Essence of Quantum Many-Body Perturbation theory

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Abstract

We here, try to derive the ubiquitous Hedin equations using Quantum Many-Body Perturbation theory (QMBPT).QMBPT is full of rich diagrams showing the symmetries of myriad interactions of particles and anti-particles, giving us insights on how to miss-match and add different interactions important to the specific system we are dealing with. This is in contrast with the usual presentation of Hedin equations derived using variational principle and quantum linear response theory, where a complete different approach of probing the system with *fictious infinitesimal* field is used.

1. Introducing Particle propagators

Schrodinger equation in the interaction picture acquires the following form

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \hat{H}_1(t)|\Psi_I(t)\rangle \tag{1}$$

where

$$\hat{H}_1(t) = e^{\frac{i}{\hbar}H_0 t}\hat{H}_1 e^{-\frac{i}{\hbar}H_0 t} \tag{2}$$

Time evolution in the interaction picture is governed by the operator that connects interaction picture kets at different times according to

$$|\Psi_I(t)\rangle = U(t,t_0)|\Psi_I(t_0)\rangle \tag{3}$$

A special symbol U which of course is our usual unitary transformation operator is introduced. One can obtain the equation of motion for U from eq.(1) and eq.(3)

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = \hat{H}_1(t)U(t,t_0) \tag{4}$$

It can be shown that the sollution of eq.(4) can be formally written as a summation given by

$$U(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 ... \int_{t_0}^{t} dt_n \mathcal{T}[\hat{H}_1(t_1)\hat{H}_1(t_2)...\hat{H}_1(t_n)] \tag{5}$$

where the $\mathcal{T}$-operation is extended to order the $\hat{H}_1$ operator with the latest time farthest to the left, and so on.

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The definition of greens function in the Heisenberg picture is

$$G(\alpha,\beta;t-t^{'}) = -\frac{i}{\hbar}\theta(t-t^{'})\left\langle \Psi_0^N \middle| a_{\alpha_H}(t)a^{\dagger}_{\beta_H}(t^{'}) \middle| \Psi_0^N \right\rangle \tag{6}$$

where the corresponding creation and anhilation operators are defined in the Heisenberg picture. It can be shown that this definition of G written in the interaction picture using U gives us

$$G(\alpha,\beta;t-t^{'}) = \lim_{T'\to-\infty(1-i\eta)} \lim_{T\to+\infty(1-i\eta)} Q(\alpha,\beta;T,T',t-t^{'}) \tag{7}$$

where

$$Q(\alpha,\beta;T,T',t-t^{'}) = -\frac{i}{\hbar}\frac{\left\langle \Phi_0^N \middle| \mathcal{T}[U(T,T')a_{\alpha_H}(t)a^{\dagger}_{\beta_H}(t^{'})] \middle| \Phi_0^N \right\rangle}{\left\langle \Phi_0^N \middle| \mathcal{T}[U(T,T') \middle| \Phi_0^N \right\rangle} \tag{8}$$

We have now achieved a perturbative series in the numerator and denominator *(as U can be written as series as given in eq.*(5)*)*. It can be shown that the numerator turns out to be a product of series of *connected* and *disconnected* diagrams while the denominator is the same *connected* diagrams which exactly cancels out as shown in eq.(9). What we mean by connected and disconnected diagrams can be seen from the example diagrams are shown in Fig.1 which is the first order terms present in the numerator.

$$G(\alpha,\beta;t-t^{'}) \\ = \frac{G^0(\alpha,\beta;t-t^{'})\times(1+\left\langle \Phi_0^N \middle| \hat{S}^{(1)} \middle| \Phi_0^N \right\rangle+...)+G^1(\alpha,\beta;t-t^{'})\times(1+\left\langle \Phi_0^N \middle| \hat{S}^{(1)} \middle| \Phi_0^N \right\rangle+...)}{(1+\left\langle \Phi_0^N \middle| \hat{S}^{(1)} \middle| \Phi_0^N \right\rangle+\left\langle \Phi_0^N \middle| \hat{S}^{(2)} \middle| \Phi_0^N \right\rangle...)} \tag{9}$$

where $S^{(n)}$ refers to the n^{th} order disconnected diagram and G^n refers to the n^{th} order connected Greens function diagram.

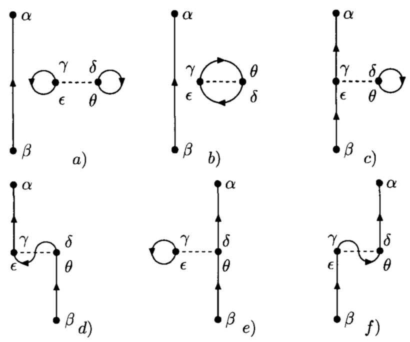

Figure 1: Six diagrams corresponding to the six terms in first order of eq.(8). Note that diagrams a) and b) are disconnected and will be canceled by contributions from the denominator of eq.(9)

Plugging in the various G^n's and converting it into interaction picture by using eq.(5), eq.(6), eq.(7), eq.(8), one can arrive at the final equation

$$
\begin{aligned}
&G(\alpha,\beta;t-t^{'}) \\
&= -\frac{i}{\hbar}\sum_{m}^{\infty}\left(-\frac{i}{\hbar}\right)^{m}\frac{1}{m!}\int dt_1 ... \int dt_m \times \left\langle \Phi_0^N \middle| \mathcal{T}[\hat{H}_1(t_1)...\hat{H}_1(t_m)a_\alpha(t)a_\beta^\dagger(t^{'})] \middle| \Phi_0^N \right\rangle_{connected}
\end{aligned} \tag{10}
$$

What this means is that only contributions to the single particle propagator that are completely linked and connected to the operators a $a_\alpha(t)$ and $a_\beta^\dagger(t)$ need be considered in this expansion. Each term in eq.(10) can be uniquely associated with a Feynman diagram as they are just products of Greens functions. This observation that any term in the perturbation expansion of G, except in zero-order, has a noninteracting propagator at the top and at the bottom of the diagram, makes it possible to introduce the self-energy Σ, which represents the sum of all the intermediate contributions. The decomposition of the single particle propagator in the noninteracting propagator G^0 and the sum of the other terms defining the self-energy, is graphically represented in Fig.2, Where the interacting G is given by double lines and the non interacting G^0 is given by single line.

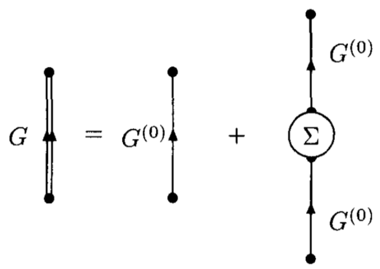

Figure 2: Diagrammatic representation of the sp propagator introducing the reducible self-energy Σ

First few terms contributing to the self energy upto second order is shown diagrammatically in Fig.3, Note we have used the fact that V is symmetric to reduce the number of diagrams. We could have chosen any diagram out of c), d), e), f) from Fig.1 to represent all of them equivalently, here we have chosen c) in Fig.3. From analyzing the diagrams in higher orders one can clearly see that higher order terms can be generated by attaching all possible combinations of a certain set of *irreducible* diagrams.

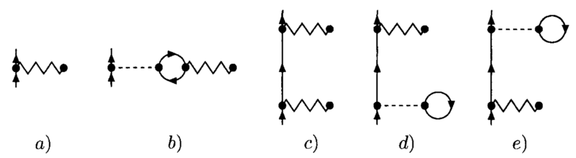

Figure 3: Diagrams contributing to the self-energy up to second order when an auxiliary potential U is employed

This here is the key to treating many-body interactions. The fact that there exists certain set of diagrams, repeated application of which, produces all the other diagrams (interactions) makes it possible for us to write the interacting G by eq.(11)

$$G(\alpha,\beta;E) = G^0(\alpha,\beta;E) + \sum_{\gamma,\delta} G^0(\alpha,\gamma;E)\Sigma^*(\gamma,\delta,E)G^0(\delta,\beta;E)$$
$$+ \sum_{\gamma,\delta,\epsilon,\theta} G^0(\alpha,\gamma;E)\Sigma^*(\gamma,\epsilon,E)G^0(\epsilon,\theta;E)\Sigma^*(\theta,\delta,E)G^0(\delta,\beta;E) \tag{11}$$

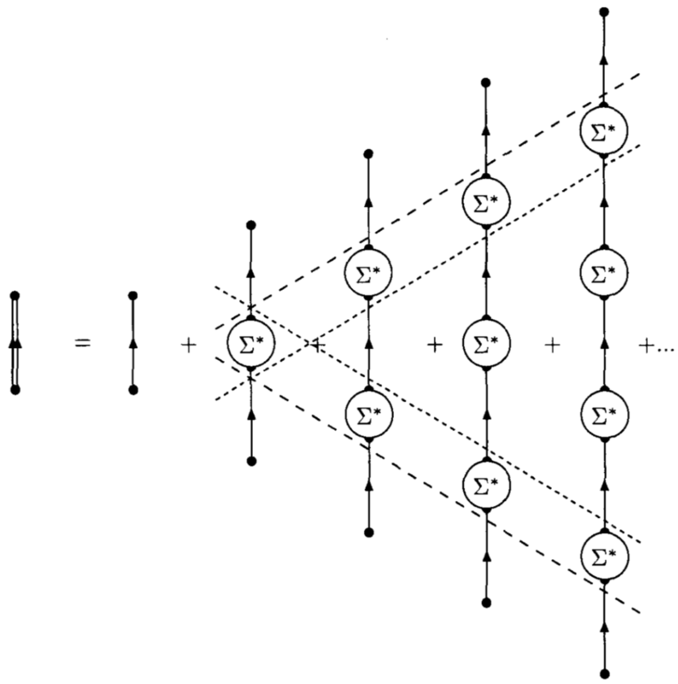

Figure 4: Decomposition of the single particle propagator in terms of irreducible self-energy contributions.

Eq.(11) is graphically represented in Fig.4, It now makes it easier for us to see that everything bellow the lower small dotted line is the same as the total sum, using which we can write (11) as (12) which is graphically shown in Fig.5. This is the diagrammatic representation of the famous Dyson series.

$$G(\alpha,\beta;E) = G^0(\alpha,\beta;E) + \sum_{\gamma,\delta} G^0(\alpha,\gamma;E)\Sigma^*(\gamma,\delta,E)G(\delta,\beta;E) \tag{12}$$

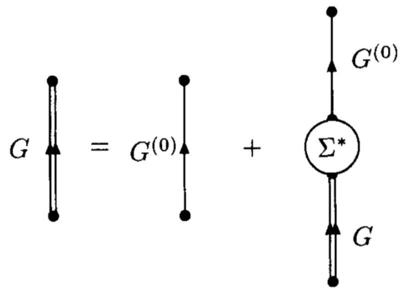

Figure 5: Diagrammatic representation of the single particle propagator in terms of the irreducible self-energy Σ^* and the noninteracting propagator G^0 representing (12)

2. Equation of motion

Equation of motion of the Greens function gives us a an elegant way to understand and come up with more logical approximations in the energy domain as compared to the time domain we have been working now. This is evident from the eq.(13)

$$i\hbar\frac{\partial}{\partial t}G(\alpha,\beta;t-t') = \int \frac{dE}{2\pi\hbar}e^{-\frac{i}{\hbar}E(t-t')}\left\{E \times G(\alpha,\beta;E)\right\} \tag{13}$$

Let us start with the hameltonian $\hat{H}$ which is decomposed into a solvable part $\hat{H}_0^{'}$ and a 2 particle interaction term $\hat{V}$. It is convenient to add and subtract an auxiliary potential $\hat{U}$ which at the end would eventually drop out of the final equations as it should.

$$\begin{aligned}\hat{H} &= \hat{H}_0^{'} + V \\ &= (\hat{H}_0^{'} + \hat{U}) + (-\hat{U} + \hat{V}) \\ &= \hat{H}_0 - \hat{U} + \hat{V}\end{aligned} \tag{14}$$

Since $\hat{H}_0$ is independent of any two particle interaction terms, it can now be diagonalized in single particle basis and be written as

$$\hat{H}_0 = \sum_{\gamma} \epsilon_\gamma a_\gamma^\dagger a_\gamma \tag{15}$$

which can then be used to calculate the time evolution of each individual $a_{\alpha_H}(t)$ which is given by

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}a_{\alpha_H}(t) &= \left[a_{\alpha_H}(t), \hat{H}\right] \\ &= e^{i\hat{H}t/\hbar}\left[a_\alpha, \hat{H}\right]e^{-i\hat{H}t/\hbar}\end{aligned} \tag{16}$$

Other commutation relations about a_α can be trivially written as

$$\left[a_\alpha, \hat{U}\right] = \sum_{\delta} \langle\alpha|\, U \,|\delta\rangle\, a_\delta \tag{17}$$

$$\left[a_\alpha, \hat{V}\right] = \sum_{\delta\theta\zeta} \langle\alpha\delta| V |\theta\zeta\rangle a_\delta^\dagger a_\zeta a_\theta \tag{18}$$

applying these results one can calculate the equation of motion of Greens function by taking the respective derivative

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}G(\alpha,\beta;t-t') &= \frac{\partial}{\partial t}\left\langle\Psi_0^N\middle|\mathcal{T}\left[a_{\alpha_H}(t), a_{\beta_H}^\dagger(t')\right]\middle|\Psi_0^N\right\rangle \\ &= \left\langle\Psi_0^N\middle|\frac{\partial}{\partial t}\left\{\theta(t-t')a_{\alpha_H}(t)a_{\beta_H}^\dagger(t') - \theta(t'-t)a_{\beta_H}^\dagger(t')a_{\alpha_H}(t)\right\}\middle|\Psi_0^N\right\rangle \end{aligned} \tag{19}$$

simplifying this using eq.(15)-(18) gives us

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}G(\alpha,\beta;t-t') = \delta(t-t')\delta_{\alpha\beta} + \epsilon_\alpha G(\alpha,\beta;t-t') - \sum_\delta \langle\alpha| U |\delta\rangle G(\delta,\beta;t-t') \\ + \frac{i}{2\hbar}\sum_{\delta\zeta\theta}\langle\alpha\delta| V |\theta\zeta\rangle \left\langle\Psi_0^N\middle|\mathcal{T}\left[a_{\delta_H}^\dagger(t)a_{\zeta_H}(t)a_{\theta_H}(t)a_{\beta_H}^\dagger(t')\right]\middle|\Psi_0^N\right\rangle \end{aligned} \tag{20}$$

2.1. Two particle Propagator

Eq.(20) is the iconic relation which represents the first step of a hierarchy in which the $N+1$-particle propagator is related to the N-particle propagator [Martin and Schwinger (1959); Migdal (1967)]. This relationship can be seen in the last term of eq.(20) which is made up of two particle created and destroyed.

$$G_{II}(\alpha t_\alpha, \beta t_\beta, \gamma t_\gamma, \delta t_\delta) = -\frac{i}{\hbar}\left\langle\Psi_0^N\middle|\mathcal{T}\left[a_{\beta_H}(t_\beta)a_{\alpha_H}(t_\alpha)a_{\gamma_H}^\dagger(t_\gamma)a_{\delta_H}^\dagger(t_\delta)\right]\middle|\Psi_0^N\right\rangle \tag{21}$$

The steps taken for the sp propagator, leading to eq. (10), may now be repreated for the two particle propagator. In attaining this expression for the two particle propagator, the Heisenberg picture addition and removal operators have to be replaced by corresponding interaction picture operators. The resulting expectation value is taken with respect to the noninteracting ground state $\left|\Phi_0^N\right\rangle$ which again reveals a cancellation between the numerator and the denominator, leading to a corresponding set of connected contributions (diagrams). The result may be written by eq.(22) which is very similar to eq.(10)

$$\begin{aligned} G_{II}(\alpha t_\alpha, \beta t_\beta, \gamma t_\gamma, \delta t_\delta) = -\frac{i}{\hbar}\sum_m^\infty\left(-\frac{i}{\hbar}\right)^m\frac{1}{m!}\int dt_1 ... \int dt_m \\ \times \left\langle\Phi_0^N\middle|\mathcal{T}[\hat{H}_1(t_1)...\hat{H}_1(t_m)a_\beta(t_\beta)a_\alpha(t_\alpha)a_\gamma^\dagger(t_\gamma)a_\delta^\dagger(t_\delta)]\middle|\Phi_0^N\right\rangle_{connected} \end{aligned} \tag{22}$$

The zeroth order term in eq.(22)

$$\begin{aligned} G_{II}^0(\alpha t_\alpha, \beta t_\beta, \gamma t_\gamma, \delta t_\delta) &= -\frac{i}{\hbar}\left\langle\Phi_0^N\middle|\mathcal{T}[a_\beta(t_\beta)a_\alpha(t_\alpha)a_\gamma^\dagger(t_\gamma)a_\delta^\dagger(t_\delta)]\middle|\Phi_0^N\right\rangle \\ &= i\hbar[G^0(\alpha,\gamma;t_\alpha-t_\gamma)G^0(\beta,\delta;t_\beta-t_\delta) - G^0(\alpha,\delta;t_\alpha-t_\delta)G^0(\beta,\gamma;t_\beta-t_\gamma)] \end{aligned} \tag{23}$$

This combination of unperturbed single particle propagators is shown diagrammatically in Fig.6. Clearly, "disconnected" should not apply to the two non-interacting propagators shown in

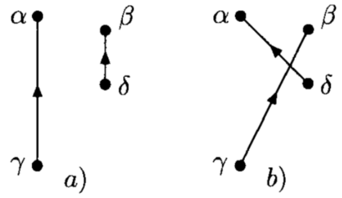

Figure 6: The two contributions to the noninteracting two particle propagator in the time formulation as given by eq.(23).

Fig.6. Similarly, higher-order contributions, which have attachments to these lines, but do not link them, are still "connected" as long as there are no other disconnected parts. Now, skipping all the algebra in which one apply wick's theorem liberally, one can calculate the first order contribution to the two particle propagator which comes out to be

$$G^1_{II}(\alpha t_\alpha, \beta t_\beta, \gamma t_\gamma, \delta t_\delta) = (\frac{-i}{\hbar})^2 \int dt_\epsilon \int dt_\zeta \int dt_\eta \int dt_\theta \frac{1}{4} \sum_{\epsilon\zeta\eta\theta} \langle \epsilon\zeta | V(t_\epsilon, t_\zeta, t_\eta, t_\theta) | \eta\theta \rangle$$
$$\times G^0(\alpha, \epsilon; t_\alpha - t_\epsilon) G^0(\beta, \zeta; t_\beta - t_\zeta) \times G^0(\eta, \gamma; t_\eta - t_\gamma) G^0(\theta, \delta; t_\theta - t_\delta) \tag{24}$$

where

$$V(t_\epsilon, t_\zeta, t_\eta, t_\theta) = \delta(t_1 - t_2)\delta(t_2 - t_3)\delta(t_3 - t_4) \langle \alpha\beta | V | \gamma\delta \rangle \tag{25}$$

It can be shown that this $V(t_\epsilon, t_\zeta, t_\eta, t_\theta)$ is the same $\hat{V}(t)$ one would get when working in interaction picture of $\hat{V}$

In establishing the result in eq.(24), Wick's theorem and the symmetry of $\hat{V}$ was used while only the connected contributions were kept. Diagrammatically, one may relate V by a box to represent the additional time arguments in the two particle interaction picture. It is easier to see this diagrammatically as one requires a 4 vertex object to connect two particle interactions (one requires 2 points each for *before* and *after* interaction making it 4). This is diagrammatically shown in Fig.7

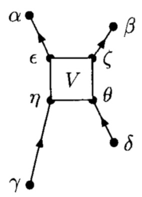

Figure 7: First-order connected contribution to the two particle propagator, linking two noninteracting propagators in the time formulation. eq.(24).

In the analysis of the single particle propagator two types of diagrams were encountered. The first kind contained the diagram representing G^0. The second contained all other connected diagrams involving higher-order self-energy insertions. The two particle propagator also contains two types of diagrammatic contributions. The first group includes the diagram with two non interacting single particle propagators shown in Fig.6. In higher order, additional terms are generated, which contribute to the same group. These terms insert all possible self-energy corrections to these noninteracting propagators, but never link the two. The sum of all these contributions generalizes the noninteracting propagators in Fig.6 to exact ones. The extension of Fig.6 is shown in part a) of Fig.9. Note that the dressing will include both the generalization of part a) and b) of Fig.6

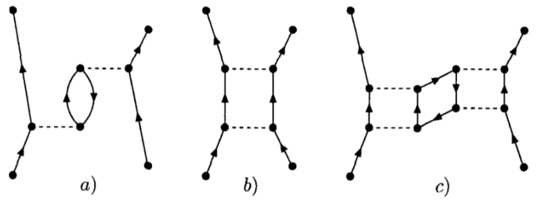

Figure 8: Higher-order connected contributions to the tp propagator which generalize the first-order term in Fig.7, to the four-point vertex function.

The other group of diagrams in higher order, generalize the first-order contribution shown in Fig.7. Each of the four noninteracting propagators will receive all possible self-energy insertions, turning them into exact single particle propagators. This however, is not the only possible extension of Fig.7. In addition to dressing the propagators, more complicated connections appear, which link the incoming two propagators, with the two outgoing ones. Examples of such generalizations are shown in Fig.8. The existence of these diagram connections show us that the most general term that one needs to use for depicting the complete sum total of the interactions of this type is again a general four point vertex function, but this time instead of V it is going to be a much more complicated beast, and one can call it the four point vertex function - Γ. The four-point vertex function includes all possible terms that connect the two incoming lines with the two outgoing ones. All intermediate sp propagators will correspondingly become fully dressed, as well as the four external ones in the diagrams shown in Fig.8. The same holds for all other higher-order contributions. This is diagrammatically shown in 9 b).

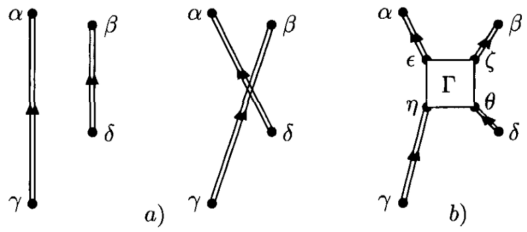

Figure 9: Two contributions to the exact two particle propagator in the time formulation. In part a) the dressed, but noninteracting, two particle propagator is shown including both direct and exchange contributions. In part b) the four-point vertex function Γ is introduced to represent the sum of all higher-order contributions, generalizing Fig.6

This quantity Γ, can be considered as the effective interaction between dressed particles in the medium. Often experimental information is available about some of the features of Γ, helping us to devise approximation schemes. It is now possible to summarize the discussion by writing G_{II} in terms of dressed single particle propagators and Γ as shown in eq.(26) this is the same as shown in Fig.9

$$
\begin{aligned}
G_{II}(\alpha t_\alpha, \beta t_\beta, \gamma t_\gamma, \delta t_\delta) = {} & (i\hbar)[G(\alpha,\gamma;t_\alpha - t_\gamma)G(\beta,\delta;t_\beta - t_\delta) - G(\alpha,\delta;t_\alpha - t_\delta)G(\beta,\gamma;t_\beta - t_\gamma)] \\
& + (i\hbar)^2 \int dt_\epsilon \int dt_\zeta \int dt_\eta \int dt_\theta \sum_{\epsilon\zeta\eta\theta} G(\alpha,\epsilon;t_\alpha - t_\epsilon)G(\beta,\zeta;t_\beta - t_\zeta) \\
& \times \langle\epsilon\zeta|\,\Gamma(t_\epsilon,t_\zeta,t_\eta,t_\theta)\,|\eta\theta\rangle \times G(\eta,\gamma;t_\eta - t_\gamma)G(\theta,\delta;t_\theta - t_\delta)
\end{aligned} \tag{26}
$$

2.2. *Putting it all together*

Well equipped with the tools to deal with the two particle propagator, We now come back to eq.(20) to complete the analysis of the equation of motion for the propagator G, leading to an important relation between the vertex function Γ and the irreducible self-energy Σ^*. We can now combine eq.(26) and eq.(20) to get eq(27)

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}G(\alpha,\beta;t-t') = {} & \delta(t-t')\delta_{\alpha\beta} + \epsilon_\alpha G(\alpha,\beta;t-t') - \sum_\delta \langle\alpha|\,U\,|\delta\rangle\, G(\delta,\beta;t-t') \\
& - i\hbar \sum_{\delta\zeta\theta} \langle\alpha\delta|\,V\,|\theta\zeta\rangle\, G(\zeta,\delta;t-t^+)G(\theta,\beta;t-t^{'}) \\
& - \frac{1}{2}(i\hbar)^2 \sum_{\delta\zeta\theta}\sum_{\kappa\lambda\mu\nu} \langle\alpha\delta|\,V\,|\theta\zeta\rangle\, G(\theta,\kappa;t-t_\kappa)G(\zeta,\lambda;t-t_\lambda)G(\nu,\delta;t_\nu - t) \\
& \times \langle\kappa\lambda|\,\Gamma(t_\kappa,t_\lambda,t_\mu,t_\nu)\,|\theta\zeta\rangle\, G(\mu,\beta;t_\mu - t')
\end{aligned} \tag{27}
$$

Things start to get interesting once we Forrier transform eq.(27) into the Energy space from the time space. Rearranging after taking the F.T one finds the incredible result that the interacting greenfunction G turns out to be a Dyson series again with a self energy Σ^* which contains all the information about the two particle greens function like V and Γ giving us eq.(28) which is the same as the one we got in eq.(12) with Σ^* given by eq.(29). Σ^* is shown in Fig.10, again not that we have used the fact that V and Γ are symmetric and have used only one diagram to represent the entire series as we did earlier in Fig.3

$$
G(\alpha,\beta;E) = G^0(\alpha,\beta;E) + \sum_{\gamma,\delta} G^0(\alpha,\gamma;E)\Sigma^*(\gamma,\delta,E)G(\delta,\beta;E) \tag{28}
$$

$$
\begin{aligned}
\Sigma^*(\gamma,\delta,E) = {} & \langle\gamma|\,U\,|\delta\rangle - i\int_{C\uparrow}\frac{dE^{'}}{2\pi}\sum_{\mu\nu}\langle\gamma\mu|\,V\,|\delta\nu\rangle\, G(\nu,\mu;E^{'}) \\
& + \frac{1}{2}\int\frac{dE_1}{2\pi}\int\frac{dE_2}{2\pi}\sum_{\epsilon,\mu,\nu,\zeta,\rho,\sigma}\langle\gamma\mu|\,V\,|\delta\nu\rangle\, G(\epsilon,\zeta;E_1)G(\nu,\rho;E_2) \\
& \times G(\sigma,\mu;E_1+E_2-E)\,\langle\zeta\rho|\,\Gamma(E_1,E_2,E,E_1+E_2-E)\,|\delta\sigma\rangle
\end{aligned} \tag{29}
$$

3. Approximation Schemes

We have now derived the exact equation for the interacting greens function (eq.(28) eq.(29)) using one unknown quantity Γ. Now it is upto various talented physicists to come up with approximations to Γ using data from experiments. This close relation of Γ to experiments exists

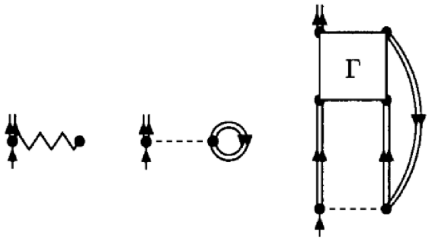

Figure 10: Diagrams representing the irreducible self-energy as given by eq.(29)

because of the fact that we have taken all the two particle correlations and added it exclusively in Γ, which makes it experimentally tractable as most experiments involve at the very least, two particle interactions. The effects of using more and more higher order terms and interactions in Γ becomes more prominent when one enters the area of *Strongly correlated* systems.

3.1. Hartree-Fock

$$\Gamma = 0 \tag{30a}$$

$$\Sigma^*(\gamma, \delta) = \langle\gamma| U |\delta\rangle - i \int_{C\uparrow} \frac{dE'}{2\pi} \sum_{\mu\nu} \langle\gamma\mu| V |\delta\nu\rangle G(\nu, \mu; E') \tag{30b}$$

The easiest of the approximations involves setting $\Gamma = 0$. This simple approximation can be used to treat systems where the two particle correlation is negligible compared to the particle exchange terms. One can show in an elegant way that this approximation is indeed the same as Hartree-Fock approximation derived by using variation principle. This is often used as a diagrammatic way of representing the Hartree fock equation as using self energy contribution as only the first two terms in eq.(29). One can clearly see from eq.(30b) that this makes the self energy independent of energy as $\Sigma^*(\gamma, \delta, E)$ merely becomes $\Sigma^*(\gamma, \delta)$. And the self energy can now uses only the first two diagrams in Fig.10. Leaving the U part in eq.(29) (first diagram in Fig.10) one can de-symetrize the second term and split it into two contributions as shown in Fig.11. We have changed the diagram notation a bit to make it relate-able to the common conventional text, the modification being using *squiggly lines* instead of dotted lines to represent V. These diagrams are identical to c) and d) terms in Fig.1 if one replaces the dotted line (V) with *squiggly lines*

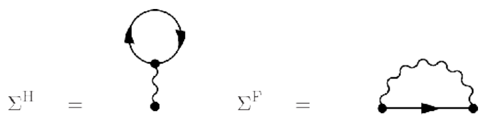

Figure 11: Diagrams representing the irreducible self-energy by setting Γ = 0 in eq.(29)

3.2. GW approximation

The next step of approximation one can do is to add the first and second order terms in the Γ diagram which brings in the energy dependence of Σ^* back, making the approximation that $\Gamma = V$

or saying that the first order correction to Γ is exactly equal to V brings us to the an approximation that goes by the name *RPA* where only the week coloumb interactions are considered by adding the bubble diagrams. Even though this approximation brings in more physics compared to the Hartree fock terms, one finds that the values are still way off when compared to the experiment. The explanation of which was given by Heiden in what turns out to be one of the most iconic papers in Many-Body Perturbation theory. The important insight from that paper is to show that it is extremely inaccurate to consider the perturbation series in terms of V (coulomb interaction) as it is extremely large and instead proposes to use W which he defines to be a *Screened coulomb interaction*. He then proceeds to reformulate eq.(29) in terms of this W. So our first task is to come up with a perturbation series with W playing the role of V, after which we can apply approximations to that to get the famous GW approximation.

The entire processes we are trying to achieve is this - pick terms in Γ that involves *Screening* interactions and add it to V to make it W after which we subtract those from Γ to get Γ^*. Let us start by defining some useful terms and latter relating them to the terms we have seen above. We start by defining W in terms of *Polarization* function P given by dyson series

$$W = V + VPW \tag{31}$$

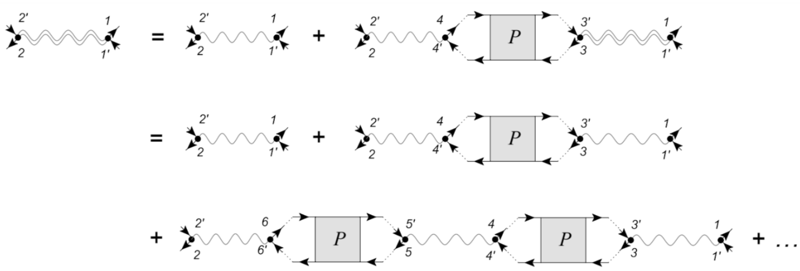

Figure 12: Diagrams representing W in terms of V and P according to eq.(31)

where we have dropped the label index and state index as it just makes seeing these results cumbersome. Eq.(31) is diagrammatically represented in Fig.12. Since we want to take a part of Γ and insert it in V, our P is made up of Γ but not all of the diagrams, only the *interaction* part and not the *exchange* part as we want to add only the interactions in W. What we mean by this can be seen from Fig.13 Here in the first diagram, exchanging particle 1 and 2 gives us back the same diagram which would correspond to an example of *exchange* term in Γ while the second diagram cannot be reproduced by exchanging particle 1 and 2 which cursosponds to the *interaction* term in Γ. So diagrams that belong to the first class are put together to from Γ^* let us aggrigate all the *exchange* diagrams and call it Γ_{ph} thus we have split our initial Γ we had in previous sections as $\Gamma^* + \Gamma_{ph}$

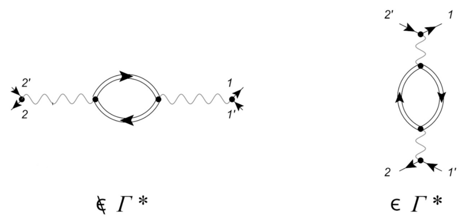

Figure 13: First diagram is an exmple term in Γ_{ph} while the second is an example in Γ^{*}

We can now write P as eq.(32) in terms of Γ^{*} that contains only the interaction diagrams as indicated above. Eq.(32) is shown in Fig.14. This is similar to the terms in G_{II} from Fig.9 This is because, it can be shown that Polarization P is the *response* to the two particle greens function if we start from using linear response theory

$$P = GG + G\Gamma^{*}G \tag{32}$$

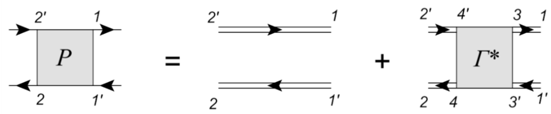

Figure 14: Diagrams representing P in terms of Γ^{*} according to eq.(32)

Looking closely at Fig.13 one can deduce a relation between Γ^{*} and Γ_{ph} given by eq.(33a) which is just saying that Γ_{ph} can be recreated by repeatedly joining Γ^{*} by two greens function (as you can see from Fig.13). This is diagrammatically represented in Fig.15. This is the famous Bethe salpeter equation. Notice that we have a new symbol Γ^{*}_{ph} instead of Γ_{ph}. This is done so to avoid recounting the V term in W as this is already counted in W as shown in Fig.12

$$\Gamma^{*} = \Gamma^{*}_{ph} + \Gamma^{*}GG\Gamma^{*}_{ph} \tag{33a}$$

$$\Gamma^{*}_{ph} = \Gamma_{ph} - V \tag{33b}$$

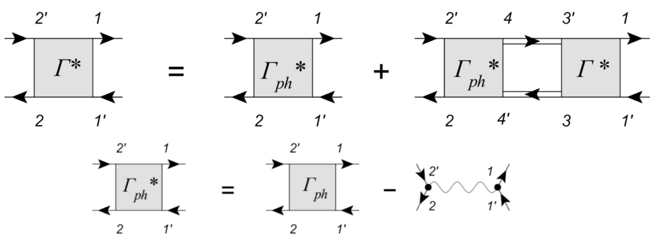

Figure 15: Bethe salpeter equation relating *exchange* and *correlation* parts of Γ according to eq.(32)

Next step is to relate all these to self energy. A very elegant way to derive this standard quantum field theoretical relation is to visually see how this evolves from differentiating the diagrams. From Fig.16, we can see that top left loop diagram as one G loop which when differentiated wrt G removes the G double line yielding the bottom left diagram. while for the top second diagram, has 3 G's thus we get 3 different terms when differentiating rt G wach time dropping a line. After doing the same procedure for higher order terms, one can see this is exactly the diagrammatic sum for Γ_{ph}.

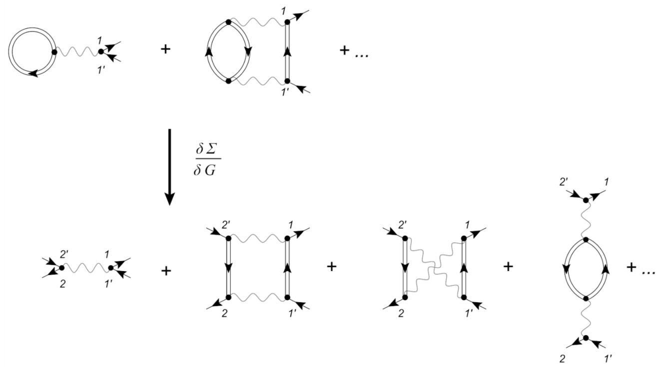

Figure 16: Selecting few Feynman diagrams we illustrate that differentiation of Σ w.r.t. G yields the particle-hole irreducible vertex Γ_{ph}.

Thus we can now write the equation relating Γ_{ph} with Σ by eq.(34a), but we need to note that our self energy is self energy sans the hartree part and hence we arrive at eq.(34b)

$$\Gamma_{ph} = \frac{\delta\Sigma}{\delta G} \tag{34a}$$

$$\Gamma_{ph} = \frac{\delta[\Sigma - \Sigma_{Hartree}]}{\delta G} \tag{34b}$$

We can now go back to eq.(29) and switch all V's to W's and at the same time switch Γ to Γ^*. Eq.(35a) rewrites eq.(29) dropping all the indexes and the U term (which can be identically set to 0) while eq.(35b) converts the same into W and Γ^*. This is diagrammatically shown in Fig.17

$$\Sigma = -VG + GG\Gamma G \tag{35a}$$

$$\Sigma = -WG + GG\Gamma^* G \tag{35b}$$

3.2.1. Putting it all together - Hedin equations and GW

We now have all the tools required to approximate and arrive at GW. With few algebraic steps and manipulations latter we can relate all the variables from previous section and formally write the set of equations defining the self energy called the Hedien equations as

$$G = G_0 + G_0\Sigma G \tag{36a}$$

$$\Sigma = iGW\Gamma \tag{36b}$$

$$W = V + WPV \tag{36c}$$

$$P = -iGG\Gamma \tag{36d}$$

$$\Gamma = 1 + \frac{\delta\Sigma}{\delta G}GG\Gamma \tag{36e}$$

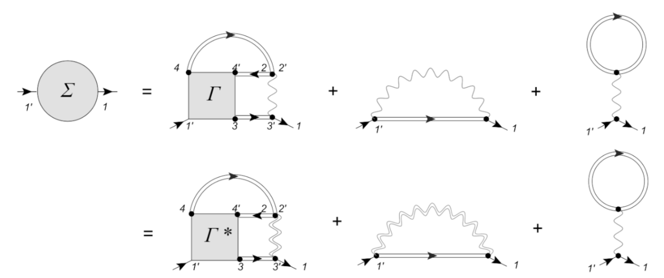

Figure 17: Self energy reformulated using W according to eq.(35b). Notice V (single squiggly line) being replaced by W (double squiggly line)

where now Γ differs from the used in eq.(29) as this is just a new renamed version of $\Gamma^* + 1$ used in eq.(33a).

Theoretically solving these set of equations iteretively to get G in eq.(36a) would give us the exact solution to our interacting problem, but it is extremely tedious and close to impossible task to solve them. So we again resort to a approximation. The approximation we are going to make is the same as in Hartree case, but this time we have a better first order approximation of Γ as we have given a part of it to W. We arrive at GW approximation by either setting Γ in eq.(36e) to 1 or Γ^* in eq.(35b) to 0

$$\Gamma \approx 1 \tag{37a}$$

$$\Gamma^* \approx 0 \tag{37b}$$

This is the so called GW approximation as we are basically setting $\Sigma = GW$ in eq.(35b) or eq.(36b). So the new set of equations we get are

$$G = G_0 + G_0 \Sigma G \tag{38a}$$

$$\Sigma = iGW \tag{38b}$$

$$W = V + WPV \tag{38c}$$

$$P = -iGG \tag{38d}$$

This approximation basically reduces a step in the big picture of exactly solving the many body interaction problem shown by the self consistent flowchart in Fig.18 taken from a review article by Jiang [3] .This is a better approximation than the previous Hartree because of the fact that we have now replaced our V with screen W makes it possible for us to better approximate the interactions in condensed matter systems.

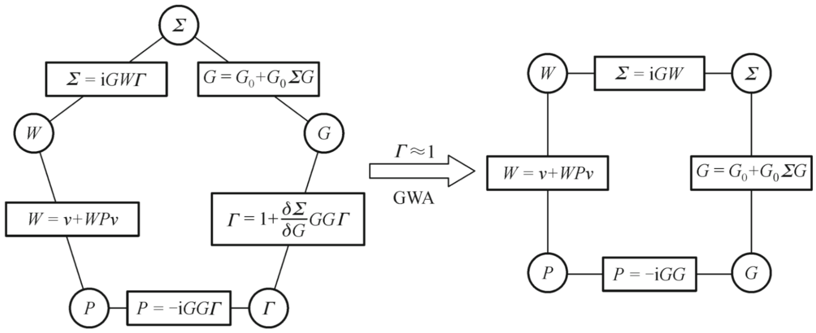

Figure 18: Schematic illustration of Hedins equations in the full form (left) and within the GW approximation (right)

4. Conclusion

We have shown how to *technically* solve the many body interaction problem exactly by using Hedin equations albeit its difficulties and later proceed to show how to derive a tractable approximation introduced by Hedin - GW. All these steps where performed from fundamental many body quantum physics. This review uses different techniques and figures introduced by Jiang [3],Mattuck [5],Dickhoff and Van Neck [1],Held et al. [2] and Martin et al. [4].

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