3 June 2017

# Hedin equations

References:


1) L. Hedin, Phys. Rev 139 A796 (1965)

2) F. Giustino, Rev. Mod phys. 89, 015003 (2017)

3) A. Stan, "Conserving approximations in non equilibrium Green's function theory" PhD thesis Univ Groningen 2009.

4) Ferdi Aryasetawan "Functional derivative technique"


Introduction: The Feynman diagrammatic method was developed in the 1950 - 1960s which is intuitive and relatively simple. But the infinite set of diagrams are difficult to keep track. It is easy to miss a diagram or give incorrect prefactor (combinatorial factors).

Hedin came up in 1965 with a closed set of equations which is equivalent to the original diagrams. Another important feature of the Hedin equations is that it is expressed in the full Green's functions G not $G_0$. This makes it easy to do approximations, such as GW method. Hedin's equations are closed only formally, because of the presence of functional derivatives, such as $\frac{\delta \Sigma}{\delta G}$.

Here I try to reproduce standard literature results for pure electron systems (ions are not moving), and the electron + phonon (without electron-electron interaction). For the most general case of eletron, phonon, and full electron-electron, eletron-phonon interacting system, I refer to the Rev Mod phys long review by Giustino.

I still prefer a discrete discription of electrons with a tight-binding model to start with

$$C^\dagger H C = \sum_{jk} c_j^\dagger H_{jk} c_k$$

where $C = \begin{pmatrix} c_1 \\ c_2 \\ \cdot \\ c_j \\ \cdot \end{pmatrix}$ is the annihilation operators vector; $c_j$ for site $j$ (or state $j$). The charge at site $j$ is given by $\hat{q}_j = (-e) c_j^\dagger c_j = (-e) n_j$ ($-e$ is electron charge)

We ignore spins, or if we wish, we can include the spin degrees of freedom in the index $j$. To describe the electron Coulomb interaction, we can introduce a scalar field $\varphi$ so that the interaction energy is

$$\sum_j \hat{q}_j \varphi_j = \sum_j (-e) c_j^\dagger c_j \varphi_j$$

However, $\varphi$ will be viewed as only an external one, we write down the Coulomb interaction explicitly rough than mediated by field $\varphi$.

so $\frac{1}{2} \sum_{jk} \frac{1}{4\pi\varepsilon_0 |\vec{r}_j - \vec{r}_k|} \hat{q}_j \hat{q}_k = \frac{1}{2} \sum_{jk} \hat{q}_j V_{jk} \hat{q}_k$

In the summation $\sum_{jK} = \sum_{j=1}^{N}\sum_{K=1}^{N}$ so both $jK$ and $Kj$ is counted so we need to divide by 2

$$H_{int} = \frac{1}{2} q^T v q \qquad q = \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_j \\ \vdots \\ q_N \end{pmatrix}$$

as a matrix multiplication

$$v = (v_{jK}) = (v(\vec{r}_j - \vec{r}_K))$$

We see one problem since $v(\vec{r}=0) \to \infty$ the terms with $j=K$, the self interaction terms, gives infinity, we formally subtract off this contribution

$$H_{int} = \frac{1}{2} q^T v q = \frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{N} v_{jK} q_j q_K$$

$$\to \quad \frac{1}{2}\sum_{j\neq K} v_{jK} q_j q_K = \frac{1}{2}\sum_{j,K} v_{jK} q_j q_K - \frac{1}{2}\sum_j v_{jj} q_j q_j$$

$$= \frac{1}{2}\sum_{j,K} \left( v_{jK} q_j q_K - \delta_{jK} v_{jK} q_j q_K \right)$$

sum over all $j$, all $K$

$v = \frac{1}{4\pi\varepsilon_0 r}$ in 3D

clearly $v_{jK} = v_{Kj}$

$$= \frac{1}{2}\sum_{j,K} v_{jK}\left(q_j q_K - \delta_{jK} q_j q_K\right) = \frac{1}{2}\sum_{j,K} v_{jK}\left(q_j q_K - \delta_{jK} q_j^2\right)$$

$$= \frac{1}{2} e^2 \sum_{jK} v_{jK}\left[c_j^+ c_j c_K^+ c_K - \delta_{jK}\left(c_j^+ c_j c_j^+ c_j\right)\right]$$

clearly $\left(c_j^+ c_j\right)^2 = c_j^+ c_j$

Since the occupation number $n_j = c_j^+ c_j$ has eigenvalues of 0 or 1 only so $n_j(1-n_j) = 0$

$n_j = n_j^2$

We find $H_{int} = \frac{1}{2} e^2 \sum_{jk} v_{jk} \left[ c_j^+ c_j \, c_k^+ c_k - \delta_{jk} c_j^+ c_k \right]$

since $c_j c_k^+ + c_k^+ c_j = \delta_{jk}$

$$H_{int} = \frac{1}{2} e^2 \sum_{jk} v_{jk} \left[ c_j^+ \left(-c_k^* c_j + \delta_{jk}\right) c_k - \delta_{jk} c_j^+ c_k \right]$$

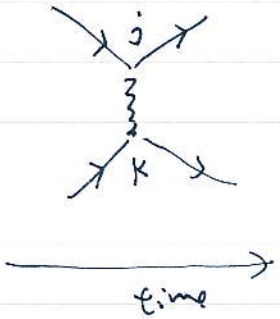
$$= \frac{1}{2} e^2 \sum_{jk} v_{jk} \left[ -c_j^+ c_k^+ c_j c_k \right] \qquad c_j c_k = -c_k c_j$$

$$= \frac{1}{2} e^2 \sum_{jk} v_{jk} c_j^+ c_k^+ c_k c_j = \frac{1}{2} e^2 \sum_{jk} c_j^+ c_k^+ v_{jk} c_k c_j$$

this is a standard form, usually written in the field $\psi(x)$ as

$$\frac{1}{2} e^2 \int dx \, dx' \, \psi^+(x) \psi^+(x') v(x, x') \psi(x') \psi(x)$$

We express the Coulomb interaction term in diagram as




we annihilate state j and k and create state k and j with amplitude $v_{jk}$. (order matters).

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Putting together, our Hamiltonian is

$$\tilde{H} = c^+ H c + \sum_j \hat{q}_j \phi_j + \frac{1}{2} e^2 \sum_{jk} c_j^+ c_k^+ v_{jk} c_k c_j$$

$\hat{q}_j = (-e) c_j^+ c_j$ We can combine the 1st term and second term, $H \to H^{\phi}_{jk} = H_{jk} + (-e) \delta_{jk} \phi_j$

$\phi$ acts only on the diagonal (on site). We will make $\phi$ time dependent $\to \phi_j(t)$.

The purpose of $\phi_j(t)$ is to be able to make functional derivative. Consider an arbitrary functional of $\phi_j(t)$

$F(\phi_j(t))$. $\quad \delta F = F(\phi_j(t) + \delta\phi_j) - F(\phi_j(t))$

$$= \sum_j \int dt \, \frac{\delta F}{\delta \phi_j(t)} \, \delta\phi_j(t)$$

this defines the functional derivatives. In fact we'll make time $t \to \tau$ on the Contour.

We define electron Green's function, contour ordered

$$G_{jk}(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau \, c_j(\tau) \, c_k^+(\tau') \rangle_{\hat{H}}$$

Here we have the full Hamilton $\hat{H} = \hat{H}^\phi + H_{int}$ which is time dependent due to the presence of $\phi$. $G$ is a functional of $\phi$, thus we can compute

$\delta G / \delta \phi_j(\tau)$.

We follow the usual diagrammatic method with $H_{int}$ as perturbation and $\hat{H}^\phi$ as the original $G_0$, then we can write the result in a Dyson equation

$$G = G^0 + G^0 M G$$

We use $M$ as self energy as we are going redefine the self energy by split $M$ into a "Hartree" term and "Fock" term, and call only the Fock term $\Sigma$.

$$M = \text{(Hartree loop)} + \Sigma$$

need to be discussed.

$$= (-i\hbar) e^2 \delta(\tau, \tau') V G(\tau, \tau^+) + \Sigma = (-e)\,\delta(\tau, \tau') \langle V \rangle$$

$$G_j(\tau, \tau^+) = \frac{i}{\hbar} \langle c_j^\dagger(\tau) \, c_j(\tau) \rangle = -\frac{1}{i\hbar} \langle q_j \rangle \left(\frac{1}{-e}\right)$$

Formally $G = G^0 + G^0 M G$

$\rightarrow G^{0-1} G = I + MG$ $\qquad M = V + \Sigma$

$= I + (V + \Sigma) G$ $\qquad G^{0-1} G^0 = I$

$\rightarrow (G^{0-1} - V) G = I + \Sigma G$

here $I \rightarrow \delta_{jk}\, \delta(\tau, \tau')$ Multiplication implies convolution in $\tau$

ie. $\Sigma G \rightarrow \int \Sigma_{jk}(\tau, \tau_1)\, G(\tau_1, \tau')\, d\tau_1$

$G^0$ is the Green's function for $H\phi$

so $\left[ i\hbar \frac{\partial}{\partial \tau} I - H - (-e)\{\phi_j(t)\} \right] G^0 = I$

so this is formally $G^{0-1}$ (except it is not in two variable convolution form)

$\{\phi_j\} = \begin{bmatrix} \phi_1 & & 0 \\ & \phi_2 & \\ & & \ddots \\ 0 & & \phi_N \end{bmatrix}$ is diagonal matrix with elements $\phi_j$

Combine with $V$ term from the original self energy $M$ we get the equation for $G$

$V_{tot} = \{V_j^{tot}\}$

$\left( I i\hbar \frac{\partial}{\partial \tau} - H - V_{tot}^{(-e)} \right) G = I + \Sigma G$

$V_j^{tot} = \phi_j + \left( v \langle q_r \rangle \right)_j$ $\qquad v$ map charge to potential

$V_j^{tot}$: total potential; $\phi_j$: external potential; induced potential $\rightarrow \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(r')}{|r - r'|}\, dr$

This is just a rewritten of the dyson equation. The only unusual points are 1) we have an external, time dependent potential 2) We split the Hartree term out and put to the left side of equation.

3) The hartree term is $VG = D_0 G$, not $WG = DG_0$

The next step is to work out the equation of motion for the Green's function $G(\tau, \tau')$. As is well-known, for the linear system, we

have simple result. If $\hat{H} = c^{+} H c$, then the countar ordered Green's sonctim satisfies the "Schrödigr" cqvation $\left(i\hbar \, I \frac{\partial}{\partial \tau} - \hat{H}\right) G(\tau, \tau') = \delta(\tau, \tau') \cdot I$ with a right-hand side $\delta$- Sourae, hote the equatim is still correct if the Hamiltn is time dependent, $H \to H(\tau)$. The meanig of the time derivatives (and integratims) is explained in my 2nd review on NEGF in "Frontier Physics".

For interacting systems such as the Coumbomb interacrims $c^{+} c^{+} c\, c$, the equatim of motim is obviously not closed. High order Green's functims involving four c's result.

A Key step and concept is the functional derivative with respect to $\varphi$. With this mathematical device, the Coulomb interaltim terms, the extra nonlinear term can be expressed as $\frac{\delta G}{\delta \varphi_j(\tau)}$, as a result a "closed" equatin is obtained for G. The rest of the steps are still complicated but the idea is to remove the referenc to $\varphi$ from the problem, and make a systms consistant of $G$, $\Sigma$, and vertex functin $\Gamma$ (at $\varphi = 0$) but still involvs functional derivatins of $\Sigma$ with respect to $G$.

Firse the equatim of motim fr $G$

$$G_{jk}(\tau, \tau') = -\frac{i}{\hbar} \left\langle T_\tau \, c_j(\tau) \, c_k^{+}(\tau') \right\rangle$$

$$= \frac{1}{i\hbar} \theta(\tau, \tau') \left\langle c_j(\tau) \, c_k^{+}(\tau') \right\rangle - \frac{1}{i\hbar} \theta(\tau', \tau) \left\langle c_k^{+}(\tau') \, c_j(\tau) \right\rangle$$

Take derivative $i\hbar \frac{\partial}{\partial \tau}$, we note $\frac{\partial}{\partial \tau}\theta(\tau,\tau') = \delta(\tau,\tau')$

$\frac{\partial}{\partial \tau}\theta(\tau',\tau) = -\delta(\tau,\tau')$ and due to the $\delta$-function

we need $C_j(\tau) C_K^\dagger(\tau) + C_K^\dagger(\tau) C_j(\tau) = \delta_{j,K}$ (ie $\tau'=\tau$)

this gives the right-hand side as $\delta(\tau,\tau') I$.

$I = \begin{bmatrix} 1 & & 0 \\ & 1 & \\ 0 & & \ddots \\ & & & 1 \end{bmatrix}$ is $N \times N$ identity matrix. So we can

write $i\hbar \frac{\partial}{\partial \tau} G(\tau,\tau') = \delta(\tau,\tau') I + \left(\frac{1}{i\hbar}\right) \langle T_\tau \dot{C}(\tau) C^\dagger(\tau') \rangle$

Note $\langle \quad \rangle$ means $Tr(\rho_H \dots)$ the time depence of $C$ is the Heisenberg evolution of the full Hamiltonian

$\hat{H} = H^\phi + H_{int} = C^\dagger H C + \sum_s (-e) \hat{q}_s \varphi_j(t) + H_{int}$

Here $\dot{C}$ is $i\hbar \frac{dC}{d\tau} = [C, \hat{H}]$

or $\dot{C}_j = \frac{dC_j}{d\tau} = \frac{1}{i\hbar}\left[C_j, C^\dagger [H^\phi] C + \frac{1}{2} e^2 \sum_{K\ell} C_K^\dagger C_\ell^\dagger V_{K\ell} C_\ell C_K\right]$

Here $H^\phi$ is the original matrix $H$ plus a diagonal term $(-e)\varphi_j(t)$ on the $(j,j)$ diagonal

So $\dot{C}_j = \frac{1}{i\hbar}\left\{\sum_K H^\phi_{jK} C_K + \frac{1}{2} e^2 \left[C_j, \sum_{K\ell} C_K^\dagger C_\ell^\dagger V_{K\ell} C_\ell C_K\right]\right.$

We have used the formula for commutator

$$[A, BC] = \{A,B\}C - B\{A,C\} = [A,B]C + B[A,C]$$

$\{A,B\} = AB + BA \qquad [A,B] = AB - BA$

The Coulomb term gives $[C_j, C_K^\dagger C_\ell^\dagger C_\ell C_K]$

$= [C_j, C_K^\dagger C_\ell^\dagger] C_\ell C_K + C_K^\dagger C_\ell^\dagger \underbrace{[C_j, C_\ell C_K]}_{=0}$

$$= \{c_j, c_k^+\} c_\ell^+ c_\ell c_k \mp c_k^+ \{c_j, c_\ell^+\} c_\ell c_k$$

$$= \delta_{jk} c_\ell^+ c_\ell c_k - \underbrace{\delta_{j\ell} c_k^+ c_\ell c_k}_{\text{swap}} = \delta_{jk} n_\ell c_k + \delta_{j\ell} n_k c_\ell$$

here $n_j = c_j^+ c_j$

Putting these result into the Heisenberg equation for $c_j$ we get

$$i\hbar \dot{c}_j = \sum_k H^\phi_{jk} c_k + \frac{1}{2} e^2 \sum_{k,\ell} \left(\delta_{jk} n_\ell c_k + \delta_{j\ell} n_k c_\ell\right) V_{k\ell}$$

$$+ \frac{1}{2} e^2 \left[\sum_\ell n_\ell c_j V_{j\ell} + \sum_k n_k c_j V_{kj}\right]$$

$$= \sum_k H^\phi_{jk} c_k + e^2 \left(\sum_\ell V_{j\ell} n_\ell\right) c_j \qquad V_{j\ell} = V_{\ell j}$$

The physical meaning of the 2nd term is clear. It is just the potential energy produced by all the charges located at $\ell$, in continuous form

$$V(\vec{r}) = \int \frac{e^2 n(\vec{r}')}{4\pi\varepsilon_0 |\vec{r} - \vec{r}'|} d^3\vec{r}'$$

Thus, the equation of motion for the contour ordered Green's function is

$$i\hbar \frac{\partial}{\partial \tau} G_{jk}(\tau, \tau') = \delta(\tau, \tau') \delta_{jk} + \left(\frac{1}{i\hbar}\right) \langle T_\tau \left[\sum_s H^\phi_{js} c_s(\tau) + e^2 \left(\sum_\ell V_{j\ell} n_\ell(\tau)\right) c_j(\tau)\right] c_k^+(\tau') \rangle$$

$$= \delta(\tau, \tau') \delta_{jk} + \sum_s H^\phi_{js} G_{sk}(\tau, \tau') + \frac{e^2}{i\hbar} \sum_\ell V_{j\ell} \langle T_\tau n_\ell(\tau) c_j(\tau) c_k^+(\tau') \rangle$$

We see a new special Green's function defined by

$$\left(-\frac{i}{\hbar}\right) \langle T \underbrace{c_\ell^+(\tau) c_\ell(\tau)}\ c_j(\tau) c_k^+(\tau') \rangle$$

As far as time ordered is concerned the operator $nc$ must move as a single identity.

Now the critical step is to express the last nonlinear term as a functional derivative $\frac{\delta G}{\delta \varphi}$. In order to work out this functional derivative explicitly, we need to have an explicit expression for $G$ as a functional of $\varphi$. To this end, we should use an interaction picture in terms of $\hat{H} = c^\dagger H c$ (not $\hat{H}^\varphi$). Another point is to note that $\varphi$ is defined for each site $j$ and each given contour time $\tau$. Since each $\tau$ is independ (but we take only continuous function in $\tau$) there is no reason to demand $\tau$ is a function of time $t$ only. So $\tau \equiv (t, \sigma)$ is branch $\sigma$-dependent. As a result, the contribution to the scattering matrix from upper branch does not cancel the lower brach. ie.

$$\mathrm{Tr}\left(\rho(-\infty) T_\tau e^{-\frac{i}{\hbar}\int_C \tilde{H}_{int}(\tau)\,d\tau}\right) \neq 1$$

so we need to divided explicitly this term in the denominator. ie. when $\varphi$ is contour dependent, the vacuum diagrams are not zero, just like in the problem of full counting statistics.

But at the end of calculation, when the functional derivatives are obtained, we can set $\varphi \equiv 0$. In this sense, the $\varphi$-dependence are always treated in the linear response regime.

With the above discussion we have $\varphi$-dependent Green's function

$$G^\varphi_{jK}(\tau, \tau') \equiv \left(-\frac{i}{\hbar}\right) \frac{\mathrm{Tr}\left[\rho(-\infty) T_\tau c_j(\tau) c^\dagger_K(\tau') e^{-\frac{i}{\hbar}\int \tilde{H}_{int}(\tau'')\,d\tau''}\right]}{\mathrm{Tr}\left[\rho(-\infty) T_\tau e^{-\frac{i}{\hbar}\int \tilde{H}_{int}(\tau'')\,d\tau''}\right]}$$

6 June 2017

Here $c(\tau)$ is in the interaction picture governed by $\hat{H}$ = $c^+ H c$, i.e.

$$c(t) = e^{+\frac{i}{\hbar}\hat{H}t} \, c \, e^{-\frac{i}{\hbar}\hat{H}t}$$

$$\tilde{H}_{int}(\tau) = \hat{H}^{\varphi}_{int} = (-e)\sum_{\ell} \hat{n}_{\ell}(\tau)\varphi_{\ell}(\tau) + \sum_{\ell} c^{+}_{(\tau)} M^{\ell}_{(\tau)} c^{\ell}_{(\tau)} u(\tau)$$

$\hat{n}_{\ell} = c^{+}_{\ell} c_{\ell}$ the $\tau$-dependence here is also in the interaction picture of $\hat{H}$. $\rho(-\infty)$ is some initial density matrix whose nature need not to be specified here. The integral $\int d\tau''$ is on the Keldysh contour


The contour ordering superoperator $\mathcal{T}_c$ applies to the operators to its right. Since $c(\tau)$ has no $\varphi$ dependence, we have made explicit the $\varphi$-dependence in only the scattering operator $S$

$$S(\tau_1, \tau_2) = \mathcal{T}_c \, e^{-\frac{i}{\hbar}\int_{\tau_1}^{\tau_2} d\tau'' \left[(-e)\sum_{\ell} n_{\ell}(\tau'')\varphi_{\ell}(\tau'') + c^{+} M c + u\right]}$$

$$G^{\varphi}(\tau, \tau') = \left(-\frac{i}{\hbar}\right) \frac{\mathrm{Tr}\left[\rho(-\infty)\, \mathcal{T}_c \, c(\tau)\, c^{+}(\tau')\, S^{\varphi}(-\infty, -\infty)\right]}{\mathrm{Tr}\left[\rho(-\infty) S^{\varphi}(-\infty, -\infty)\right]}$$

Note that $S^{\varphi}(-\infty, -\infty) = S^{\varphi}(-\infty^{-}, +\infty^{-}) \, S^{\varphi}(+\infty^{+}, -\infty^{+}) \neq 1$

lower branch, upper branch

We make variation with respect to $\varphi$

$$\delta G^{\varphi} = \left(-\frac{i}{\hbar}\right)\left[\frac{\mathrm{Tr}\left[\rho\, \mathcal{T}_c\, c(\tau)\, c^{+}(\tau')\, \delta S S^{\dagger}\right]}{\mathrm{Tr}\left[\rho S\right]} - \frac{\mathrm{Tr}\left[\rho\, \mathcal{T}_c\, c(\tau)\, c^{+}(\tau') S^{\dagger}\right]}{\left(\mathrm{Tr}\left[\rho S\right]\right)^2} * \mathrm{Tr}\left[\rho \delta S\right]\right]$$

The variation of the scattering matrix with respect to $\varphi$ is

$$\delta S = T_\tau \delta \left( e^{-\frac{i}{\hbar}\int d\tau'' \left[ (-e)\sum_\ell n_\ell(\tau'')\varphi_\ell(\tau'') + \vec{c}^{+}(\tau'')\vec{M}(\tau'')\vec{c}(\tau'') \right]} \right)$$

$$= T_\tau \left[ -\frac{i}{\hbar}\int d\tau_1 \, (-e) \sum_r n_r(\tau_1)\, \delta\varphi_r(\tau_1)\, e^{-\frac{i}{\hbar}\int d\tau'' \, \tilde{H}^{\varphi}_{int}(\tau'')} \right]$$

$$= \int d\tau_1 \frac{\delta S}{\delta \varphi_r(\tau_1)} \delta\varphi_r(\tau_1)$$

Thus we can identify the functional derivative of $S$ with respect to $\varphi$ as

$$\frac{\delta S}{\delta \varphi_r(\tau_1)} = T_\tau \left[ \left(-\frac{i}{\hbar}\right)(-e)\, n_r(\tau_1)\, e^{-\frac{i}{\hbar}\int d\tau'' \tilde{H}^{\varphi}_{int}(\tau'')} \right]$$

since $\delta S$ is linear in $\delta\varphi_r$ it is clear $\delta G^{\varphi}$ is also linear in $\delta\varphi_r$. we have

$$\frac{\delta G^{\varphi}_{jk}(\tau,\tau')}{\delta\varphi_r(\tau_1)} = \left(-\frac{i}{\hbar}\right)\left[ \frac{Tr[\rho T_\tau c_j(\tau) c^{+}_k(\tau') \left(-\frac{i}{\hbar}\right)(-e) n_r(\tau_1) S]}{Tr[\rho S]} \right.$$

$$\left. - \frac{Tr(\rho T_\tau c_j(\tau) c^{+}_k(\tau') S)}{Tr(\rho S)} \cdot \frac{Tr(\rho T_\tau \left(-\frac{i}{\hbar}\right)(-e) n_r(\tau_1) S)}{Tr(\rho S)} \right]$$

$$= \left(\frac{1}{i\hbar}\right)\left\{ \left\langle T_\tau n_r(\tau_1) c_j(\tau) c^{+}_k(\tau') \right\rangle_{\tilde{H}_{int}} \frac{ie}{\hbar} - \left(\frac{-e}{i\hbar}\right)\langle n_r(\tau_1)\rangle \left\langle T_\tau c_j(\tau) c^{+}_k(\tau') \right\rangle \right\}$$

back to full Hamiltonian $H_c + \vec{\Sigma}\vec{q}\phi + c\vec{M}c\cdot\vec{u}$

$$\langle \cdots \rangle_{\tilde{H}_{int}} = \frac{Tr(\rho \cdots)}{Tr(e \cdots)} \leftarrow \text{includes a denominator}$$

$$= \frac{1}{i\hbar}\left\langle T_\tau n_r(\tau_1) c_j(\tau) c^{+}_k(\tau') \right\rangle \frac{ie}{\hbar} + \underbrace{e\langle n_r(\tau_1)\rangle}_{-\langle q_r(\tau_1)\rangle} G^{\varphi}_{jk}(\tau,\tau')\left(\frac{1}{i\hbar}\right)$$

In the equation of motion for $G^{\varphi}$, we need the term $\frac{1}{i\hbar}\left\langle T_\tau \underbrace{n_\ell(\tau) c_j(\tau)} c^{+}_k(\tau') \right\rangle$ on page 279.

As stated earlier, as far as counter order is concerned the product of the operator $\underbrace{n\,c}$ must behave as a single identity. This means we always need to put $n$ to the left of $c$. This can be achieved if the time for $n$ is slightly late than $c$, so we take $\tau_1 = \tau^+$

The equation of motion becomes

$$i\hbar \frac{\partial}{\partial \tau} G_{jk}(\tau,\tau') = \delta(\tau,\tau')\delta_{jk} + \sum_s H^{\phi}_{js} G_{sk}(\tau,\tau') + e^2 \sum_l V_{jl} \left[ \frac{\hbar}{ie} \frac{\delta G_{jk}(\tau,\tau')}{\delta \varphi_l(\tau^+)} + \underbrace{\langle \hat{n}_l(\tau) \rangle}_{\parallel} G_{jk}(\tau,\tau') \right]$$

$e^2 \sum_l V_{jl} \langle n_l \rangle$ is Hartree term

$$\tau^+ = \tau + \Delta$$

Note $\delta G = \sum \int d\tau \frac{\delta G}{\delta \varphi} \delta\varphi$ so $\left[\frac{\delta G}{\delta \varphi}\right] = \left[\frac{G}{\varphi t}\right]$

so $$i\hbar \frac{\partial G_{jk}(\tau,\tau')}{\partial \tau} - \left(\sum_s H^{\phi}_{js} G_{sk}(\tau,\tau')\right) + e^2 \left(\sum_l V_{jl} \langle n_l \rangle\right) G_{jk}(\tau,\tau') + \frac{e}{i}\hbar \sum_l V_{jl} \frac{\delta}{\delta \varphi_l(\tau^+)} G_{jk}(\tau,\tau') = \delta(\tau,\tau')\delta_{jk}$$

We can write this in matrix / vector form as

$$\left[ i\hbar \frac{\partial}{\partial \tau} I - H^{tot} + ie\hbar \{V_j \cdot \frac{\delta}{\delta \varphi(\tau^+)}\} \right] G(\tau,\tau') = \delta(\tau,\tau') I$$

$$H^{tot}_{jk} = H_{jk} + \delta_{jk}\left[(-e)\varphi_j + \underbrace{e^2 \sum_l V_{jl} \langle n_l \rangle}_{\parallel}\right]$$

$$(-e) V(q_j)$$

$$= H_{jk} + \delta_{jk} V^{tot}_j (-e)$$

$$V^{tot}_j = \phi_j + \underbrace{(V \langle q \rangle)_j}_{\text{matrix}} \leftarrow \text{vector} \qquad \leftarrow \text{Hartree potential}$$

7 June 2017

By taken the functional derivative of $G$, we were able to convert the nonlinear term $\langle T_\tau (n(\tau) c(\tau) c^\dagger(\tau')\rangle$ into a linear form and the equation

$$\left( i\hbar \, I \frac{\partial}{\partial \tau} - \tilde{H} \right) G(\tau, \tau') = I \, \delta(\tau, \tau')$$

Here $\tilde{H}$ is a matrix and different operator on $\varphi$

$\tilde{H} = H$ + diagal term

The $j^{th}$ diagal term $= (-e) \left[ \varphi_j \right.$ ← extal potential $+ \left[ U \langle q \rangle \right]_j$ ← hartree term

$$+ i\hbar \left[ V \cdot \frac{\delta}{\delta \varphi} \right)_j \Big]$$

functional derivatis

$$\left[ U \cdot \frac{\delta}{\delta \varphi} \right]_j = \sum_l U_{jl} \frac{\delta}{\delta \varphi_l} .$$

This is a very important equation, since, it makes $G$ "closed". But the price we pay is that it is in a very high-dimensional space, since $G$ should be viewed as the complete function of $\varphi_j(\tau)$.

This equation, according to Hedin, is originally due to Schwinger, 1959. Here the equation is expressed in slightly different notation is equivalent to (A10) in Hedin's Phys. Rev paper (1965).

The next few steps is to identify the self energy $\Sigma$ and get rid of $\varphi$ in favour of other variable. Compare the differential form of the Dyson equation, we are almost there except in Dyson equation, we have $-\Sigma G$, but here

(te) $ih\left\{\left(V\cdot\frac{\delta}{\delta\varphi}\right)_j G(\tau,\tau')\right\} = -\Sigma G$ full form with indices

$\rightarrow e^{ih\sum_{jl} V_{jl}\frac{\delta}{\delta\varphi_l(\tau^+)}} G_{jk}(\tau,\tau') = -\sum_s \Sigma_{js}(\tau\tau'')\, G_{sk}(\tau'',\tau')\, d\tau''$

The left side is $\frac{\delta G}{\delta\varphi}$ but right side is $\Sigma\cdot G$

In order to have something times $G$, we use a trick.

to express $\frac{\delta G}{\delta\varphi}$ by $\frac{\delta G^{-1}}{\delta\varphi}$. Here $G^{-1}$ means

$$\int G(\tau,\tau'')\, G(\tau'',\tau')^{-1} d\tau'' = I\,\delta(\tau,\tau')$$

multiply in matrix element
convolute in time $\tau''$

compare $d\left(\frac{1}{x}\right) = \frac{-1}{x^2}dx$

Symbolically, $G G^{-1} = 1$

so $\delta G\, G^{-1} + G\,\delta G^{-1} = 0$ (Leibnitz rule)

or $\delta G = -G\,\delta G^{-1} G$ multiply $G$ from left

so $\frac{\delta G(\tau,\tau')}{\delta\varphi_l(\tau_1)} = -\int\!\!\int G(\tau,\tau_2)\,\frac{\delta G^{-1}(\tau_2\tau_3)}{\delta\varphi_l(\tau_1)}\, G(\tau_3\tau')\, d\tau_2 d\tau_3$

here on the left matrix multiplication on space index in $G$ is implied. Put this back into the left side we get

$$e^{ih\left\{\left(V\cdot\frac{\delta}{\delta\varphi(\tau^+)}\right)_j\right\}} G(\tau,\tau') = ?$$

To simplify notation, we use

$1 \equiv (j_1,\tau_1)$ $\quad G_{j_1 j_2}(\tau_1,\tau_2) \rightarrow G(1,2)$

$\int d3 \rightarrow \sum_{j_3}\int d\tau_3$

also $V(1,2) \rightarrow v_{j_1 j_2}\,\delta(\tau_1,\tau_2)$

introduce

so $e^{ih\int v(1^+,3)\frac{\delta}{\delta\varphi(3)} G(1,2)\, d3} = -\int \Sigma(1,3)\, G(3,2)\, d3$

$\uparrow$ transfer $\tau_1^+$ into 1.

With these shorthand notations we have

$$e i\hbar \int d3 \left[ v(1^+, 3) \left[ - G(1,4) \frac{\delta G^{-1}(4,5)}{\delta \varphi(3)} G(5,2) \right] d4\, d5 \right.$$

$$= - \int d3\, \Sigma(1,3) G(3,2)$$

Rename 5 as 3, 3 → 4

we identify

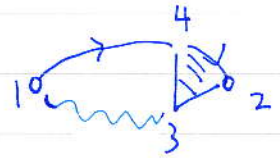
$$\Sigma(1,3) = e i\hbar \iint v(1^+, 5) G(1,4) \frac{\delta G^{-1}(4,3)}{\delta \varphi(5)} d5\, d4$$

or rename the numbers again 3 → 2, 5 → 3

$$\Sigma(1,2) = i\hbar e \int d3 \int d4\; v(1^+, 3) G(1,4) \frac{\delta G^{-1}(4,2)}{\delta \varphi(3)}$$

This is a formal exact expression for electron self energy. Equivalent to Eq (A16)

We should think of $e = -1$ in Hedin's notation.

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Our next step is to evoke the theory of screening. So the interaction $v$ becomes the screened one, we called $D$, the full photon (scalar) Green's function. Satisfies the Dyson equation, symbolically

$$D = v + v \Pi D \qquad D \to D_{jk}(\tau, \tau')$$

$$v \to V_{jk} \delta(\tau, \tau')$$

here we take this as a definition and try to define an equation for the self energy $\Pi$. $\Pi \to \Pi_{jk}(\tau, \tau')$

We define the dielectric constant (matrix as)

$$\epsilon = 1 - v\Pi$$

so $\epsilon D = v$ and define $\epsilon^{-1} = 1 + v\chi$

Here $\chi$ is density (charge) correlation function

The relation between $\chi$ and $\Pi$ is

$$\chi = \Pi \epsilon^{-1} = \Pi + \Pi V \chi$$

$\epsilon$ has been defined such that

and $\epsilon^T q = q^{ex}$ ← external charge

↑ induced charge ↑ actual

$D = V + V \chi V$

$\epsilon \phi = \phi^{ex}$

actual external

↓ ↓

$V^{tot}$ $\varphi$ new notation

For further see Mahan-Li-Yu.pdf.

Here $\chi_{jk}(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau \delta q_j(\tau) \cdot \delta q_k(\tau') \rangle$

here $\delta q = q - \langle q \rangle$ we need a proof that this is true. $\chi$ and $\Pi$ is symmetric, like $D$, but $\epsilon$ is not.

The total actual potential is

$$V_j^{tot}(\tau) = \phi_j(\tau) + \sum_k v_{jk} \langle q \rangle_k(\tau)$$

or symbolically $V_{tot}(1) = \varphi(1) + \int d2\, v(1,2) \langle \hat{q}(2) \rangle$

Since $\epsilon \phi = \phi^{ex} \Rightarrow \int \epsilon(1,2)\, \delta V_{tot}(2)\, d2 = \delta \varphi(1)$

$$\frac{\delta \varphi(1)}{\delta V_{tot}(2)} = \epsilon(1,2)$$

$$\epsilon^{-1}(1,2) = \frac{\delta V_{tot}(1)}{\delta \varphi(2)}$$

I hope the notation is consistent

since $\int \epsilon^{-1}(1,2)\, \epsilon(2,3)\, d2 = \int d2 \left[ \frac{\delta V_{tot}(1)}{\delta \varphi(2)} \frac{\delta \varphi(2)}{\delta V_{tot}(3)} \right]$

$= \delta(1,3)$

With this relation (or definition of) $\epsilon^{-1}$ to $\frac{\delta V^{tot}}{\delta \varphi}$, we get

$$\epsilon^{-1}(1,2) = \frac{\delta V_{tot}(1)}{\delta \varphi(2)} = \delta(1,2) + \int d3\, v(1,3) \frac{\delta \langle q(3) \rangle}{\delta \varphi(2)}$$

↓

We keep $\varphi$ small, to 1 linear order in $\varphi$, we can apply the linear response theory so

$\frac{\delta \langle q(3) \rangle}{\delta q(2)} = \chi(3,2)$ since $\delta \langle q(3) \rangle = \int \chi(3,2)\, \delta q(2)\, d2$

Thus $\epsilon^{-1} = 1 + v\chi$ is verified and $\chi$ is indeed the fluctuation of charge.

The standard notation for the screened potential is $W$ which I called $D$. Let us $W$. Then

$$W = \epsilon^{-1} v = (1 + v\chi) v = v + v\chi v$$
$$= v + v \Pi W$$

We need to change $v$ to $W$ in the self energy $\Sigma$ formula. To do this we make a change of variable from $\varphi$ to $V^{tot} = \varphi + \int d2\, v(1,2) \langle \hat{q} \rangle$

So → use the chain rule: $\frac{\delta}{\delta \varphi(3)} = \int \frac{\delta V^{tot}(4)}{\delta \varphi(3)} \frac{\delta}{\delta V^{tot}(4)}\, d4$

$$= \int d4\, \epsilon^{-1}(4,3) \frac{\delta}{\delta V^{tot}(4)}$$

we have:

→ $W(1,2) = \int d3\, \epsilon^{-1}(1,3)\, v(3,2)$

We define the vertex function as $\Gamma(1,2;3) \equiv - \frac{\delta G^{-1}(12)}{\delta V^{tot}(3)}$

using these relations we have

using the fact that $v$, $\Pi$, $\chi$ and thus are symmetric with respect to the two arguments 1 and 2 we can also write $W = v\epsilon^{-1}$ or

$W(1,2) = \int d3\, v(1,3)\, \epsilon^{-1}(3,2)$ wrong

Using the above relation, we are ready to write down the first of the Hedin equations for the electron self energy $\Sigma(1,2)$ as

from page 293

$$\Sigma(1,2) = ihe \int d3 \int d4\; v(1^+,3)\, G(1,4)\, \frac{\delta G^{-1}(4,2)}{\delta \varphi(3)}$$

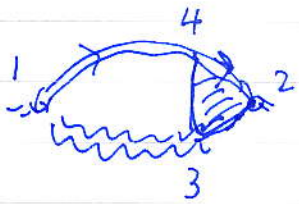
$$= (-e)\, ih \int d3 \int d4 \int d5\; v(1^+,3)\, G(1,4)\, \underbrace{\epsilon^{-1}(5,3)}_{1}\, \Gamma(4,2;5)$$

$\epsilon$ symmetri argument

$$= (-e)\, ih \int d4 \int d5\; W(1^+,5)\, G(14)\, \Gamma(42;5)$$

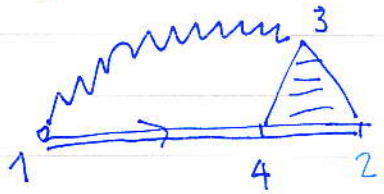
rename $5 \to 3$ $\quad [v(3,1^+) = v(1^+,3),\ W$ is symmetric, $\epsilon$ is not symmetric]

$$\Sigma(1,2) = (-e)\, ih \int d3 \int d4\; W(1^+,3)\, G(1,4)\, \Gamma(4,2;3)$$




This result is known before Hedin. eg. in AGD, by purely diagrammatic argument. Hedin obtained the same result analytic/agebraically. See page 88, 89 in AGD [Abrikosov, Gorkov, Dzyaloshinski]. This result was also presented diagrammatically in Fetter and Walecka.

Both diagram




To determine $W$, we need $\Pi$, by

$$W = v + v\Pi \cdot W$$

We thus need an exact analytic expression for the polarization diagram $\Pi(1,2)$. We can get a functional derivative for $\Pi$ as

$$W = v\epsilon^{-1} \Rightarrow W(1,2) = \int v(1,3) \frac{\delta V_{tot}(3)}{\delta \varphi(2)}\, d3$$

$$= \int v(1,3) \left[ \delta(3,2) + \int d4\; v(3,4) \frac{\delta \langle \hat{q}(4) \rangle}{\delta \varphi(2)} \right] d3$$

$$= v(1,2) + \int d3\, d4\, d5\; v(1,3)\, v(3,4)\, \frac{\delta \langle \hat{q}(4) \rangle}{\delta V_{tot}(5)}\, \underbrace{\frac{\delta V_{tot}(5)}{\delta \varphi(2)}}$$

$= V(1,2) + \int d3\, d4 \; V(1,3) \frac{\delta \langle \hat{q}(4) \rangle}{\delta V_{ext}(5)}$

$W = \epsilon^{-1} V$

$W(1,2) = \int \epsilon^{-1}(1,3)\, V(3,2)\, d3 = \int \frac{\delta V_{ext}(1)}{\delta \varphi(3)} V(3,2)\, d3$

$= \int d3 \left[ \delta(1,3) + \int d4\, V(1,4) \frac{\delta \langle q(4) \rangle}{\delta \varphi(3)} \right] V(3,2)$

$= V(1,2) + \int d4\, V(1,4) \frac{\delta \langle q(4) \rangle}{\delta \varphi(3)} V(3,2)$

Compare with $W = V + V \chi V$ we see $\chi(1,2) = \frac{\delta \langle q(1) \rangle}{\delta \varphi(2)}$

as before

$= V(1,2) + \int d4\, d5\, V(1,4) \frac{\delta \langle q(4) \rangle}{\delta V_{ext}(5)} \cdot \frac{\delta V_{ext}(5)}{\delta \varphi(3)} V(3,2)$

$= V(1,2) + \int d4 \int d5\, V(1,4) \frac{\delta \langle q(4) \rangle}{\delta V_{ext}(5)} \underbrace{\epsilon^{-1}(5,3) V(3,2)}_{W(5,2)}$

$5 \to 4 \quad 4 \to 3$

$= V(1,2) + \int d3 \int d4\, V(1,3) \frac{\delta \langle q(3) \rangle}{\delta V_{ext}(4)} W(4,2)$ $\qquad \epsilon = 1 - V\Pi$

So $\Pi(3,4) = \frac{\delta \langle q(3) \rangle}{\delta V_{ext}(4)}$ So $\Pi$ maps total potential to induced charge

See Mahan-I-Yu.pdf page 193 for this interpretation.

To calculate this functional derivative

$\langle q(1) \rangle = (-e)(-i\hbar)\, G(1,1^+)$ $\qquad G^< = \frac{i}{\hbar} \langle c^+ c \rangle$

but $\frac{\delta G(1,2)}{\delta V_{ext}(3)} = -\int d4\, d5\; G(1,4) \frac{\delta G^{-1}(45)}{\delta V_{ext}(3)} G(5,2)$

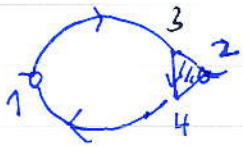
again this is because $G G^{-1} = I$ and $\delta G\, G^{-1} + G\, \delta G^{-1} = 0$

So $\Pi(1,2) = \frac{\delta \langle q(1) \rangle}{\delta V_{ext}(2)} = e i\hbar \frac{\delta G(1,1^+)}{\delta V_{ext}(2)} = -e i\hbar \int d4\, d5 \left[ G(1,4) \frac{\delta G^{-1}(45)}{\delta V_{ext}(2)} G(5,1^+) \right]$

using the definition for $\Gamma$, $\Gamma(1\,2;3) = -\dfrac{\delta G^{-1}(1,2)}{\delta V_{tot}(3)}$

we get $\Pi(1,2) = e\,i\hbar \int d3\,d4\; G(1,3)\,\Gamma(3\,4;2)\,G(4,1^{+})$

This is the 2nd Hedin equation for the self energy of photon.



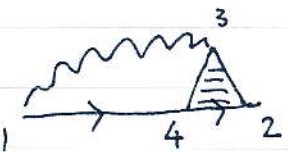

We see that we started with $\varphi$ as the fundamental variable but the transformation to $V_{tot}$ is an important step to take.

The last equation is a self-consistent equation for $\Gamma$ itself.

The logic is like this. Originally we have one functional derivative equation for the Green's function $G^{\varphi}$, as an equation of motion as given on page 287, 289. However, this functional derivative equation is in a very high dimension ( $G$ is a function of each $\varphi(\tau)$ ). Can we solve such equation on computer?

With the help of new variable $V_{tot}(1) = \varphi(1) + \int v(1,2)\langle q(2)\rangle\, d2$ and the dielectric function $\epsilon^{-1}(1,2) = \dfrac{\delta V_{tot}(1)}{\delta \varphi(2)}$, we can express two self-energies the electronic one and photon one by the vertex function $\Gamma(1,2;3) = -\dfrac{\delta G^{-1}(1,2)}{\delta V_{tot}(3)}$. Diagrammatically this is

$\Sigma(1,2) = (-e)\,i\hbar$

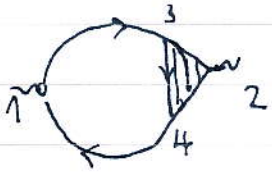



$G^{(1,2)} =$


$W(1,2) =$


$= W(2,1)$

$\Pi(1,2) = e\,i\hbar$




$\Gamma(1\,2;3) =$

However, the complexity does not go away. It is now reside in $\Gamma$. To get an equation for the vertex function $\Gamma(1,2;3)$ we need the Dyson equation

$$G = G_0 + G_0(\{V_{tot}\}(-e)t + \Sigma)G$$

Here $G_0$ is from $c^+Hc$ not including the external field $\varphi$ and Hartree term $v\varphi$. We have put these two terms in $V_{tot} = \varphi + v\varphi$. This term acting only as a diagonal matrix elements in space $j$ and time $\tau$ so the curly braces $\{V_{tot}\}$. From the above we find the inverse as

$$G^{-1}(1,2) = G_0^{-1}(1,2) + eV_{tot}(1)\delta(1,2) - \Sigma(1,2)$$

$\delta(1,2) \to \delta_{j,k}\,\delta(\tau_1,\tau_2)$ is the $\delta$-function in space & time. Take variation, since $G_0^{-1}$ does not depends on $\varphi$, and $V_{tot}(1)$ is to be the independent variable for the variation set get

$$\Gamma(1,2;3) = -\frac{\delta G^{-1}(12)}{\delta V_{tot}(3)} = (-e)\delta(1,3)\delta(1,2) + \frac{\delta\Sigma(1,2)}{\delta V_{tot}(3)}$$

If we omit the 2nd term, with $\Gamma(12;3) = -e\,\delta(12)\,\delta(1,3)$ we simply recover the self-consistent Born approximation (SCBA). But there is a slight difference. The Hartree term is still $\varphi + \int v\langle\varphi\rangle$ (with $\varphi = 0$). not $\int W\langle\varphi\rangle$! I.e. the potential should not be renormalized or screened, i.e. $D$ should be $D_0 = V$. As we see the Dyson equation in the form above is an exact equation. There is no reason to change $v$ in $V_{tot}$ to $W = D$!

To transfer the functional derivative from $\frac{\delta\Sigma}{\delta V_{tot}}$ to $\frac{\delta\Sigma}{\delta G}$ we need to think what does $\Sigma$ depends on.

If we do the standard diagrammatic expansion the self-energy is expressed by the non-interacting Green's functions $G_0^g$ and $V$. $V$ does not depends on $g$. $g$ is transformed to a new variables $V_{tot}$ one-to-one. However, we need the full Greens function $G^g$. We assume we can invert the Dyson equation

$$G = G_0 + G_0 \Sigma(G_0, V) G$$

taking $V$ as parameter i.e. $G_0 \equiv G_0(G, V)$

Substitute this back to the self energy $\Sigma(G_0, V)$ we can express it as solely a function of $G$ and $V$. i.e.

$$\Sigma = \Sigma(G_0, V) = \Sigma(G, v)$$

since $v$ is indepnt of $g$ thus $V_{tot}$ we have the chain rule

$$\frac{\delta \Sigma(1,2)}{\delta V_{tot}(3)} = \iint \frac{\delta G(45)}{\delta V_{tot}(3)} \frac{\delta \Sigma(1,2)}{\delta G(4,5)} \, d4 \, d5$$

However, if we express the self energy as $\Sigma(G, W)$ as in Hedin's original paper, then $W$ also depends on $g$ the chain rule is not so simple as we also need $\frac{\delta W}{\delta V_{tot}}$. Then

$$\frac{\delta \Sigma(12)}{\delta V_{tot}(3)} = \int d4 \int d5 \left[ -G(4,6) \frac{\delta G^{-1}(67)}{\delta V_{tot}(3)} G(7,5) \frac{\delta \Sigma(1,2)}{\delta G(4,5)} \right] d(5\,67)$$

$$= \int d(4567) \, G(4,6) \Gamma(6,7;3) G(7,5) \frac{\delta \Sigma(1,2)}{\delta G(4,5)}$$

so $\Gamma(1,2;3) = (-e)\,\delta(1,3)\,\delta(1,2)$ + above term

This is the last Hedin equation

Diagramatically we have for the vertex function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Starting page 263, we defined the tight-binding model with Coulomb interaction (with self-interaction removed). We then derive the equation of motion for $G$, replacing the nonlinear term by functionally derivating. This is a self-contained equation. However, we prefer an expression for self energy. A trick is used to transfer $\delta G$ to $\delta G^{-1}$ by noting $GG^{-1} = I$. Then we need the physics of screening, i.e. $\epsilon = 1 - v\Pi$, $\frac{1}{\epsilon} = 1 + v\chi$, etc. From this we can change from $g$ to $V_{tot}$ and expresses two self-energies in terms of $G$, $W$ and vertex function $\Gamma$. Finally, we get an equation for $\Gamma$. I think I have derived Hedin equations with sufficient details and justifications.

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We have demonstrated a detailed derivation of the Hedin equations for the free electron + Coulomb interaction system. Our next task is to give a derivation of the electron-phonon system (without electron-electron interaction).

Since electron-phonon interaction is structurally identical to electron-scalar field system, I also expect identical result for the phonon system with $D$ takes the position of $W$.

However, there is one puzzling aspect in the phonon case. There is no equivalence of the potential $V_{tot}(1)$ and hartree term in phonon case. We need to see how these differences are resolved.

We consider a finite cluster with a tight-binding electron system $\hat{H}_e = c^\dagger H c$ here $H$ is a finite $N$ by $N$ hermitian matrix $H^\dagger = H \rightarrow H_{ik}^* = H_{ki}$

$c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$ $c^\dagger = (c_1^\dagger, c_2^\dagger, \cdots c_N^\dagger)$ is row vector.

The free phonon is $\hat{H}_p = \frac{1}{2} p^T p + \frac{1}{2} u^T K u$ here $K$ is real and symmetric $K^T = K$, we call the matrix $K$ Dynamic matrix and $u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_j \\ \vdots \end{pmatrix} \equiv \vec{u}$ is a finite column vector. And the equation of motion for the phonon takes the usual Hamilton form

$$\dot{u} = \frac{\partial H_p}{\partial p} \qquad \dot{p} = -\frac{\partial H_p}{\partial u}$$

or $\dot{u} = p, \quad \dot{p} = \ddot{u} = -Ku$

Electron-phonon interaction is $H_{ep} = \sum M_{jk}^\alpha c_j^\dagger c_k u_\alpha$

$= c^\dagger \vec{M} c \cdot \vec{u}$

We do not assume periodicity. The advantage of such a notation is its generality. If the system does have periodicity, we can incorporated such fact at the very end, which only means the eigen mods, defined by

$$S^\dagger H S = \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \\ & & & \varepsilon_i \end{pmatrix} \qquad T^T K T = \begin{pmatrix} \omega_1^2 & & 0 \\ & \omega_2^2 & \\ 0 & & \ddots \\ & & & \omega_n^2 \end{pmatrix}$$

Is such that the wave vector $\vec{K}$ is a good "quantum number" Here $S^\dagger S = S S^\dagger = I, \quad T^T T = T T^T = I$

Our task is to obtain the associated Hedin equations for the Hamiltonian $\hat{H} = c^\dagger H c + \frac{1}{2}(p^2 + u^T K u) + c^\dagger \vec{M} c \cdot \vec{u}$ which relate the Green's functions $G$, $D$, and self-energies $\Sigma$ and $\Pi$, and finally the vertex function $\Gamma$. I claim it is nearly the same as before for the electron-Coulomb case but we need a proof.

Here we sort of follow the notes by Yu Ya dated 14 May 2017 (http://besides.wesfc2.com/) entitled "Hedin equations for interacting Electron-phonon systems."

In order to dynamically perturb the system, we introduce a center dependent force $f_\ell(\tau)$ coupled to the phonon coordinates $u_\ell$, i.e. we add one extra term to the Hamiltonian $\hat{H}$

$$\hat{H}' = -\sum_\ell f_\ell(\tau)\, \hat{u}_\ell$$

$\hat{u}_\ell$ is in Schrödinger picture and in $f(\tau)$, $\tau$ is explicit time (time dependent force). Since $[\hat{u}] = \sqrt{M}\cdot L$, the units for $f$ is $[f] = \frac{E}{\sqrt{M}}$ so that $[fu]$ is energy.

Here $f_\ell(\tau)$ plays the rule of $\varphi$ (see page 265) couple to the charge $\hat{q}$ in the Coulomb case. The role of $V_{tot}$ is now played by $\langle \hat{u}_\ell \rangle$ that is conjugate to $f$ (very much like the $\langle q \rangle$).

Our first step is to derive the equation of motion for the Hamiltonian $\hat{H} + \hat{H}' = c^\dagger H c + \frac{1}{2}(p^2 + u^T K u) + c^\dagger \vec{M} c \cdot \vec{u} - \vec{f}(t)\cdot\vec{u}$

Since $i\hbar \frac{dc}{dt} = [c, \hat{H} + \hat{H}'] = Hc + \vec{M} c \cdot \vec{u}$ the extra perturbation does not give new terms.

$[u, p] = i\hbar I$



while $\frac{d^2 u}{dt^2} = \frac{dp}{dt} = \frac{1}{i\hbar}[p, \hat{H} + \hat{H}'] = -Ku - c^\dagger M c - f$

all three terms are vectors

From these, we obtain the equation of motion for the contour ordered Green's functions as

$$i\hbar \frac{\partial}{\partial \tau} G_{jk}(\tau, \tau') - \sum_s H_{js} G_{sk}(\tau, \tau') - \left(-\frac{i}{\hbar}\right) \sum_{ls} M^l_{js} \left\langle T_\tau c_s(\tau)\, u_l(\tau)\, c^\dagger_k(\tau') \right\rangle = \delta_{jk} \delta(\tau, \tau')$$

$$\frac{\partial^2}{\partial \tau^2} D_{jk}(\tau, \tau') + \sum_s K_{js} D_{sk}(\tau, \tau') + \left(-\frac{i}{\hbar}\right) \sum_{ll'} M^j_{ll'} \left\langle T\left(c^\dagger_l(\tau)\, c_{l'}(\tau)\right) u_k(\tau') \right\rangle$$

$$= -\delta_{jk} \delta(\tau, \tau') + \left(-\frac{i}{\hbar}\right) f_j(\tau) \langle u_k(\tau') \rangle$$

Here the Green's function are defined in the usual way

$$G_{jk}(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau\, c_j(\tau)\, c^\dagger_k(\tau') \rangle$$

$$D_{jk}(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau \left( u_j(\tau) - \langle u_j(\tau) \rangle \right) \left( u_k(\tau') - \langle u_k(\tau') \rangle \right) \rangle$$

Since $\langle u_j(\tau) \rangle \neq 0$. we subtract off so that $D$ as a Dyson equation

$$\langle \cdots \rangle = \frac{\mathrm{Tr}(\rho \cdots S)}{\mathrm{Tr}(\rho S)} \qquad S = T_\tau e^{-\frac{i}{\hbar} \int \left(-\vec{f}(\tau'') u(\tau'')\right) d\tau''}$$

here $S$ is governed by $\hat{H}'$ only and the operator $c$, $c^\dagger$, $u$ evolving according $\hat{H}$. We see

$$\delta S = T_\tau \sum_j \int d\tau'' \left(\frac{i}{\hbar} \delta f_j(\tau'')\, u_j(\tau'')\right) \cdot S$$

or $\frac{\delta S}{\delta f_j(1)} = T_\tau \left(\frac{i}{\hbar} u(1) S\right)$ This analog to Eq $\frac{\delta S}{\delta g}$ on page 285.

We now ask how does the average position $\langle u_j(\tau) \rangle$ changes with the application of a time dependent force $f_k(\tau')$? The answer is

precisely given by linear response theory with the response function $D_{\bar{\jmath}K}(x,\tau')$. We derive this result by the definition of the average $\langle u\rangle$ and use functional derivative. We note that $\langle u\rangle$ is not constant since $f$ is time dependent.

To work out this linear response since $\langle u\rangle_{\hat{H}} \neq 0$ in general even when $f\equiv 0$ but $\langle u\rangle$ under the total Hamiltn is a constant, we consider

$$\langle \Delta u\rangle = \langle u\rangle_{\hat{H}+\hat{H}'} - \langle u\rangle_{\hat{H}} = \langle (u - \langle u\rangle_{\hat{H}})\rangle_{\hat{H}+\hat{H}'}$$

finite $f$ $\quad$ $f\equiv 0$ for all $\tau$ and $j$

So $\Delta u = u - \langle u\rangle_{\hat{H}}$ the fluctuation is with respect to the time independent full Hamiltn $\hat{H} = \hat{H}_e + \hat{H}_p + \hat{H}_{ep}$.

so

$$\langle \Delta u(\tau)\rangle = \frac{Tr(\rho T_\tau (u(t) - \langle u\rangle_{\hat{H}})\, S)}{Tr(\rho S)}$$

Now we make variation with respect to $f$ so

$$\delta\langle \Delta u(\tau)\rangle = \frac{Tr(\rho T_\tau (u(\tau) - \langle u\rangle_H)\,\delta S)}{Tr(\rho S)} - \frac{Tr(\rho(u-\langle u\rangle)S)}{Tr(\rho S)^2} Tr(\rho\,\delta S)$$

Note that in the interaction picture with interaction as $H' = -\sum_j f_j(\tau)\, U_j$ and the Heisenberg evolution by $\hat{H}$ for the operator $u(\tau) \to u(t) = e^{+\frac{i}{\hbar}\hat{H}t}\, u\, e^{-\frac{i}{\hbar}\hat{H}t}$ the only $f$ dependence is in $S$ and we already get

$$\delta S = \left(\frac{i}{\hbar}\right)\int d2\; u(2)\,\delta f(2)\cdot S$$

$1 \equiv (j, \tau_1)$

$$\delta \langle \Delta u(q) \rangle = \int d2 \frac{i}{\hbar} \delta f(2) \left[ \frac{Tr(\rho T_\tau u(q)\, u(2) \cdot S')}{Tr(\rho S')} - \frac{Tr(\rho \Delta u(1) S)}{Tr(\rho S)} \times \frac{Tr(\rho u(2) S)}{Tr(\rho S')} \right]$$

It is clear $\delta \langle u \rangle_H = 0$
It is just a number do not vanish with $\delta f$

so $\delta F \equiv F(f + \delta f) - F(f)$

$$\delta \langle \Delta u(1) \rangle = \delta \langle u(1) \rangle = \int d2 \left(\frac{i}{\hbar}\right) \delta f(2) \left[ \langle T_\tau u(1) u(2) \rangle - \langle u(1) \rangle \langle u(2) \rangle \right]$$

$$= - \int d2\, D(1,2)\, \delta f(2)$$

here $D(1,2) = \left(-\frac{i}{\hbar}\right) \langle T_\tau \left( u(1) - \langle u(1) \rangle \right) \left( u(2) - \langle u(2) \rangle \right) \rangle$

Note $\Delta u(1) = u(1) - \langle u(1) \rangle$ only when $f \equiv 0$. In the definition of $D$ $\langle u(1) \rangle$ is over variations $f$, ie

$$\langle \dots \rangle = \frac{Tr(\rho \dots S')}{Tr(\rho S')} \quad \text{in which } S' \text{ contains } f.$$

This result recovers the usual linear response theory result if we say that the force $f(\tau) = f^\sigma(t)$ is independent of the branch index $\sigma$. Then

$$\delta \langle \Delta u^+(t) \rangle = - \left[ \int_{-\infty}^{\infty} dt'\, D^{++}(t,t') f(t') - \int_{-\infty}^{\infty} dt'\, D^{+-}(t,t') f(t') \right]$$

remember $\int d\tau' = \sum_\sigma \int_{-\infty}^{\infty} dt' \cdot \sigma \qquad \sigma = \pm$

$$\delta \langle \Delta u^+(t) \rangle = - \int_{-\infty}^{\infty} dt' \left[ D^t(t,t') - D^<(t,t') \right] f(t')$$

$$= - \int_{-\infty}^{\infty} dt'\, D^r(t,t') f(t')$$

This is precisely the retarded Green's function.

$$+ \begin{bmatrix} + & - \\ D^t & D^< \\ D^> & D^{\bar{t}} \end{bmatrix}$$

According to the definition of functional derivative we have

$$\frac{\delta \langle u(1) \rangle}{\delta f(2)} = -D(1,2)$$

Since we have the general relation $D^t + D^{\bar{t}} = D^> + D^<$
or $D^r = D^t - D^< = D^> - D^{\bar{t}}$ we see the response of the position of atoms is independent of the branch index $\sigma$

$$\delta \langle u^{\bar{}}(t) \rangle = \delta \langle u^{+}(t) \rangle \rightarrow \delta u^{\sigma}(t) = -\sum_{\sigma'} \int dt' D^{\sigma\sigma'}(t,t') f(t')$$

$$= -\int_{-\infty}^{+\infty} dt' \left[ D^{-+}(t,t') - D^{--}(t,t') \right] f(t') = -\int_{-\infty}^{+\infty} D^r(t,t')^{\vee} dt' f(t')$$

$$\downarrow$$

$$D^> - D^{\bar{t}}$$

---

We now work out the functional derivatins of the contour ordered Green's functions $\frac{\delta G}{\delta f}$, $\frac{\delta D}{\delta f}$ and see how it is related to the nonlinear terms in the equation of motion for the Green's functions. We write out the Green's function in the form

$$G(1,2) = -\frac{i}{\hbar} \frac{\langle T_\tau [c(1)\, c^+(2)\, S] \rangle}{\langle S \rangle}$$

here avgs $\langle \cdots \rangle = \mathrm{Tr}(\rho \cdots)$

$$S = e^{-\frac{i}{\hbar}\int (-f(3)\, u(3))\, d3}$$

$$\int d3 \equiv \sum_{j_3} \int d\tau_3$$

The contour order super operator apply to all the operator to the right of it.

Here $1 \equiv (j_1, \tau_1)$ etc There $c(1)$, $u(3)$ etc are in the Heisenberg picture governed by full Hamilton $\hat{H}$ on page 313. So the only dependence of the time-dependent force is in the Scattering "matrix" $S$. We make the variation with respect to $G$, obtain

$$\delta G(1,2) = -\left(\frac{i}{\hbar}\right)\left[\frac{\langle T_\tau\left(c(1)\, c^+(2)\, \delta S\right)\rangle}{\langle S\rangle} - \frac{\langle T_\tau c(1)\, c^+(2)\, S\rangle}{\langle S\rangle^2}\langle \delta S\rangle\right]$$

Now $\delta S = \frac{i}{\hbar}\int (\delta f(3))\, u(3)\, d3 \cdot S$

so $\delta G(1,2) = \int d3\, \delta f(3)\left(\frac{i}{\hbar}\right)\left[-\left(\frac{i}{\hbar}\right)\frac{\langle T_\tau\left[c(1)\, c^+(2)\, u(3)\, S\right]\rangle}{\langle S\rangle}\right.$

$$\left. + \frac{i}{\hbar}\,\frac{\langle T_\tau\, c(1)\, c^+(2)\, S\rangle}{\langle S\rangle}\,\frac{\langle u(3)\, S\rangle}{\langle S\rangle}\right]$$

$$\equiv \int d3\, \frac{\delta G(1,2)}{\delta f(3)}\cdot \delta f(3)$$ ← this is the definition of functional derivative

Thus $\frac{\delta G(1,2)}{\delta f(3)} =$ [illegible]

$$= \frac{1}{\hbar^2}\left\langle T\, c(1)\, c^+(2)\, u(3)\right\rangle_{H+H'} + \left(-\frac{i}{\hbar}\right) G(1,2)\,\langle u(3)\rangle_{H+H'}$$

$\frac{1}{\hbar^2} = \frac{i}{\hbar}\cdot\left(-\frac{i}{\hbar}\right)$

Here $\langle \cdots \rangle_{H+H'} = \frac{\langle \cdots S\rangle}{\langle S\rangle}$ is the averages with respect the total Hamiltonian $H + H'$, $H' = -\vec{f}\cdot\vec{u}$

Compare with the equation of motion we get

$$i\hbar\frac{\partial}{\partial\tau} G_{jk}(\tau,\tau') - \sum_s H_{js}\, G_{sk}(\tau,\tau') + \sum_l M^l_{js}\Big($$

$$i\hbar\,\frac{\delta G_{sk}(\tau,\tau')}{\delta f_l(\tau)} - G_{sk}(\tau,\tau')\,\langle u_l(\tau)\rangle\Big) = \delta_{jk}\,\delta(\tau,\tau')$$

Note that we got a new term $\langle u_l(\tau)\rangle$ in here (Hartree term)

$\Delta u = u - \langle u\rangle$.

Similarly $D(1,2) = -\frac{i}{\hbar}\frac{\langle T_\tau \Delta u(1)\Delta u(2)\, S\rangle}{\langle S\rangle}$ and

$$\delta D(1,2) = -\frac{i}{\hbar}\left[\frac{\langle T_\tau \Delta u(1)\Delta u(2)\,\delta S\rangle}{\langle S\rangle} - \frac{\langle T_\tau \Delta u(1)\Delta u(2)\, S\rangle\langle \delta S\rangle}{\langle S\rangle^2}\right]$$

Since $\delta S \propto u$ we get a $\langle T_\tau\, u\, u\, u\rangle$. Such term is not needed.

14 June 2017

We can write the equation of motion for $G$ in a more compact notation with matrices, it is

$$\left[ i\hbar \frac{\partial}{\partial \tau} \cdot I - \left( H + \vec{M} \cdot \langle \vec{u}(\tau) \rangle - i\hbar \vec{M} \cdot \frac{\delta}{\delta \vec{f}(\tau)} \right) \right] G(\tau, \tau') = I\, \delta(\tau, \tau')$$

Here $I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \\ 0 & & 1 \ddots \end{pmatrix}$ is $N \times N$ identity matrix

$H$ is the single particles Hamilt. the usual hartree term (see page 273) of $v\langle q \rangle$ is now $\vec{M} \cdot \langle \vec{u} \rangle$, which is not on-site, but still $N \times N$ matrix by making $\vec{M} \equiv (M^l)$ dotted into the vector $\frac{\delta}{\delta \vec{f}} \equiv \left(\frac{\delta}{\delta f_l}\right)$ the result is matrix operator is acting on the matrix $G$. the result is $\delta(1,2) \equiv \delta_{j_1 j_2} \delta(\tau_1, \tau_2)$, the $\delta$-function is space and contour time.

Our next task is to transform so that we can identify the self energy $\rightarrow$ $\begin{cases} G = G_0 + G_0 \Sigma G \\ D = D_0 + D_0 \Pi D \end{cases}$.

The equation of motion for $D$ also requires the same functional derivative, not a different one. From page 315 we get

$$\frac{\partial^2}{\partial \tau^2} D_{jk}(\tau, \tau') + \sum_s K_{js} D_{sk}(\tau, \tau') + \sum_{l l'} M^j_{l l'} \left( i\hbar \frac{\delta G^{(\tau \tau^+)}_{ll'}}{\delta f_k(\tau')} - G_{ll}(\tau, \tau^+) \langle u(\tau') \rangle_k \right) - \left(\tfrac{i}{\hbar}\right) \ldots f_j(\tau) \langle u(\tau') \rangle_k$$

this two terms are cancelled due to $\Delta u = u - \langle u \rangle$ !!

$$= -\delta_{jk}\, \delta(\tau, \tau')$$

Note since in the interaction we have $c^+ M c$ we must put the 2nd $\tau$ to slight later than $\tau$, we use $\tau^+ = \tau + \Delta\tau$.

Note we do "inner product" with $G$ and "outer product" with $u$.

We can also write this equation compactly as matrix equation as

This should not be here, because I have taken the derivative

subtract term

$$\left[\frac{\partial^2}{\partial\tau^2}\underline{I} + K\right] D(\tau,\tau') - \left[\mathrm{Tr}(\vec{M}\,G(\tau,\tau^+)) + \frac{i}{\hbar}\vec{f}(\tau)\right] \otimes \langle \vec{u}(\tau')\rangle$$

(outer product)

$$+ i\hbar\,\mathrm{Tr}\left(\vec{M}\otimes\frac{\delta}{\delta f(\tau')}G(\tau,\tau^+)\right) = -\underline{I}\,\delta(\tau,\tau')$$

[Here the trace is over the electron degrees of freedom only. The meaning of this equation is obscure, particularly the $\langle u(\tau')\rangle$ term.] The two equations, G and D do not close themselves, because of the extra $\langle u(\tau)\rangle$. We thus need an equation for $u$, which is

$$\frac{d^2}{d\tau^2}\langle u(\tau)\rangle = -K\langle u(\tau)\rangle + i\hbar\,\mathrm{Tr}(\vec{M}\,G(\tau,\tau^+)) - f(\tau)$$

Is this equation really necessary? Yes. In steady state $\langle u(\tau)\rangle$ because independent of $\tau$ with $f\equiv 0$

we need to determine $\langle\vec{u}\rangle$ by

$$-K\langle\vec{u}\rangle + i\hbar\,\mathrm{Tr}(\vec{M}\,G(\tau,\tau^+)) = 0$$

or $$\langle\vec{u}\rangle = i\hbar\,K^{-1}\,\mathrm{Tr}(\vec{M}\,G(\tau,\tau^+))$$

} This gives the hartree diagram

---

We need a more careful derivation of equation of motion for D

$$\Delta u = u - \langle u\rangle$$

$$D_{jk}(\tau,\tau') = -\frac{i}{\hbar}\langle T_\tau \Delta u_j(\tau)\Delta u_k(\tau')\rangle$$

$$= \frac{1}{i\hbar}\left[\theta(\tau,\tau')\langle \Delta u_j(\tau)\,\Delta u_k(\tau')\rangle + \theta(\tau',\tau)\langle \Delta u_k(\tau')\,\Delta u_j(\tau)\rangle\right]$$

$$\frac{\partial}{\partial\tau}D_{jk}(\tau,\tau') = \frac{1}{i\hbar}\left[\delta(\tau,\tau')\langle \Delta u_j(\tau)\Delta u_k(\tau') - \Delta u_k(\tau')\Delta u_j(\tau)\rangle\right]$$

$\tau' = \tau$

$$+\frac{1}{i\hbar}\left[\theta(\tau,\tau')\langle \Delta\dot{u}_j(\tau)\,\Delta u_k(\tau')\rangle + \theta(\tau',\tau)\langle \Delta u_k(\tau')\Delta\dot{u}_j(\tau)\rangle\right]$$

$$= \frac{1}{i\hbar}\left[\delta(\tau,\tau')\cdot 0\right] + \frac{1}{i\hbar}\left[T_\tau \Delta\dot{u}_j(\tau)\,\Delta u_k(\tau')\rangle\right]$$

So the first derivative is

$$\frac{\partial}{\partial\tau} D_{jk}(\tau,\tau') = \frac{1}{i\hbar}\langle T_\tau\, \Delta\dot{u}_j(\tau)\, \Delta u_k(\tau')\rangle$$

because of the $\delta$-function we can set $\tau' = \tau$

Take $\frac{\partial}{\partial\tau}$ again $\quad \frac{\partial^2}{\partial\tau^2} D_{jk}(\tau,\tau') = \delta(\tau,\tau')\frac{1}{i\hbar}\langle[\Delta\dot{u}_j(\tau), \Delta u_k(\tau')]\rangle$

$$+ \frac{1}{i\hbar}\langle T_\tau\, \Delta\ddot{u}_j(\tau)\, \Delta u_k(\tau')\rangle$$

$$[\Delta\dot{u}_j(\tau), \Delta u_k(\tau)] = [\dot{u}_j(\tau) - \langle\dot{u}_j(\tau)\rangle,\ u_k(\tau) - \langle u_k(\tau)\rangle]$$

since $\langle u\rangle$ and $\langle\dot{u}\rangle$ are ordinary numbers, it commutes with the operators so $[\Delta\dot{u}_j(\tau), \Delta u_k(\tau')] = [\dot{u}_j(\tau), u_k(\tau')]$

$= -i\hbar\,\delta_{jk}$ $\qquad$ we note $\dot{u}_j(\tau) \equiv p_j(\tau)$

This gives the first term on the right hand side as $I\,\delta(\tau,\tau')$.

The Heisenberg equation for $u$ is given on page 315, i.e.,

$$\frac{d^2u}{dt^2} = \ddot{u} = -Ku - c^\dagger M c - f \qquad \text{all at time } \tau$$

($\frac{d}{dt}$ and $\frac{d}{d\tau}$ are the same)

Here $u$ is in the full Heisenberg picture, $\langle\ \rangle = \mathrm{Tr}(\rho\cdots)$ is independent of time.

so $\Delta\ddot{u} = \ddot{u} - \langle\ddot{u}\rangle$

$$= -Ku - c^\dagger M c - f + K\langle u\rangle + \langle c^\dagger M c\rangle + f$$

all at time $\tau$. $f$ is a scalar, not operator so $\langle f\rangle = f$

we get

$$\frac{\partial^2}{\partial\tau^2} D_{jk}(\tau,\tau') = -\delta_{jk}\,\delta(\tau,\tau') + \frac{1}{i\hbar}\langle T_\tau\left[-\sum_s K_{js} u_s(\tau) - \sum_{ll'} C^\dagger_{rl} M^j_{ll'} C_{rl'}(\tau)\right]\Delta u_k(\tau')\rangle$$

$$+ \frac{1}{i\hbar}\langle T_\tau\left[\sum_s K_{js}\langle u_s(\tau)\rangle + \sum_{ll'} C^\dagger_l(\tau) M^j_{ll'} C_{l'}(\tau)\right]\Delta u_k(\tau')\rangle$$

$$\langle\ddot{u}_j(\tau) + f_j(\tau)\rangle$$

write $\Delta\ddot{u} = -K(\underbrace{u - \langle u\rangle}_{\Delta u}) - c^\dagger M c + \langle c^\dagger M c\rangle$

we get

$$\frac{\partial^2}{\partial\tau^2} D_{jk}(\tau,\tau') = \delta_{jk}\,\delta(\tau,\tau') + \frac{1}{i\hbar}\left\langle T_\tau\left[-K_{js}\,\Delta u_s(\tau)\right]\Delta u_k(\tau')\right\rangle$$

$$+ \frac{1}{i\hbar}\sum_{ll'}\left\langle T_\tau\left(-c_l^\dagger(\tau)\,M^j_{ll'}\,c_{l'}(\tau)\,\Delta u_k(\tau')\right\rangle\right.$$

$$+ \frac{1}{i\hbar}\sum_{ll'}\left\langle T_\tau\, c_l^\dagger(\tau)\,M^j_{ll'}(\tau\tau)\right\rangle\left\langle \Delta u_k(\tau')\right\rangle = 0$$

The last term is zero since $\langle \Delta u_k(\tau')\rangle = \langle u_k(\tau') - \langle u_k(\tau')\rangle\rangle$

$= \langle u_k(\tau')\rangle - \langle u_k(\tau')\rangle$

$= 0$

we write

$$\frac{\partial^2}{\partial\tau^2} D_{jk}(\tau,\tau') = \delta_{jk}\,\delta(\tau,\tau') - \sum_s K_{js} D_{sk}(\tau,\tau')$$

$$- \frac{1}{i\hbar}\sum_{ll'}\left\langle T_\tau\, M^j_{ll'}\, c_l^\dagger(\tau)\, c_{l'}(\tau)\, u_k(\tau')\right\rangle + \frac{1}{i\hbar}\sum_{ll'} M^j_{ll'}\left\langle T_\tau\, c_l^\dagger(\tau) c_{l'}(\tau)\right\rangle \times \langle u_k(\tau')\rangle$$

Using the result on page 323, i.e.

$$i\hbar\frac{\delta G(1,2)}{\delta f(3)} = \frac{i}{\hbar}\left\langle T(c(1)\,c^\dagger(2)\,u(3)\right\rangle + \cdots G(1,2)\langle u(3)\rangle$$

or take $1 \equiv (\tau, l)$, $2 \equiv (\tau^+, l')$ $3 = (\tau', k)$

we can write the $c^\dagger c\, u$ term as

$$+\frac{1}{i\hbar}\sum_{ll'} M^j_{ll'}\left\langle T_\tau\, c_{l'}(\tau)\, c_l^\dagger(\tau^+)\, u_k(\tau')\right\rangle$$

chose sign here

$$= -\sum_{ll'} M^j_{ll'}\left[\, i\hbar\,\frac{\delta G_{ll}(\tau,\tau^+)}{\delta f_k(\tau')} - G_{l'l}(\tau,\tau^+)\langle u_k(\tau')\rangle\right]$$

note index swap

note the last term in the equation of motion for $D$ is

$$\frac{1}{i\hbar}\sum_{ll'} M^j_{ll'}\left\langle T_\tau\, c_l^\dagger(\tau)\, c_{l'}(\tau)\right\rangle = -\frac{1}{i\hbar}\sum_{ll'} M^j_{ll'}\left\langle T_\tau\, c_{l'}(\tau)\, c_l(\tau^+)\right\rangle$$

$= -\sum M^j_{ll'} G_{l'l}(\tau,\tau^+)$. It is cancelled exactly by the extra term in $\frac{\delta G}{\delta f}$. So we get

$$\frac{\partial^2}{\partial\tau^2} D(\tau,\tau') = -I\,\delta(\tau,\tau') - K\,D(\tau,\tau') - i\hbar\, \mathrm{Tr}_e\left(M \otimes \frac{\delta G(\tau,\tau^+)}{\delta \vec{f}(\tau')}\right)$$

outer product of two vectors

This agrees with that on page 327.
Unlike the equation for $u$, there is no linear driven term $f(\tau)$!

Having worked out the equation of motion for $G$ and $D$, the electron & phonon Green's functions, expressing the nonlinear terms in terms of functional derivative $\frac{\delta}{\delta f(x)} G$. This step is the key insight of Hedin, the rest of steps are merely some algebraic manipulation and definition. The step parallel to what we have done for the electron Coulomb interactions.

First, we make a change of variational independent variable $f_K(\tau) \to f(1)$ $(1) \equiv (\tau, K)$ to $\langle u_K(\tau)\rangle = \langle u(1)\rangle$

This is done by the linear response page 315 - 321

$$\frac{\delta \langle u(1)\rangle}{\delta f(2)} = -D(1,2)$$

Usually in linear response theory, the right-hand side is evaluated at $f \equiv 0$. However, we might also need high order derivatives, such as $\frac{\delta^2 \langle u(1)\rangle}{\delta f(1)\,\delta f(2)}$ so that right-hand side can still be a functional of $f$ as well (which should be correct). The precise mapping from $f$ to $\langle u\rangle$ is (which could be nonlinear if $D$ still depends on $f$)

$$\langle u\rangle_f - \underbrace{\langle u\rangle_{f=0}}_{\text{constant}} = -\int D(1,2)\, f(2)\, d2$$

Having specified how we do change of variables from $f$ to $\langle u \rangle$, we take functional derivative with respect to $\langle u \rangle$ instead of $f$, $\delta\langle u \rangle = \langle u \rangle_{f+\delta f} - \langle u \rangle_f$

$\delta\langle u(1) \rangle$ is the infinitesimal variation of $\langle u \rangle$.

so functional derivative equation for $G$ on page 325 because

$$\vec{M} \cdot \frac{\delta}{\delta \vec{f}(\tau)} = \int \vec{M} \cdot \frac{\delta \langle w(3) \rangle}{\delta \vec{f}(\tau)} \frac{\delta}{\delta \langle u(3) \rangle} \, d3$$

$$= \int d3 \sum_{\ell} M^{\ell}_{jk} \left( - D(3, (\tau \ell)) \right) \frac{\delta}{\delta \langle u(3) \rangle}$$

the self energy term is now $1 \equiv (\tau, j)$ $2 \equiv (\tau', k)$

$$-ih \sum_{\ell s} M^{\ell}_{jg} \left( -D(3, (\tau, \ell)) \right) \frac{\delta}{\delta \langle u(3) \rangle} G(\tau, \tau')_{sk} \, d3$$

Let introduce the bare vertex function as

$$M(1\,2;3) = M^{j_3}_{j_1 j_2} \delta(\tau_1 \tau_2) \delta(\tau_1 \tau_3)$$

This term can be written more compactly as

$$+ih \iiint M(1,4;5) D(3,5) \frac{\delta}{\delta \langle u(3) \rangle} G(4,2) \, d(3\,4\,5)$$

In order to identify the self energy of the form

$$\int \Sigma(1,3) G(3,2) \, d3$$

we need a Green's function $G$, but here $G$ is inside the functional derivation, $\delta G$. the standard trick, see Hedin, is

$$G^{-1} G = I$$

so $\delta G^{-1} \cdot G + G^{-1} \delta G = 0 \rightarrow -G \delta G^{-1} G = \delta G$

or $$\frac{\delta G(4,2)}{\delta \langle u(3) \rangle} = \int\int G(4,6) \frac{\delta G^{-1}(6,7)}{\delta \langle u(3) \rangle} G(7,2) \, d(6\,7)$$

so the self energy term becomes, after substitute the above

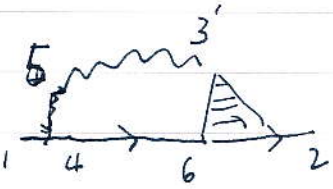
$$\Sigma(1,3)\, G(3,2)\, d3 = i\hbar \int d(3456\,7) \Big[ M(14;5)\, D(3,5) \times \Big(-G(4,6)\, \frac{\delta G^{-1}(6,7)}{\delta \langle u(3)\rangle}\, G(7,2)\Big)\Big]$$

re naming the dummy variables in the right hand term

$7 \to 3, \quad 3 \to 3'$

$$\Sigma(1,3) = -i\hbar \int d(3'456)\, M(14;5)\, D(3',5)\, G(4,6)\, \frac{\delta G^{-1}(6,3')}{\delta \langle u(3')\rangle}$$

$1 \downarrow 2$ remove again $3 \to 2$




Note that, ignoring the photon lines (functions) the electron line form a matrix multiplation (trace)

$$\Sigma(1 \to 2) \equiv M(14,\cdots)\, G(4,6)\, \frac{\delta G^{-1}(6,2)}{\delta \cdots}$$

The above diagram should be compared with that on page 299.

We define the vertex function such that to lowest order it is the same as $M(12;3)$, from the equation of motion on top of page 325, we get

$$G^{-1}(\tau,\tau') = \underbrace{i\hbar \frac{\partial}{\partial \tau} I}_{\text{purely symbolic}} - H - \vec{M}\cdot\langle \vec{u}(\tau)\rangle - \underbrace{i\hbar\, \vec{M}\cdot \frac{\delta}{\delta f \cdots}}_{\text{high order}}$$

$$\downarrow$$

$$G^{-1}(1,2) = \underbrace{\cdots\cdots}_{\text{independent of } \langle \vec{u}\rangle} - \int M(1,2;3)\langle u(3)\rangle\, d3 + \text{high order}$$

$\uparrow$ diagonal in time $\tau$

So $\dfrac{\delta G^{-1}(1,2)}{\delta \langle u(3)\rangle} = -M(1,2;3)$ so we can define vertex function

$$\Gamma(1,2;3) = -\frac{\delta G^{-1}(1,2)}{\delta \langle u(3)\rangle}$$

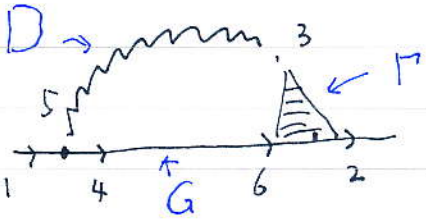
electron, out $\uparrow$ photon

With this definition the self energy is

we use $D(1,2) = D(2,1)$

$$\Sigma(1,2) = ih \int d(3456)\, M(14;5)\, D(5,3)\, G(4,6)\, \Gamma(62;3)$$

$$= ih \int d(3456)\, M(14;5)\, G(4,6)\, \Gamma(62;3)\, D(5,3)$$




This is identical to the electron case if $M \to (-e)$ and diagrams in the three indices of $M$. If we take $\Gamma(62;3) \approx M(62;3)$ it is so-called GW method.

Now we do similar manipulation for the phonon equation motion. The phonon self energy term is from page 327

$$\underbrace{\Pi D} = ih\, Tr_e\left(\vec{M} \otimes \frac{\delta}{\delta f(\tau')} G(\tau\tau^+)\right)$$

This is symbolic only we rewrite compact notation

$$= ih \sum_{ss'} M^{i}_{ss'} \sum_{k} \frac{\delta G_{s's}(\tau,\tau^+)}{\delta f_k(\tau')} = ih \int d(34)\, \underbrace{M(34;1)}_{\text{two } \delta\text{-functions}} \frac{\delta G(43^+)}{\delta f(2)}$$

two $\delta$-functions and time

$\tau^+$ mean slight late than $\tau$.

Do the change of independent variable for $f$ to $\langle u \rangle$ we get

$$\frac{\delta G}{\delta f(2)} = \int \frac{\delta \langle u(5)\rangle}{\delta f(2)} \frac{\delta G}{\delta \langle u(5)\rangle}\, d5$$

$$= -\int d5\, D(5,2) \frac{\delta G}{\delta \langle u(5)\rangle}$$

change again from $\delta G$ to $\delta G^{-1}$

$$= -\int d5\, D(5,2) \left[ -G(4,6) \frac{\delta G^{-1}(6,7)}{\delta \langle u(5)\rangle} G(7,3^+) \right] d6\, d7$$

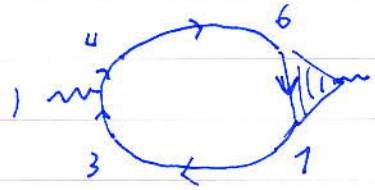
So $(\Pi D)[1,2] = ih \int d(34567) \left[ M(3,4;1)\, D(5,2)\, G(4,6) \right.$

$$\left. (-\Gamma(6,7;5))\, G(7,3^+) \right]$$

Compare with the definition of $\Pi$ we find

$$\Pi(1,5) = (-i\hbar)\int d(3467)\, M(34;1)\, G(4,6)\, \Gamma(6,7;5)\, G(7,3^+)$$

rename $5 \to 2$




This is the polarization diagram with vertex correction

This should be compared with that for electron-electron Coulomb system on page 303. (remember $M \to (-e)\,\delta(1,3)\,\delta(1,4')$ $\delta(1,3) \to \sum_{\lambda_1\lambda_3} \delta(\tau_1,\tau_3)$. This demonstrated mathematical equivalence of the pure Coulomb system & phonon system (as well as scalar photon system).

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The last step is to work out a equation for the functional derivative vertex function

$$\Gamma(1,2;3) = -\frac{\delta G^{-1}(1,2)}{\delta \langle u(3)\rangle}$$

Symbolically we have the Dyson equation

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \int M(1,2;3)\langle u(3)\rangle\, d3 - \Sigma(1,2)$$

"Hartree" term "Fock" term

and

$$\left(i\hbar\frac{\partial}{\partial t} I - H\right) G_0(1,2) = \delta(1,2)$$

$G_0$ is the Green's function without the force perturbation $f$ or $\langle u\rangle$. So it is independent of $\langle u\rangle$ so

$$\Gamma(1,2;3) = -\frac{\delta G^{-1}(1,2)}{\delta\langle u(3)\rangle} = M(1,2;3) + \frac{\delta\Sigma(1,2)}{\delta\langle u(3)\rangle}$$

This equation is similar to that for Coulomb system on page 305. To compute the functional derivative $\frac{\delta\Sigma}{\delta\langle u\rangle}$ we need one more change of variables from $\langle u\rangle$ to $G$.

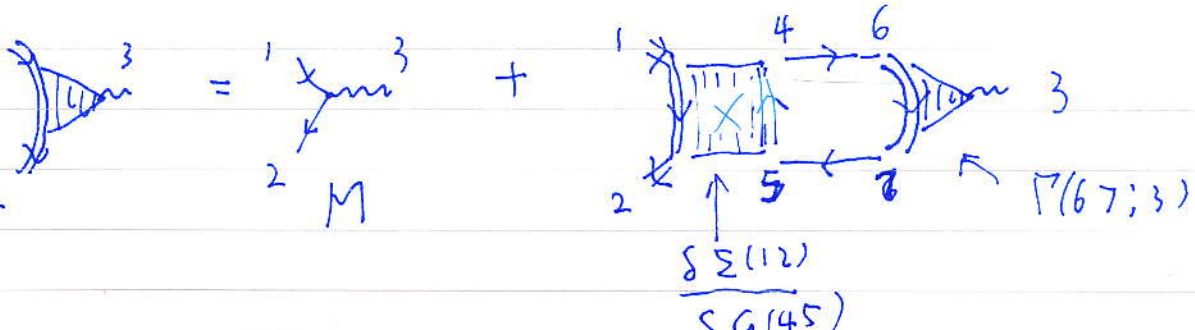
$$\frac{\delta\Sigma(1,2)}{\delta\langle u(3)\rangle} = \int d(45)\frac{\delta G(45)}{\delta\langle u(3)\rangle}\frac{\delta\Sigma(1,2)}{\delta G(4,5)}$$ here, in order to have this equation to make sense, we need to view $\Sigma$ as a functional of $G$ only (with other quantity independent of $\langle u\rangle$. Since $\langle u\rangle$ is related to $D$ so $\Sigma$ cannot be a functional of $D$, otherwise we also need to do $\frac{\delta\Sigma}{\delta D}$. The idea is that we can express $\Sigma$ in terms of $G_0$ and $D_0$ (as well as $\langle u_0\rangle$!) since $G = G_0 + G_0\Sigma_{tot}G$ (here $\Sigma_{tot}$ include the Hartree term, $\Sigma$ does not) by inverting this relation $G_0 \equiv G_0(G)$, we can eliminate $G_0$ in favor of $G$, then $\Sigma = \Sigma(G, D_0)$. Note that we don't invert $D_0$, the functional derivative is in the above sense.

[This is certainly the argument used leading to the usual equation but Hedin's original 1965 paper don't have it]. $D_0$ is independent of $f$ or $\langle u\rangle$. Why $\Sigma$ is a function of $G$ and $D_0$, and not $\Sigma(G, \langle u\rangle, D_0)$ is puzzling to me! Thus if the above argument is correct, then we get using the usual trick

$$\frac{\delta\Sigma(1,2)}{\delta\langle u(3)\rangle} = \int d(45)\left[-G(4,6)\frac{\delta G^{-1}(6,7)}{\delta\langle u(3)\rangle}G(7,5)\frac{\delta\Sigma(1,2)}{\delta G(4,5)}\right]d6\,d7$$

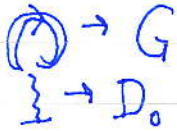
$$= \int d(4567)\frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)\Gamma(67;3)G(7,5)$$

and with $\Gamma(1,2;3) = M(12;3) + \frac{\delta\Sigma(1,2)}{\delta\langle u(3)\rangle}$ we get the last Hedin equation

$\Gamma(12;3) =$ 

We have split the electron self energy into a "Hartree" term and Fock term, only the Fock term is denoted by $\Sigma$. the hartree term is given, for the electron-phonon problem as

$$\int M(1\,2;\,3)\,\langle u(3)\rangle\, d3$$

This does not look like the usual lollipop diagram  but in fact it is this diagram just as in the electron Hartree term. An important point is that it is  with double line for electron and single line for phonon. $G \cdot D_0$. For systems with space translationally invariant systems, such as periodic crystal lattice. This term is 0 (when $f \equiv 0$ of course) See AGD, page 79, 119. However, the argument used there cannot be applied to nanostructure without periodicity. So we keep it.

To show the hartree term is actully the Feynman diagram  , we assume that we have our findl results for all the formulas and have set the deriving force $f \equiv 0$. then the system is time translationally invariant, thus $\langle u(\tau)\rangle$ is independ of time $\tau$; it is just a number (in fact, vector $\langle \vec{u} \rangle$.). So in steady state without the driven force, $\langle u\rangle$ satisfies equation (see page 327)

$$0 = \frac{d^2}{d\tau^2}\langle u(\tau)\rangle = -K\langle u(\tau)\rangle + i\hbar\, \mathrm{Tr}_e\left(\vec{M} G(\tau, \tau^+)\right) = 0$$

The trace here is over the electron degrees of freedom.

We can solve for $\langle u \rangle$ to get

$$\vec{\langle u \rangle} = it K^{-1} \mathrm{Tr}(\vec{M} G(\tau, \tau^+))$$

But $D_0^r(\omega) = ((\omega + i\eta) I - K)^{-1} = -(K)^{-1}$ when $\omega = 0$

So $\langle u_j \rangle = -it \left[ D_0^r(\omega=0) \right]_{jk} \sum_{ss'} M^K_{ss'} G_{s's}(\tau'', \tau''^+)$ result is $\infty$ Legendre of $\tau''$.

we get $\int M(1,2;3) \langle u(3) \rangle \, d3$

$$\Rightarrow \sum_\ell M^\ell_{jk} \delta(\tau_1, \tau_2) \delta(\tau, \tau_3) \langle u_\ell(\tau_3) \rangle \, d\tau_3 = \sum_\ell M^\ell_{jk} \delta(\tau, \tau_2) \langle u_\ell(\tau_1) \rangle$$

$\tau_1 \to \tau, \quad \tau_2 \to \tau' \quad \to \sum_\ell M^\ell_{jk} \delta(\tau, \tau') \langle u_\ell(\tau) \rangle$

$$\to \sum_{\ell ss'} (-it) M^\ell_{jk} \delta(\tau, \tau') D^r_{\ell k'}(\omega=0) M^{k'}_{ss'} G_{s's}(\tau'', \tau''^+)$$

$$= (-it) \sum_{\ell ss'} M^\ell_{jk} D^{0r}_{\ell k'}(\omega=0) M^{k'}_{ss'} G_{s's}(\tau'', \tau''^+)$$

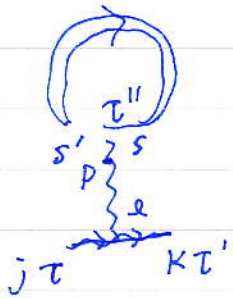
$\sum_{\ell ss'} \to \delta(\tau, \tau')$

$$= (-it) \delta(\tau, \tau') \sum_{\ell s} M^\ell_{jk} \int_{-\infty}^{+\infty} D^{0r}_{\ell p}(t) \, dt \, M^p_{ss'} G_{s's}(\tau'', \tau''^+)$$

$t \uparrow$ time

This is precisely the value of the diagram


→ label the point




Why only $D^{0r}$ ??

According to the Feynman rule, the value of the graph is

each vertex has only one time variable.

$$(-ih)\,\delta(\tau,\tau')\sum_{epss'} M^{e}_{ik}\int D^{0}_{ep}(\tau,\tau'')\,M^{p}_{ss'}\,\underbrace{G_{s's}(\tau'',\tau''^{+})}_{\text{in hyp } \tau''}\,d\tau''$$

So $\int D^{0}_{ep}(\tau,\tau'')\,d\tau'' =$ [illegible]

$$= \int_{-\infty}^{+\infty} D_0^{\sigma+}(t-t'')\,dt'' - \int_{-\infty}^{\infty} D_0^{\sigma-}(t-t'')\,dt''$$

$$= \int_{-\infty}^{\infty} [\,D_0^{\sigma+}(t) - D_0^{\sigma-}(t')\,]\,dt$$

if $\sigma = +$ we have $D_0^{++} - D_0^{+-} = D_0^{t} - D_0^{<} = D_0^{r}$

if $\sigma = -$ we also have $D^{-+} - D^{--} = D_0^{>} - D_0^{\bar{t}} = D_0^{r}$

$$\equiv \int_{-\infty}^{\infty} D_0^{r}(t)\,dt = D_0^{r}(\omega=0). \qquad \text{Q.E.D.}$$

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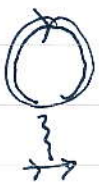
Important lesson learned. If we do GW then the Hartree term is  $= D_0 G$

the wiggly line is not double line but a single line.

So the self-consistent Born approximation used by me, Lü Jingtao, Zhang Lifa is wrong. Since we used double line  . The double line leads to double counting for some diagrams, such as  . With the double line ($D$) we get a factor of 2 for this diagram but it should be 1. The Hedin equation derivation gaves a rigorous justification why the Hartree term should be in single line $D_0$!