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Derivations for Personal Learning

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Chapter 1

Dyson to GQME: 12/13

The Generalized Quantum Master Equation (GQME) is given by

$$\dot{\mathcal{C}}(t) = \mathcal{C}(t)\Omega_1 - \int_0^t d\tau\, \mathcal{C}(t-\tau)\mathcal{K}_1(\tau) + D(t) \tag{1.1}$$

where the correlation function is defined as

$$\mathcal{C}(t) = (\hat{\mu} \mid \hat{\mu}(t)), \tag{1.2}$$

the higher-order moments are

$$\Omega_n \equiv \left((i\mathcal{L})^n \hat{\mu}, \hat{\mu}\right) / (\hat{\mu}, \hat{\mu}) \tag{1.3}$$

with the auxiliary kernels

$$K_n(t) \equiv \left((i\mathcal{L})^n \hat{f}(t), \hat{\mu}\right) / (\hat{\mu}, \hat{\mu}) \tag{1.4}$$

$\hat{f}(t)$ in the above equation is referred to as the random force operator

$$\hat{f}(t) \equiv e^{it\mathcal{L}\mathcal{L}} \mathcal{Q} i\mathcal{L}\hat{\mu} \tag{1.5}$$

with $\mathcal{Q} = \mathcal{I} - \mathcal{P}$ being the complementary projection operator. But this becomes complicated, so Wenjie found that we can express $\mathcal{K}_1(t)$ without time evolution using $\hat{f}(0) = \mathcal{Q} i\mathcal{L}\hat{\mu}$ and, we get

$$K_n(0) = \Omega_{n+1} - \Omega_n \Omega_1 \tag{1.6}$$

Therefore, we only need to consider $\dot{K}_1(t)$, which can be obtained directly:

$$\dot{K}_1(t) = \frac{(i\mathcal{L}\dot{\hat{f}}(t), \hat{\mu})}{(\hat{\mu}, \hat{\mu})} = K_2(t) - \Omega_1 K_1(t) \tag{1.7}$$

Similarly, we can show that the auxiliary kernels are coupled through

$$\dot{K}_n(t) = K_{n+1}(t) - \Omega_n K_1(t). \tag{1.8}$$

We expect that the higher order auxiliary kernels will decay quickly, so we can truncate the series at some finite n. The moments of the memory kernel are

$$\Omega_n = \frac{((i\mathcal{L})^n \hat{\mu}, \hat{\mu})}{(\hat{\mu}, \hat{\mu})}, \tag{1.9}$$

with $\mathcal{L}$ being the Liouville superoperator with $\mathcal{L}\hat{\mu} = \left[\hat{H}, \hat{\mu}\right]$. The construction of the numerator in equation 1.9 can be thought of as the generation of a Krylov subspace up to level n, i.e. we need to build up $\mathcal{K}_n(\mathcal{L}, \hat{\mu}) = \text{span}\{\hat{\mu}, (i\mathcal{L})\hat{\mu}, (i\mathcal{L})^2\hat{\mu}, \ldots, (i\mathcal{L})^{n-1}\hat{\mu}\}$, where $\hat{\mu} = \hat{c}$ or $\hat{c}^\dagger$. In the case if we choose $\hat{\mu} = \hat{c}$, we get the lesser Green's function

$$\mathcal{C}(t) = (\hat{c}, \hat{c}(t)) \equiv \langle \hat{c}^\dagger(0)\hat{c}(t)\rangle = \frac{G^<(t)}{i} \tag{1.10}$$

whereas if we chose $\hat{\mu} = \hat{c}^\dagger$, we get the greater Green's function

$$\mathcal{C}(t) = (\hat{c}^\dagger, \hat{c}^\dagger(t)) \equiv \langle \hat{c}(0)\hat{c}^\dagger(t)\rangle = -\frac{G^>(t)}{i} \tag{1.11}$$

Then we can construct the retarded Green's function as

$$G_R(t) = \Theta(t)\left(G^<(t) - G^>(t)\right) \tag{1.12}$$

Using Krylov subspace methods, one never has to construct the Liouvillian matrix, but instead can directly compute the extremal eigenvalues and eigenvectors of $\mathcal{L}$ by considering the action of $\mathcal{L}$ on the Krylov subspace.

1.1 Explicit Construction of the Liouville Superoperator

Consider that we are working with the upfolded Hamiltonian

$$\mathbf{H} = \begin{pmatrix} \mathbf{f} & \mathbf{W} \\ \mathbf{W}^\dagger & \mathbf{d} \end{pmatrix} \tag{1.13}$$

where we again have a physical space $\mathbf{f}$ and a bath space $\mathbf{d}$, whose coupling is given by $\mathbf{W}$. Tell me what would happened if we considered the action of this on the composite operator vector defined lower? Lets consider making a Krylov subspace, corresponding to repeated applications of the Liouville superoperator to the initial operator $\hat{\boldsymbol{\mu}}$. Now, The idea is to define a composite operator vector

$$\hat{\boldsymbol{\mu}} \equiv \begin{pmatrix} \hat{\mu}_1 \\ \hat{\mu}_2 \end{pmatrix} = \begin{pmatrix} \hat{c} \\ \hat{c}^\dagger \end{pmatrix}, \tag{1.14}$$

where $\hat{c}$ is the annihilation operator and $\hat{c}^\dagger$ is the creation operator. Notice that the equation of motion for the Green's function is

$$(i\partial_t - \hat{H}_0)G(t,t') = \delta(t-t') + \int_{-\infty}^{\infty} d\tau\, \Sigma(t,\tau)\, G(\tau,t') \tag{1.15}$$

$$\rightarrow G(\dot{t},t') = -i\hat{H}_0 G(t,t') - i\delta(t-t') + \int_{-\infty}^{\infty} d\tau'\, \Sigma(t,\tau')\, G(\tau',t') \tag{1.16}$$

So our task becomes to figure out how

$$-i\hat{H}_0 G(t,t') - i\delta(t-t') + \int_{-\infty}^{\infty} d\tau' \, \Sigma(t,\tau') \, G(\tau',t') = \mathcal{C}(t)\Omega_1 - \int_0^t d\tau \, \mathcal{C}(t-\tau)\mathcal{K}(\tau) + D(t) \quad (1.17)$$

I feel like it should be the case that $-i\hat{H}_0 G(t,t') = \mathcal{C}(t)\Omega_1$. Do you think that this should be the case or no? Because I think we can agree that the equation that comes first should be the same as the equation of motion for the greens function. And then try to apply a decomposed Hamiltonia like $H = H_0 + V$ to the first equation, so that we can see what happens.

To simple by things as much as possible initially consider that we only use the noninteracting Hamiltonian $\hat{H}_0 = \epsilon \hat{c}^\dagger \hat{c}$ in the action of the Liouvillian.

$$\Omega_1 = \frac{((i\mathcal{L})\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})}{(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})} = \frac{\Big((i[\hat{H}_0, \hat{\boldsymbol{\mu}}], \hat{\boldsymbol{\mu}}\Big)}{(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})} \quad (1.18)$$

If we just consider the numerator, we see that

$$\Big((i[\hat{H}_0, \hat{\boldsymbol{\mu}}], \hat{\boldsymbol{\mu}}\Big) = \Big(i[\hat{H}_0, \hat{c}], \hat{c}\Big) + \Big(i[\hat{H}_0, \hat{c}^\dagger], \hat{c}^\dagger\Big) \quad (1.19)$$

Considering just the first term

$$\Big(i[\hat{H}_0, \hat{c}], \hat{c}\Big) = -i\epsilon([\hat{c}^\dagger \hat{c}, \hat{c}], \hat{c}) = -i\epsilon(\hat{c}, \hat{c}) = -i\epsilon\,(1 - f(\epsilon)) \quad (1.20)$$

and the second term

$$\Big(i[\hat{H}_0, \hat{c}^\dagger], \hat{c}^\dagger\Big) = -i\epsilon([\hat{c}^\dagger \hat{c}, \hat{c}^\dagger], \hat{c}^\dagger) = -i\epsilon(\hat{c}^\dagger, \hat{c}^\dagger) = -i\epsilon f(\epsilon) \quad (1.21)$$

which can be summarized as

$$\Big(i[\hat{H}_0, \hat{\boldsymbol{\mu}}], \hat{\boldsymbol{\mu}}\Big) = -i\epsilon \implies \Omega_1 = -i\epsilon \quad (1.22)$$

Now, the equation of motion for the interacting Green's function is given by

$$\left(i\frac{\partial}{\partial t} - h_0\right) G(t,t') = \delta(t-t') + \int dt'' \Sigma(t,t'') G(t'',t') \quad (1.23)$$

$$\frac{\partial}{\partial t} G(t,t') = \underbrace{-ih_0 G(t,t')}_{\Omega_1 C(t)} - i\delta(t-t') + \int dt'' \Sigma(t,t'') G(t'',t') \quad (1.24)$$

Now come if we consider the higher-order moments

$$\Omega_n \equiv \frac{((i\mathcal{L})^n \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})}{(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})} = \frac{(i)^n \, (\mathcal{L}^n \hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})}{(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\mu}})} = (i)^n \Big([\hat{H}, [\hat{H}, [\hat{H}, \cdots, \hat{\boldsymbol{\mu}}]]] \cdots\Big) \quad (1.25)$$

where it is implied that we are applying the commutator n times. We want to answer the form for the $\hat{\mathbf{H}}^{G_0 W_0}$ Hamiltonian, which has the super matrix form of

$$\begin{bmatrix} \mathbf{f} + \boldsymbol{\Sigma}_\infty & \mathbf{W} \\ \mathbf{W}^\dagger & \mathbf{d} \end{bmatrix} \quad (1.26)$$

and the memory kernel

$$\mathcal{K}(t) = \left(\mathbf{A} \left| \mathcal{L}\mathcal{Q} e^{i\mathcal{Q}\mathcal{L}t} \mathcal{Q}\mathcal{L} \right| \mathbf{A}\right), \quad (1.27)$$

where $\mathcal{Q} = \mathcal{I} - \mathcal{P}$ is the complementary projection operator.

Chapter 2

UEG

Throughout, I am working in the retarded time formalism. We are working with a plane wave basis, where each state has its own wavevector.

2.1 MF

Even before doing HF, I generate my basis of plane waves, and their wave vectors in 3D are just a list of integers, three entries long. From HF, I get a set of MO coefficients $C_{\boldsymbol{k}_\mu \boldsymbol{k}_p}$ and orbital energies $\epsilon_{\boldsymbol{k}_p}$.

2.2 RPA

For the UEG, I am first looping over all momentum transfer vectors $\boldsymbol{k}_q$. To learn which excitations are valid for the given $\boldsymbol{k}_q$, we first loop over occupied states $\boldsymbol{k}_i$. Virtual states $\boldsymbol{k}_a$ are already determined by that point; we compute $\boldsymbol{k}_a \equiv \boldsymbol{k}_i + \boldsymbol{k}_q$, and based of of whether it is a valid virtual index, we either add it to our list or continue. The criterion for validity is that the wave vector must be outside the Fermi sphere, but still within our plane wave basis, i.e. within the KE cutoff. We do the same for the second pair of indices $\boldsymbol{k}_j, \boldsymbol{k}_b$. Then, we can form the Casida eigenproblem for each $\boldsymbol{k}_q$.

$$\begin{pmatrix} \boldsymbol{A}(\boldsymbol{k}_q) & \boldsymbol{B}(\boldsymbol{k}_q) \\ -\boldsymbol{B}(\boldsymbol{k}_q) & -\boldsymbol{A}(\boldsymbol{k}_q) \end{pmatrix} \begin{pmatrix} \boldsymbol{X}(\boldsymbol{k}_q) & \boldsymbol{Y}(\boldsymbol{k}_q) \\ \boldsymbol{Y}(\boldsymbol{k}_q) & \boldsymbol{X}(\boldsymbol{k}_q) \end{pmatrix} \begin{pmatrix} \boldsymbol{\Omega}(\boldsymbol{k}_q) & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{\Omega}(\boldsymbol{k}_q) \end{pmatrix} = \begin{pmatrix} \boldsymbol{X}(\boldsymbol{k}_q) & \boldsymbol{Y}(\boldsymbol{k}_q) \\ \boldsymbol{Y}(\boldsymbol{k}_q) & \boldsymbol{X}(\boldsymbol{k}_q) \end{pmatrix} \tag{2.1}$$

The $\boldsymbol{A}(\boldsymbol{k}_q)$ and $\boldsymbol{B}(\boldsymbol{k}_q)$ matrices are defined as

$$A_{\boldsymbol{k}_i \boldsymbol{k}_a, \boldsymbol{k}_b \boldsymbol{k}_j}(\boldsymbol{k}_q) = (\epsilon_{\boldsymbol{k}_a} - \epsilon_{\boldsymbol{k}_i})\, \delta_{\boldsymbol{k}_i \boldsymbol{k}_j} \delta_{\boldsymbol{k}_a \boldsymbol{k}_b} + \frac{4\pi}{|\boldsymbol{k}_q|^2} \tag{2.2}$$

$$B_{\boldsymbol{k}_i \boldsymbol{k}_a, \boldsymbol{k}_j \boldsymbol{k}_b}(\boldsymbol{k}_q) = \frac{4\pi}{|\boldsymbol{k}_q|^2} \tag{2.3}$$

After solving the Casida eigenvalue problem, I perform the bioorthogonalization procedure, which ensures that

$$(\boldsymbol{X}(\boldsymbol{k}_q) - \boldsymbol{Y}(\boldsymbol{k}_q))^\dagger\, (\boldsymbol{X}(\boldsymbol{k}_q) + \boldsymbol{Y}(\boldsymbol{k}_q)) = \boldsymbol{I} \tag{2.4}$$

Now, I have a list of excitation energies Ω and corresponding right eigenvectors $\boldsymbol{X}, \boldsymbol{Y}$ for each momentum transfer $\boldsymbol{k}_q$. But for the self energy, we actually need rather the transition densities $\rho(\boldsymbol{k}_q)$, which are lists (with length μ) of scalars, defined as

$$\rho_\nu(\boldsymbol{k}_q) = \sum_{\boldsymbol{k}_i \boldsymbol{k}_a} \left(X^\nu_{\boldsymbol{k}_i \boldsymbol{k}_a}(\boldsymbol{k}_q) + Y^\nu_{\boldsymbol{k}_i \boldsymbol{k}_a}(\boldsymbol{k}_q) \right). \tag{2.5}$$

So to get them, I just need to contract over the indices $\boldsymbol{k}_i, \boldsymbol{k}_a$.

2.3 GW

2.3.1 Correlation self energy

Because I am only interested in computing the diagonal spectral function for a certain index $\boldsymbol{k}_p$, I only need to compute the diagonal correlation self energy $\Sigma^{\text{corr}}(\boldsymbol{k}_p, \omega)$, for the given frequency ω, which is given by

$$\Sigma^{\text{corr}}(\boldsymbol{k}_p, \omega) = \sum_{\boldsymbol{k}_q} \sum_{\nu}^{\text{RPA}} \frac{4\pi}{|\boldsymbol{k}_q|^2} |\rho_\nu(\boldsymbol{k}_q)|^2 \left[\frac{f_{\boldsymbol{k}_p - \boldsymbol{k}_q}}{\omega + \Omega_\nu(\boldsymbol{k}_q) - \epsilon_{\boldsymbol{k}_p - \boldsymbol{k}_q} + i\eta} + \frac{1 - f_{\boldsymbol{k}_p - \boldsymbol{k}_q}}{\omega - \Omega_\nu(\boldsymbol{k}_q) - \epsilon_{\boldsymbol{k}_p - \boldsymbol{k}_q} + i\eta} \right] \tag{2.6}$$

where $f_{\boldsymbol{k}}$ is the Fermi occupation (1 for occupied, 0 for virtual). The terms correspond to hole and particle contributions, respectively. Note that all of the $\boldsymbol{k}_q$ may not be taken into account in this summation. To generate the $\boldsymbol{k}_q$ list, our criterion was that it needs to connect an occupied state $\boldsymbol{k}_i$ to a virtual state $\boldsymbol{k}_a$. Suppose $\boldsymbol{k}_i = [-1, -1, -1]$ and $\boldsymbol{k}_a = [0, 0, 2]$, then $\boldsymbol{k}_q = \boldsymbol{k}_i - \boldsymbol{k}_a = [-1, -1, -3]$. But if we now consider the state $\boldsymbol{k}_p = [0, 0, 1]$, then $\boldsymbol{k}_p - \boldsymbol{k}_q = [1, 1, 4]$, which may be beyond the KE cutoff, and thus not in our basis. So we must skip this $\boldsymbol{k}_q$ in the summation for the correlation self energy.

2.3.2 Spectral function

Finally, the spectral function is given by

$$A(\boldsymbol{k}_p, \omega) = \frac{1}{\pi} \frac{|\operatorname{Im} \Sigma(\boldsymbol{k}_p, \omega)|}{\left(\omega - \epsilon_{\boldsymbol{k}_p} - \operatorname{Re} \Sigma(\boldsymbol{k}_p, \omega)\right)^2 + \left(\operatorname{Im} \Sigma(\boldsymbol{k}_p, \omega)\right)^2} \tag{2.7}$$

2.4 GW+C

2.4.1 Cumulant

By relating the Dyson equation to the Taylor series expansion of the exponential (both to first order), we can write:

$$\boldsymbol{G}^0(t)\boldsymbol{C}(t) = \iint \mathrm{d}t_1 \mathrm{d}t_2 \boldsymbol{G}^0(t - t_1) \boldsymbol{\Sigma}^c(t_1 - t_2) \boldsymbol{G}^0(t_2) \tag{2.8}$$

We know that all of the operators are diagonal in momentum space for the UEG, so insertion of the resolution of the identity just gives us:

$$\boldsymbol{G}^0(\boldsymbol{p},t)\boldsymbol{C}(\boldsymbol{p},t) = \iint \mathrm{d}t_1 \mathrm{d}t_2 \boldsymbol{G}^0(\boldsymbol{p},t-t_1)\boldsymbol{\Sigma}^c(\boldsymbol{p},t_1-t_2)\boldsymbol{G}^0(\boldsymbol{p},t_2) \tag{2.9}$$

$$= \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t}\boldsymbol{G}^0(\boldsymbol{p},\omega)\boldsymbol{\Sigma}^c(\boldsymbol{p},\omega)\boldsymbol{G}^0(\boldsymbol{p},\omega) \tag{2.10}$$

$$\implies \boldsymbol{C}(\boldsymbol{p},t) = i\int \frac{\mathrm{d}\omega}{2\pi} \frac{\boldsymbol{\Sigma}^c(\boldsymbol{p},\omega+\epsilon_{\boldsymbol{p}}^{HF})}{(\omega+i\eta)^2} e^{-i\omega t} \tag{2.11}$$

$$= i\int \frac{d\omega}{2\pi} \frac{1}{(\omega+i\eta)^2} e^{-i\omega t} \left\{ \sum_{\boldsymbol{q}} \sum_{\nu}^{\mathrm{RPA}} \underbrace{\frac{4\pi}{|\boldsymbol{q}|^2}|\rho_\nu(\boldsymbol{q})|^2}_{M^2_{\boldsymbol{q}\nu}} \left[\frac{f_{\boldsymbol{p}-\boldsymbol{q}}}{\omega \underbrace{+\Omega_\nu(\boldsymbol{q}) + (\epsilon_{\boldsymbol{p}} - \epsilon_{\boldsymbol{p}-\boldsymbol{q}}) + i\eta}_{-\Delta^{\mathrm{occ}}_{\boldsymbol{q}\nu}}} \right. \right. \tag{2.12}$$

$$\left. \left. + \frac{1-f_{\boldsymbol{p}-\boldsymbol{q}}}{\omega \underbrace{-\Omega_\nu(\boldsymbol{q}) + (\epsilon_{\boldsymbol{p}} - \epsilon_{\boldsymbol{p}-\boldsymbol{q}}) + i\eta}_{-\Delta^{\mathrm{virt}}_{\boldsymbol{q}\nu}}} \right] \right\}$$

$$= i\sum_{\boldsymbol{q}\nu} M^2_{\boldsymbol{q}\nu} \int \frac{d\omega}{2\pi} e^{-i\omega t} \left[\frac{f_{\boldsymbol{p}-\boldsymbol{q}}}{(\omega+i\eta)^2(\omega-\Delta^{\mathrm{occ}}_{\boldsymbol{q}\nu})} + \frac{1-f_{\boldsymbol{p}-\boldsymbol{q}}}{(\omega+i\eta)^2(\omega-\Delta^{\mathrm{virt}}_{\boldsymbol{q}\nu})} \right] \tag{2.13}$$

$$= \sum_{\boldsymbol{q}\nu} \zeta^{\mathrm{occ}}_{\boldsymbol{p}\boldsymbol{q}\nu} \left[e^{-i\Delta^{\mathrm{occ}}_{\boldsymbol{q}\nu} t} - 1 + i\Delta^{\mathrm{occ}}_{\boldsymbol{q}\nu} t \right] + \sum_{\boldsymbol{q}\nu} \zeta^{\mathrm{virt}}_{\boldsymbol{p}\boldsymbol{q}\nu} \left[e^{-i\Delta^{\mathrm{virt}}_{\boldsymbol{q}\nu} t} - 1 + i\Delta^{\mathrm{virt}}_{\boldsymbol{q}\nu} t \right] \tag{2.14}$$

For the final expression, we have defined $\zeta^{\mathrm{occ}}_{\boldsymbol{p}\boldsymbol{q}\nu} = \left(\frac{f_{\boldsymbol{p}-\boldsymbol{q}} M_{\boldsymbol{q}\nu}}{\Delta^{\mathrm{occ}}_{\boldsymbol{q}\nu}}\right)^2$ and $\zeta^{\mathrm{virt}}_{\boldsymbol{p}\boldsymbol{q}\nu} = \left(\frac{(1-f_{\boldsymbol{p}-\boldsymbol{q}}) M_{\boldsymbol{q}\nu}}{\Delta^{\mathrm{virt}}_{\boldsymbol{q}\nu}}\right)^2$. This allows us to arrive at the something similar to the Landau form of the cumulant.

A few notes on how to evaluate the contour integral: there is a double pole at $\omega_1 = -i\eta$ and a simple pole at $\omega_2 = -\Delta - i\eta$. Closing the contour in the lower half-plane because $\mathrm{Im}\left(\omega_1\right), \mathrm{Im}\left(\omega_2\right) < 0$, and applying Cauchy's residue theorem, leads to

$$\int \frac{\mathrm{d}\omega}{2\pi} e^{-\mathrm{i}\omega t} \frac{1}{\left(\omega-\omega_1\right)^2} \frac{1}{\omega-\omega_2} = (-\mathrm{i}) \left\{ \left[\partial_\omega \left(\frac{e^{-\mathrm{i}\omega t}}{\omega-\omega_2} \right) \right]_{\omega=\omega_1} + \left[\frac{e^{-\mathrm{i}\omega t}}{\left(\omega-\omega_1\right)^2} \right]_{\omega=\omega_2} \right\} \tag{2.15}$$

$$= \frac{(-\mathrm{i})}{\left(\omega_1-\omega_2\right)^2} \left\{ \left[(-\mathrm{i}t)\left(\omega_1-\omega_2\right) - 1 \right] e^{-\mathrm{i}\omega_1 t} + e^{-\mathrm{i}\omega_2 t} \right\} \tag{2.16}$$

$$\implies \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \frac{1}{\left[\omega - (0-\mathrm{i}\eta)\right]^2} \frac{f}{\omega-\Delta} = \frac{-\mathrm{i}f}{\Delta^2} \left(e^{-\mathrm{i}\Delta t} + \mathrm{i}\Delta t - 1 \right) \tag{2.17}$$

2.4.2 Green's function

Now, we plug in our derived expression for $C(\boldsymbol{p}, t)$ into the cumulant ansatz for the retarded Green's function:

$$
\begin{aligned}
G^{GW+C}(\boldsymbol{p}, t) &= G^{HF}(\boldsymbol{p}, t) e^{C(\boldsymbol{p},t)} && (2.18)\\
&= -i\Theta(t) e^{-i\epsilon^{HF}_{\boldsymbol{p}} t + C(\boldsymbol{p},t)} && (2.19)\\
&= -i\Theta(t) e^{-i\epsilon^{HF}_{\boldsymbol{p}} t + \sum_{\boldsymbol{q}\nu} \zeta^{\text{occ}}_{\boldsymbol{pq}\nu} \left(e^{-i\Delta^{\text{occ}}_{\boldsymbol{q}\nu} t} + i\Delta^{\text{occ}}_{\boldsymbol{q}\nu} t - 1 \right) + \sum_{\boldsymbol{q}\nu} \zeta^{\text{virt}}_{\boldsymbol{pq}\nu} \left(e^{-i\Delta^{\text{virt}}_{\boldsymbol{q}\nu} t} + i\Delta^{\text{virt}}_{\boldsymbol{q}\nu} t - 1 \right)} && (2.20)\\
&= -i\Theta(t) Z^{QP}_{\boldsymbol{p}} e^{-i\epsilon^{QP}_{\boldsymbol{p}} t} e^{\sum_{\boldsymbol{q}\nu} \zeta^{\text{occ}}_{\boldsymbol{pq}\nu} e^{-i\Delta^{\text{occ}}_{\boldsymbol{q}\nu} t} + \sum_{\boldsymbol{q}\nu} \zeta^{\text{virt}}_{\boldsymbol{pq}\nu} e^{-i\Delta^{\text{virt}}_{\boldsymbol{q}\nu} t}} && (2.21)\\
& && (2.22)
\end{aligned}
$$

where we have the weight of the quasiparticle peak $Z^{QP}_{\boldsymbol{p}} = \exp\left(-\sum_{\boldsymbol{q}\nu} \zeta^{\text{occ}}_{\boldsymbol{pq}\nu} - \sum_{\boldsymbol{q}\nu} \zeta^{\text{virt}}_{\boldsymbol{pq}\nu} \right)$ and the quasiparticle energy $\epsilon^{QP}_{\boldsymbol{p}} = \epsilon^{HF}_{\boldsymbol{p}} - \left(\sum_{\boldsymbol{q}\nu} \zeta^{\text{occ}}_{\boldsymbol{pq}\nu} \Delta^{\text{occ}}_{\boldsymbol{q}\nu} + \sum_{\boldsymbol{q}\nu} \zeta^{\text{virt}}_{\boldsymbol{pq}\nu} \Delta^{\text{virt}}_{\boldsymbol{q}\nu} \right)$.

We pause to make some important connections. Notice

$$
\begin{aligned}
Z^{QP}_{\boldsymbol{p}} &= \exp\left(-\sum_{\boldsymbol{q}\nu} \zeta^{\text{occ}}_{\boldsymbol{pq}\nu} - \sum_{\boldsymbol{q}\nu} \zeta^{\text{virt}}_{\boldsymbol{pq}\nu} \right) && (2.23)\\
&= \exp\left(-\sum_{\boldsymbol{q}\nu} \left(\frac{f_{\boldsymbol{p}-\boldsymbol{q}} M_{\boldsymbol{q}\nu}}{\Delta^{\text{occ}}_{\boldsymbol{q}\nu}} \right)^2 - \sum_{\boldsymbol{q}\nu} \left(\frac{(1 - f_{\boldsymbol{p}-\boldsymbol{q}}) M_{\boldsymbol{q}\nu}}{\Delta^{\text{virt}}_{\boldsymbol{q}\nu}} \right)^2 \right) && (2.24)\\
&= \exp\left(\left[\frac{\partial \Sigma^c(\boldsymbol{p}, \omega)}{\partial \omega} \right]_{\omega = \epsilon^{HF}_{\boldsymbol{p}}} \right) && (2.25)
\end{aligned}
$$

and

$$
\begin{aligned}
\epsilon^{QP}_{\boldsymbol{p}} &= \epsilon^{HF}_{\boldsymbol{p}} - \left(\sum_{\boldsymbol{q}\nu} \zeta^{\text{occ}}_{\boldsymbol{pq}\nu} \Delta^{\text{occ}}_{\boldsymbol{q}\nu} + \sum_{\boldsymbol{q}\nu} \zeta^{\text{virt}}_{\boldsymbol{pq}\nu} \Delta^{\text{virt}}_{\boldsymbol{q}\nu} \right) && (2.26)\\
&= \epsilon^{HF}_{\boldsymbol{p}} - \left(\sum_{\boldsymbol{q}\nu} \frac{f_{\boldsymbol{p}-\boldsymbol{q}} M^2_{\boldsymbol{q}\nu}}{\Delta^{\text{occ}}_{\boldsymbol{q}\nu}} + \sum_{\boldsymbol{q}\nu} \frac{(1 - f_{\boldsymbol{p}-\boldsymbol{q}}) M^2_{\boldsymbol{q}\nu}}{\Delta^{\text{virt}}_{\boldsymbol{q}\nu}} \right) && (2.27)\\
&= \epsilon^{HF}_{\boldsymbol{p}} + \Sigma^c(\boldsymbol{p}, \epsilon^{HF}_{\boldsymbol{p}}) && (2.28)
\end{aligned}
$$

where we have used the fact that $\Sigma^c(\boldsymbol{p}, \omega) = \sum_{\boldsymbol{q}\nu} \frac{f_{\boldsymbol{p}-\boldsymbol{q}} M^2_{\boldsymbol{q}\nu}}{\omega + \Omega_\nu(\boldsymbol{q}) - \epsilon_{\boldsymbol{p}-\boldsymbol{q}}} + \sum_{\boldsymbol{q}\nu} \frac{(1 - f_{\boldsymbol{p}-\boldsymbol{q}}) M^2_{\boldsymbol{q}\nu}}{\omega - \Omega_\nu(\boldsymbol{q}) - \epsilon_{\boldsymbol{p}-\boldsymbol{q}}} \implies \left[\frac{\partial \Sigma^c(\boldsymbol{p}, \omega)}{\partial \omega} \right]_{\omega = \epsilon^{HF}_{\boldsymbol{p}}} = -\sum_{\boldsymbol{q}\nu} \left(\frac{f_{\boldsymbol{p}-\boldsymbol{q}} M_{\boldsymbol{q}\nu}}{\Delta^{\text{occ}}_{\boldsymbol{q}\nu}} \right)^2 - \sum_{\boldsymbol{q}\nu} \left(\frac{(1 - f_{\boldsymbol{p}-\boldsymbol{q}}) M_{\boldsymbol{q}\nu}}{\Delta^{\text{virt}}_{\boldsymbol{q}\nu}} \right)^2$.

Next, we want to perform a Fourier transform.

$$G^{GW+C}(\boldsymbol{p},\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G^{GW+C}(\boldsymbol{p},t) \tag{2.29}$$

$$= -iZ_{\boldsymbol{p}}^{QP} \int_0^{\infty} dt\, e^{i(\omega-\epsilon_{\boldsymbol{p}}^{QP})t} e^{\sum_{\boldsymbol{q}\nu}\zeta_{\boldsymbol{pq}\nu}^{\text{occ}} e^{-i\Delta_{\boldsymbol{q}\nu}^{\text{occ}}t} + \sum_{\boldsymbol{q}\nu}\zeta_{\boldsymbol{pq}\nu}^{\text{virt}} e^{-i\Delta_{\boldsymbol{q}\nu}^{\text{virt}}t}} \tag{2.30}$$

$$= -iZ_{\boldsymbol{p}}^{QP} \int_0^{\infty} dt\, e^{i(\omega-\epsilon_{\boldsymbol{p}}^{QP})t} \left(1 + \sum_{\boldsymbol{q}\nu}\zeta_{\boldsymbol{pq}\nu}^{\text{occ}} e^{-i\Delta_{\boldsymbol{q}\nu}^{\text{occ}}t} + \sum_{\boldsymbol{q}\nu}\zeta_{\boldsymbol{pq}\nu}^{\text{virt}} e^{-i\Delta_{\boldsymbol{q}\nu}^{\text{virt}}t} + \dots\right) \tag{2.31}$$

$$= -iZ_{\boldsymbol{p}}^{QP} \int_0^{\infty} dt\, e^{[-\eta+i(\omega-\epsilon_{\boldsymbol{p}}^{QP})t]} \tag{2.32}$$

$$- iZ_{\boldsymbol{p}}^{QP} \sum_{\boldsymbol{q}\nu}\zeta_{\boldsymbol{pq}\nu}^{\text{occ}} \int_0^{\infty} dt\, e^{[-\eta+i(\omega-\epsilon_{\boldsymbol{p}}^{QP}-\Delta_{\boldsymbol{q}\nu}^{\text{occ}})t]}$$

$$- iZ_{\boldsymbol{p}}^{QP} \sum_{\boldsymbol{q}\nu}\zeta_{\boldsymbol{pq}\nu}^{\text{virt}} \int_0^{\infty} dt\, e^{[-\eta+i(\omega-\epsilon_{\boldsymbol{p}}^{QP}-\Delta_{\boldsymbol{q}\nu}^{\text{virt}})t]} + \dots$$

$$= \frac{Z_{\boldsymbol{p}}^{QP}}{\omega-\epsilon_{\boldsymbol{p}}^{QP}+i\eta} + \sum_{\boldsymbol{q}\nu}\frac{Z_{\boldsymbol{p}}^{QP}\zeta_{\boldsymbol{pq}\nu}^{\text{occ}}}{\omega-\epsilon_{\boldsymbol{p}}^{QP}-\Delta_{\boldsymbol{q}\nu}^{\text{occ}}+i\eta} + \sum_{\boldsymbol{q}\nu}\frac{Z_{\boldsymbol{p}}^{QP}\zeta_{\boldsymbol{pq}\nu}^{\text{virt}}}{\omega-\epsilon_{\boldsymbol{p}}^{QP}-\Delta_{\boldsymbol{q}\nu}^{\text{virt}}+i\eta} + \dots \tag{2.33}$$

$$= \frac{Z_{\boldsymbol{p}}^{QP}}{\omega-\epsilon_{\boldsymbol{p}}^{QP}+i\eta} + \sum_{\boldsymbol{q}\nu}\frac{Z_{\boldsymbol{pq}\nu}^{\text{occ-sat}}}{\omega-\epsilon_{\boldsymbol{pq}\nu}^{\text{occ-sat}}+i\eta} + \sum_{\boldsymbol{q}\nu}\frac{Z_{\boldsymbol{pq}\nu}^{\text{virt-sat}}}{\omega-\epsilon_{\boldsymbol{pq}\nu}^{\text{virt-sat}}+i\eta} + \dots \tag{2.34}$$

where we define the satellite energies $\epsilon_{\boldsymbol{pq}\nu}^{\text{occ-sat}} = \epsilon_{\boldsymbol{p}}^{QP} + \Delta_{\boldsymbol{q}\nu}^{\text{occ}}$ and $\epsilon_{\boldsymbol{pq}\nu}^{\text{virt-sat}} = \epsilon_{\boldsymbol{p}}^{QP} + \Delta_{\boldsymbol{q}\nu}^{\text{virt}}$, as well as the satellite weights $Z_{\boldsymbol{pq}\nu}^{\text{occ-sat}} = Z_{\boldsymbol{p}}^{QP}\zeta_{\boldsymbol{pq}\nu}^{\text{occ}}$ and $Z_{\boldsymbol{pq}\nu}^{\text{virt-sat}} = Z_{\boldsymbol{p}}^{QP}\zeta_{\boldsymbol{pq}\nu}^{\text{virt}}$.

2.4.3 Spectral function

The spectral function is obtained as (the virtual satellites spectral function, whose derivation will mirror that of the occupied satellites, are omitted for the sake of brevity)

$$A^{GW+C}(\boldsymbol{p},\omega) = -\frac{1}{\pi}\operatorname{Im} G^{GW+C}(\boldsymbol{p},\omega) \tag{2.35}$$

$$= -\frac{1}{\pi}\operatorname{Im}\left[\frac{Z^{QP}_{\boldsymbol{p}}}{\omega-\epsilon^{QP}_{\boldsymbol{p}}+i\eta}+\sum_{\boldsymbol{q}\nu}\frac{Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}}{\omega-\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}+i\eta}+\dots\right] \tag{2.36}$$

$$= -\frac{1}{\pi}\operatorname{Im}\left[\frac{\operatorname{Re} Z^{QP}_{\boldsymbol{p}}+i\operatorname{Im} Z^{QP}_{\boldsymbol{p}}}{\omega-\operatorname{Re}\epsilon^{QP}_{\boldsymbol{p}}+i\left(\eta-\operatorname{Im}\epsilon^{QP}_{\boldsymbol{p}}\right)}+\sum_{\boldsymbol{q}\nu}\frac{\operatorname{Re} Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}+i\operatorname{Im} Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}}{\omega-\operatorname{Re}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}+i\left(\eta-\operatorname{Im}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)}+\dots\right] \tag{2.37}$$

$$= -\frac{1}{\pi}\operatorname{Im}\left[\frac{\left(\operatorname{Re} Z^{QP}_{\boldsymbol{p}}+i\operatorname{Im} Z^{QP}_{\boldsymbol{p}}\right)\left(\omega-\operatorname{Re}\epsilon^{QP}_{\boldsymbol{p}}-i\left(\eta-\operatorname{Im}\epsilon^{QP}_{\boldsymbol{p}}\right)\right)}{\left(\omega-\operatorname{Re}\epsilon^{QP}_{\boldsymbol{p}}\right)^2+\left(\operatorname{Im}\epsilon^{QP}_{\boldsymbol{p}}\right)^2}\right. \tag{2.38}$$

$$\left.+\sum_{\boldsymbol{q}\nu}\frac{\left(\operatorname{Re} Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}+i\operatorname{Im} Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)\left(\omega-\operatorname{Re}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}-i\left(\eta-\operatorname{Im}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)\right)}{\left(\omega-\operatorname{Re}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)^2+\left(\operatorname{Im}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)^2}+\dots\right] \tag{2.39}$$

$$= -\frac{1}{\pi}\left[\frac{\left(\operatorname{Re} Z^{QP}_{\boldsymbol{p}}\right)\left(\operatorname{Im}\epsilon^{QP}_{\boldsymbol{p}}\right)+\left(\operatorname{Im} Z^{QP}_{\boldsymbol{p}}\right)\left(\omega-\operatorname{Re}\epsilon^{QP}_{\boldsymbol{p}}\right)}{\left(\omega-\operatorname{Re}\epsilon^{QP}_{\boldsymbol{p}}\right)^2+\left(\operatorname{Im}\epsilon^{QP}_{\boldsymbol{p}}\right)^2}\right. \tag{2.40}$$

$$\left.+\sum_{\boldsymbol{q}\nu}\frac{\left(\operatorname{Re} Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)\left(\operatorname{Im}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)+\left(\operatorname{Im} Z^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)\left(\omega-\operatorname{Re}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)}{\left(\omega-\operatorname{Re}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)^2+\left(\operatorname{Im}\epsilon^{\text{occ-sat}}_{\boldsymbol{pq}\nu}\right)^2}+\dots\right] \tag{2.41}$$

Chapter 3

TDVP

We start with the definition of the action functional:

$$S = \int_{t_1}^{t_2} dt L(\psi, \bar{\psi}) \tag{3.1}$$

where Dirac took the Lagrangian as $L(\psi, \bar{\psi}) = \langle \psi(t) | i\frac{\partial}{\partial t} - H | \psi(t) \rangle$. It can be shown that taking arbitrary independent variations of S with respect to $|\psi\rangle$ and $\langle\psi|$ and demanding that the functional be stationary yields the time-dependent Schrödinger equation (and its complex conjugate). This Lagrangian is real if the wave function is normalized, but it is convenient to not habe this restriction, but in that case the Lagrangian becomes complex. To avoid this complication, we define a new real Lagrangian

$$L(\psi, \bar{\psi}) = \frac{i}{2} \frac{\langle \psi \mid \dot{\psi} \rangle - \langle \dot{\psi} \mid \psi \rangle}{\langle \psi \mid \psi \rangle} - \frac{\langle \psi | H | \psi \rangle}{\langle \psi \mid \psi \rangle} \tag{3.2}$$

Note that this knew Lagrangian reduces to the old one one the wave function is normalized. We can now derive the equations of motion obtained from requiring the action with the new Lagrangian L to be stationary,

$$0 = \delta S = \int \delta L dt = \int dt \left(\frac{1}{2} \frac{\{\langle \delta\psi \mid \dot{\psi} \rangle + \langle \psi \mid \delta\dot{\psi} \rangle - \langle \delta\dot{\psi} \mid \psi \rangle - \langle \dot{\psi} \mid \delta\psi \rangle\}}{\langle \psi \mid \psi \rangle} \right. \tag{3.3}$$

$$\left. - \frac{\delta\langle \psi | H | \psi \rangle}{\langle \psi \mid \psi \rangle} - \left(\frac{i}{2} \frac{\langle \psi \mid \dot{\psi} \rangle - \langle \dot{\psi} \mid \psi \rangle}{\langle \psi \mid \psi \rangle} - \frac{\langle \psi | H | \psi \rangle}{\langle \psi \mid \psi \rangle} \right) \frac{\delta\langle \psi \mid \psi \rangle}{\langle \psi \mid \psi \rangle} \right)$$

$$= \int dt \left(\frac{i\langle \delta\psi \mid \dot{\psi} \rangle - \langle \delta\psi | H | \psi \rangle}{\langle \psi \mid \psi \rangle} - \frac{\langle \psi | i\partial/\partial t - H | \psi \rangle}{\langle \psi \mid \psi \rangle^2} \langle \delta\psi \mid \psi \rangle \right) + \text{c.c.} \tag{3.4}$$

$$\implies \left(i\frac{\partial}{\partial t} - H \right) |\psi\rangle = \frac{\langle \psi | i\partial/\partial t - H | \psi \rangle}{\langle \psi \mid \psi \rangle} |\psi\rangle \tag{3.5}$$

Briefly, doing some integration by parts allowed us to go from the first to the second step, and then by assuming that the variations of the bra and cat can be arbitrary and independent we get the third equation. Now, if we tack on a time-dependent phase factor to the wave

function to get

$$|\phi(t)\rangle = |\psi(t)\rangle \exp\left[i\int^t d\tau \, \frac{\langle\psi|i\partial_\tau - H|\psi\rangle}{\langle\psi|\psi\rangle}\right] \tag{3.6}$$

it is normalized and satisfies the TDSE. [1] So we have shown that this new Lagrangian formulation allows us to work with wave functions that are not normalized and can differ by a phase.

[1] We can start by computing the time derivative as

$$i\frac{\partial}{\partial t}|\phi\rangle = i\frac{\partial}{\partial t}\Big(|\psi\rangle\, e^{i\int^t \frac{\langle\psi|i\partial_\tau - H|\psi\rangle}{\langle\psi|\psi\rangle}d\tau}\Big) \tag{3.7}$$

$$= i(\partial_t|\psi\rangle)e^{i\int^t\cdots} + |\psi\rangle \underbrace{i\partial_t e^{i\int^t\cdots}}_{-\frac{\langle\psi|i\partial_t - H|\psi\rangle}{\langle\psi|\psi\rangle}e^{i\int^t\cdots}} \tag{3.8}$$

$$= e^{i\int^t\cdots}\left[i\partial_t|\psi\rangle - \frac{\langle\psi|i\partial_t - H|\psi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle\right] \tag{3.9}$$

$$= e^{i\int^t\cdots}[H|\psi\rangle] = H|\phi\rangle \tag{3.10}$$

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