{\upsilon_{C}}\right) & \text{for } \omega-\varepsilon_{0}>0\\ \dfrac{(-i)}{2}n_{e}\left(\dfrac{\varepsilon_{0}-\omega}{\upsilon_{C}}\right)^{s}\exp\left(\dfrac{\omega-\varepsilon_{0}}{\upsilon_{C}}\right) & \text{for } \omega-\varepsilon_{0}<0\end{cases}$$

$$G^r = \frac{1}{\omega - \varepsilon_0 - \Sigma^r_{ph} - \Sigma^r_T}$$

$$\Sigma^r_T = -\frac{i\Gamma}{2}$$

$$\Sigma^r_{ep} = \Sigma^r_{ep} = \Sigma^r_{ep} = \begin{cases} \frac{(-i)}{2}(1-N_e)\left(\frac{\omega-\varepsilon_0}{\upsilon_C}\right)^s \exp\left(-\frac{\omega-\varepsilon_0}{\upsilon_C}\right) & \text{for } \omega-\varepsilon_0 > 0 \\ \frac{(-i)}{2} N_e \left(\frac{\varepsilon_0-\omega}{\upsilon_C}\right)^s \exp\left(\frac{\omega-\varepsilon_0}{\upsilon_C}\right) & \text{for } \omega-\varepsilon_0 < 0 \end{cases}$$

For the time independent case

$$A(\omega) = G^r(\omega)$$

$$n_e = \sum_{L,R} \Gamma^\alpha \int \frac{d\varepsilon}{2\pi} f_\alpha(\varepsilon) \left|A_\alpha(\varepsilon)\right|^2 = \int \frac{d\varepsilon}{2\pi}\left[\Gamma^L f_L(\varepsilon) + \Gamma^R f_R(\varepsilon)\right]\left|A_\alpha(\varepsilon)\right|^2$$