Expanding model

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1 Second quantization

Fermionic many-body quantum states are described by Slater determinants catching the antisymmetric nature of the fermions. Let as an example:

$$\Psi(q_1, q_2, ..., q_N) = \sqrt{N!}\mathcal{A}\prod_{i=1}^{N}\psi_i(q_i) = \frac{1}{\sqrt{N!}}\sum_{p\in\mathcal{P}_N}(-1)^p\prod_{i=1}^{N}\psi_{p(i)}(q_i) \equiv |\psi_1\cdots\psi_N| \tag{1}$$

where $\phi_i(j)$ is the j-th electron occupying the i-th orbital of some orthogonal basis and $\mathcal{P}_N$ is the group of permutations between N elements. Here also we have introduced the antisymmetrization operator, which transforms a simple product of wave functions[1] into a Slater determinant. This exhibits the following properties.

- The application of $\mathcal{A}$ over an Slater determinant is giving the same since an Slater determinant is already an antisymmetric function, so $\mathcal{A}^2 = \mathcal{A}$.
- Since Slater determinant has not any coefficient with imaginary part $\mathcal{A}$ is a purely real operator, so $\mathcal{A}^\dagger = \mathcal{A}$.
- Physical operators are even under permutations, so them commute with $\mathcal{A}$ which is odd under permutations.

In second quantization we start with vacuum, $|0\rangle$ and we can put particles on the system at some state, say μ, using the creation operators: $c_\mu^\dagger$ applied over vacuum, $c_\mu^\dagger|0\rangle = |0, ..., n_\mu = 1, ...\rangle$, which is the state with one particle in state μ. This is named number of occupation representation. The particles can be removed by the annihilation operators c_μ. In the case of fermions we have the following anti-commutation relations:

$$\{c_\mu, c_\nu\} = 0 \quad \{c_\mu^\dagger, c_\nu^\dagger\} = 0 \quad \{c_\mu, c_\nu^\dagger\} = \delta_{\mu\nu} \tag{2}$$

so consequently $c_\mu^\dagger c_\mu^\dagger = -c_\mu^\dagger c_\mu^\dagger = 0$, which is the Pauli exclusion principle. With this formalism we can simply express the many-body states with a product between some creation operators applied over vacuum.

$$|\Psi\rangle = \left(\prod_{i=1}^{N} c_{\mu_i}^\dagger\right)|0\rangle \tag{3}$$

1.1 Wick's theorem

In order to simplify the algebraic manipulations in this formalism we can use the Wick's theorem.

First of all we have to define the "normal order" of a product of creation and annihilation operators. This stablish that all annihilation operators go to the right and creation operators to the left. To put an example guess $A = c_1 c_2^\dagger c_3$, so $:A: = :c_1 c_2^\dagger c_3: = -c_2^\dagger c_1 c_3$. This is useful because the expected value of any normal ordered operator respect to the vacuum is 0.

Now we can define the contraction between A and B as

$$\overbrace{AB} = AB - :AB: \tag{4}$$

where it is easy to see that $\overbrace{c_\mu c_\nu^\dagger} = \delta_{\mu\nu}$ meanwhile $\overbrace{c_\mu c_\nu} = \overbrace{c_\mu^\dagger c_\nu} = \overbrace{c_\mu^\dagger c_\nu^\dagger} = 0$.

Finally we can announce the theorem: a second quantized operator A with $2N$ annihilation and creation operators is equivalent to the sum of all possible combinations with $0, 1, 2, ..., N$ contractions in normal order.

$$A = \sum_{n=0}^{N} :A^{\bar{n}}: \tag{5}$$

[1] A product of wave functions is introducing distinguishably on the particles.

Here $A^{\bar{n}}$ means the sum of all possible combinations with n contractions of operator A. Look now that expected value is very simple to compute: $\langle 0|A|0\rangle = A^{\bar{N}}$. As all normal ordered operators have null expected value only the terms with N contractions remain. Also as those terms have all operators contracted the concept of normal ordering can be forbidden.

1.1.1 Time dependent Wick's theorem

The contraction between two time dependent annihilation/creation operators now involve time-ordering operator $\mathcal{T}$.

$$\mathcal{T}\left[A(t)B(t')\right] = \Theta(t-t')A(t)B(t') \pm \Theta(t'-t)B(t')A(t) \tag{6}$$

Here $+$ is for bosons and $-$ is for fermions (on this work we deal with fermions) and $\Theta(t) = 1$ for $t \geq 0$; 0 for $t < 0$ is the Heaviside function.

$$\overbrace{A(t)B}(t') = \mathcal{T}\left[A(t)B(t')\right] - :A(t)B(t'): \tag{7}$$

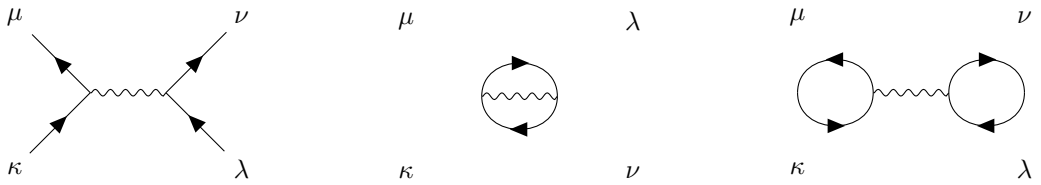
It is easy to see that the contractions between two annihilation or two creation operators will be null meanwhile a "mixed" contraction is not necessary null. The diagramatic representation of this contractions is to join the lines of the two contracted operators. As example we show in Fig.1 the contractions $\overbrace{c_\mu^\dagger c_\nu^\dagger c_\lambda} c_\kappa$ (1b) and $\overbrace{c_\mu^\dagger c_\nu^\dagger c_\lambda c_\kappa}$ (1c).

This version of the theorem says that, being A an operator product of $2N$ annihilation and/or creation operators

$$\mathcal{T}[A] = \sum_{n=0}^{N} :A^{\bar{n}}: \tag{8}$$

so the computation of the time-ordered expected value of this operator becomes into the sum of all fully contracted terms.

$$\langle \mathcal{T}[A] \rangle = A^{\bar{N}} \tag{9}$$



(a) (b) (c)

Figure 1: Feynman diagrams for: a) Two electron interaction $c_\mu^\dagger c_\nu^\dagger c_\lambda c_\kappa$, b),c) The two possible full contracted term

1.2 One-body operators

One body operators are defined as the sum of one-particle operators.

$$F(q_1, ..., q_N) = \sum_i f_i \tag{10}$$

Now, applying the properties of $\mathcal{A}$ we can compute the matrix element between two Slater determinants.

$$\begin{aligned} \langle \Phi|F|\Psi\rangle &= \sum_i \sum_{p\in\mathcal{P}_N} (-1)^p \int \cdots \int \left(\prod_j \phi_j^*(q_j)\right) f_i \left(\prod_k \psi_{p(k)}(q_k)\right) \mathrm{d}q_1 \cdots \mathrm{d}q_N \\ &= (-1)^{p'} \sum_i \int \cdots \int \left(\prod_{l\neq i} \phi_l^*(q_l)\psi_{p'(l)}(q_l)\right) \phi_i^*(q_i) f_i \psi_{p'(i)}(q_i) \mathrm{d}q_1 \cdots \mathrm{d}q_N \end{aligned} \tag{11}$$

By orthogonality there is only one permutation, p' that does not vanish. Also Φ and Ψ can only differ in an most one wave-function.

In second quantization the one-body operators can be interpreted as the action to annihilate a particle in state ν and create one in state μ weighted by the corresponding matrix element.

$$F = \sum_{\mu,\nu} f^{\mu}_{\nu} c^{\dagger}_{\mu} c_{\nu} \tag{12}$$

$$f^{\mu}_{\nu} = \int \psi^{*}_{\mu}(q) f \psi_{\nu}(q) \mathrm{d}q \tag{13}$$

We can check the matrix element of this operator between two many body states[2].

$$\langle 0| \sum_{\mu,\nu} c_{\alpha_1} \cdots c_{\alpha_N} c^{\dagger}_{\mu} c_{\nu} c^{\dagger}_{\beta_N} \cdots c^{\dagger}_{\beta_1} |0\rangle f^{\mu}_{\nu} = \sum_{\mu,\nu} f^{\mu}_{\nu} \sum_{p \in \mathcal{P}_N} (-1)^p \sum_i \delta^{\mu}_{\alpha_i} \delta^{\beta_{p(i)}}_{\nu} \prod_{l \neq i} \delta^{\beta_{p(l)}}_{\alpha_l} \tag{14}$$

This can be proved by a simple application of Wick's theorem taking into account that only for one index permutation the contractions do not vanish.

1.3 Two-body operators

In this case we define our operator as:

$$G(q_1, ..., q_N) = \sum_{i<j} g_{ij} \tag{15}$$

and we can compute the matrix element as in the case of one-body operators.

$$\begin{aligned} \langle \Phi | G | \Psi \rangle &= \sum_{i<j} \sum_{p \in \mathcal{P}_N} \int \cdots \int \left(\prod_{k=1}^{N} \phi^{*}_{k}(q_k) \right) g_{ij} \left(\prod_{l=1}^{N} \psi_{p(l)}(q_l) \right) \mathrm{d}q_1 \cdots \mathrm{d}q_N \\ &= (-1)^{p'} \sum_{i<j} \int \cdots \int \left(\prod_{k \neq i,j} \phi^{*}_{k}(q_k) \psi_{p'(k)}(q_k) \right) \phi^{*}_{i}(q_i) \phi^{*}_{j}(q_j) g_{ij} \times \\ &\qquad \times \left[\psi_{p'(i)}(q_i) \psi_{p'(j)}(q_j) - \psi_{p'(i)}(q_j) \psi_{p'(j)}(q_i) \right] \mathrm{d}q_1 \cdots \mathrm{d}q_N \end{aligned} \tag{16}$$

Now there are two permutations that allow this integral to not vanish, p' and $p'T_{ij}$ where T_{ij} is the transposition between i, j. Also Φ and Ψ can differ at most by two wave-functions.

In second quantization it is translated to destroy two particles at states λ, κ and create other two at states μ, ν weighted by the matrix element $g^{\mu\nu}_{\lambda\kappa}$.

$$G = \frac{1}{2} \sum_{\mu,\nu} \sum_{\lambda,\kappa} g^{\mu\nu}_{\lambda\kappa} c^{\dagger}_{\mu} c^{\dagger}_{\nu} c_{\kappa} c_{\lambda} \tag{17}$$

$$g^{\mu\nu}_{\lambda\kappa} = \int \int \psi^{*}_{\mu}(q_1) \psi^{*}_{\nu}(q_2) g_{12} \psi_{\lambda}(q_1) \psi_{\kappa}(q_2) \mathrm{d}q_1 \mathrm{d}q_2 \tag{18}$$

Look that a factor 1/2 is added since $g^{\mu\nu}_{\lambda\kappa} = g^{\nu\mu}_{\kappa\lambda}$. The matrix element between two many-body states are:

$$\begin{aligned} &\frac{1}{2} \langle 0| \sum_{\substack{\mu,\nu \\ \lambda,\kappa}} c_{\alpha_1} \cdots c_{\alpha_N} c^{\dagger}_{\mu} c^{\dagger}_{\nu} c_{\kappa} c_{\lambda} c^{\dagger}_{\beta_N} \cdots c^{\dagger}_{\beta_1} |0\rangle g^{\mu\nu}_{\lambda\kappa} \\ &\qquad = \frac{1}{2} \sum_{\substack{\mu,\nu \\ \lambda,\kappa}} g^{\mu\nu}_{\lambda\kappa} \sum_{p \in \mathcal{P}_N} (-1)^p \sum_{i,j} \delta^{\mu}_{\alpha_i} \delta^{\nu}_{\alpha_j} \left[\delta^{\beta_{p(i)}}_{\lambda} \delta^{\beta_{p(j)}}_{\kappa} - \delta^{\beta_{p(i)}}_{\kappa} \delta^{\beta_{p(j)}}_{\lambda} \right] \prod_{k \neq i,j} \delta^{\beta_{p(k)}}_{\alpha_k} \end{aligned} \tag{19}$$

It is easy to see that this only is kept by two permutations (you can interchange α by β and λ by κ at the same time).

1.4 Schrödinger and Heisenberg pictures

Schrödinger picture of quantum mechanics is the one where the quantum states are evolving in time meanwhile operators are kept constant. This is hold by Schrödinger equation

$$\imath \partial_t |\psi(t)\rangle = \mathcal{H} |\psi(t)\rangle \tag{20}$$

[2]Recall that the Kronecker's delta holds: $\delta^{j}_{i} = \int \psi^{*}_{i}(q) \psi_{j}(q) \mathrm{d}q$

which describes the time evolution of a quantum state in function of the hamiltonian of the system. Then, the expected value of an operator depends on time because the quantum states depend on time.

$$\langle A(t)\rangle = \langle\psi(t)|A|\psi(t)\rangle = \int \psi^*(q,t)A(q)\psi(q,t)\mathrm{d}q \tag{21}$$

In second quantization Schrödinger picture is awful since vacuum evolving in time does make no sense. It is more comfortable to work with operators that evolve in time and constant states, the named Heisenberg picture. To do this let's define, in Schrödinger picture, the temporal evolution of a state as $|\psi(t)\rangle = U(t)|\psi\rangle$, being $|\psi\rangle = |\psi(t=0)\rangle$ and U the time evolution operator. Introducing this into the Schrödinger equation $\imath\partial_t U(t) = \mathcal{H}U(t)$ and taking into account the initial condition $U(0) = \mathbb{I}$ which is trivial by definition we can make a Taylor expansion of $U(t)$ taking into account that $\partial_t^n U(t) = (-\imath\mathcal{H})^n U(t)$ (this can be proofed by induction).

$$U(t) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\partial_t^n U(t=0)\right) t^n = \sum_{n=0}^{\infty} \frac{(-\imath)^n}{n!}\mathcal{H}^n t^n = \mathrm{e}^{-\imath\mathcal{H}t} \tag{22}$$

Now from the expected value of an operator we can take its temporal evolution on Heisenberg picture: $A(t) = U^\dagger(t)AU(t)$.

$$\langle A(t)\rangle = \langle\psi|U^\dagger(t)AU(t)|\psi\rangle = \langle\psi|A(t)|\psi\rangle \tag{23}$$

Also we can take the Schrödinger equation in Heisenberg picture: $\partial_t A(t) = \imath[\mathcal{H}, A](t)$.

$$\imath\partial_t A(t) = \imath\left(\partial_t U^\dagger(t)\right)AU(t) + U^\dagger(t)A\left(\partial_t U(t)\right) = -U^\dagger(t)\left(\mathcal{H}A + A\mathcal{H}\right)U(t) = -[\mathcal{H}, A](t) \tag{24}$$

Now let a hamiltonian

$$\mathcal{H} = \sum_{i,j}\varepsilon_j^i c_i^\dagger c_j + \frac{1}{2}\sum_{\substack{i,j\\k,l}} v_{kl}^{ij} c_i^\dagger c_j^\dagger c_l c_k \tag{25}$$

and compute the temporal evolution of c_μ. For this we should take a look how commutation behaves.

$$[c_i^\dagger c_j, c_\mu] = -\{c_i^\dagger, c_\mu\}c_j = -\delta_{i\mu}c_j \tag{26}$$

$$[c_i^\dagger c_j^\dagger c_l c_k, c_\mu] = [c_i^\dagger c_j^\dagger, c_\mu]c_l c_k = \left(\delta_{j\mu}c_i^\dagger - \delta_{i\mu}c_j^\dagger\right)c_l c_k \tag{27}$$

Let's write the final solution as

$$c_\mu(t) = \sum_\nu a_\nu^\mu(t)c_\nu \tag{28}$$

and following the Schrödinger equation

$$\dot{c}_\mu(t) = \imath\sum_j \varepsilon_j^\mu c_j(t) + \frac{\imath}{2}\sum_{i,k,l}\left(v_{kl}^{i\mu} - v_{kl}^{\mu i}\right)c_i^\dagger(t)c_l(t)c_k(t) \tag{29}$$

1.5 Basis change and field operators

In first quantization, where quantum states are vectors of Hilbert space, from a given basis $\{|\xi_i\rangle, i = 1, ..., n\}$ the identity can be defined as

$$\mathbb{I} = \sum_{i=1}^{n}|\xi_i\rangle\langle\xi_i| \tag{30}$$

which can be easily checked by applying it over some general state $|\psi\rangle = \sum_j \langle\xi_j|\psi\rangle|\xi_j\rangle$:

$$\sum_{i=1}^{n}|\xi_i\rangle\langle\xi_i|\psi\rangle = \sum_{i,j}\langle\xi_i|\xi_j\rangle\langle\xi_j|\psi\rangle|\xi_i\rangle = \sum_{i,j}\delta_j^i\langle\xi_j|\psi\rangle|\xi_i\rangle = \sum_j\langle\xi_j|\psi\rangle|\xi_j\rangle = |\psi\rangle \tag{31}$$

Now let define a new basis $\{|\mu_i\rangle, i = 1, ..., n\}$. If one would transit from ξ basis to μ basis introduce the identity is a good tool. Let's do it with $|\psi\rangle$:

$$\begin{aligned} |\psi\rangle &= \sum_i \langle\xi_i|\psi\rangle \left(\sum_j |\mu_j\rangle\langle\mu_j|\right)|\xi_i\rangle = \sum_j \left(\sum_i \langle\xi_i|\psi\rangle\langle\mu_j|\xi_i\rangle\right)|\mu_j\rangle \\ &= \sum_j \langle\mu_j| \left(\sum_i |\xi_i\rangle\langle\xi_i|\right)|\psi\rangle|\mu_j\rangle = \sum_j \langle\mu_j|\psi\rangle|\mu_j\rangle \end{aligned} \tag{32}$$

In vector language we can identify the change basis matrix elements $D_i^j = \langle\mu_j|\xi_i\rangle$ being $D^\dagger$[3] the matrix that goes from ξ basis to μ basis.

$$|\mu_j\rangle = \sum_i (D_i^j)^* |\xi_i\rangle = \sum_i \langle\xi_i|\mu_j\rangle|\xi_i\rangle \tag{33}$$

In second quantization the one-particle states are written as the creation operator over the vacuum: $|\mu_j\rangle = c_{\mu_j}^\dagger|0\rangle$ and $|\xi_i\rangle = c_{\xi_i}^\dagger|0\rangle$; so the basis change is performed in the same way.

$$c_{\mu_j}^\dagger = \sum_i (D_i^j)^* c_{\xi_i}^\dagger = \sum_i \langle\xi_i|\mu_j\rangle c_{\xi_i}^\dagger \qquad c_{\mu_j} = \sum_i D_i^j c_{\xi_i} = \sum_i \langle\mu_j|\xi_i\rangle c_{\xi_i} \tag{34}$$

Now we can recall that states $|\mathbf{x}\rangle$ are the eigenstates of position operator, and by construction of quantum mechanics the wave function of an state can be defined as $\psi(\mathbf{x}) = \langle\mathbf{x}|\psi\rangle$[4]. It allows us to define the field operators, not more that operators that create/annihilate a particle in some position.

$$\Psi^\dagger(\mathbf{x}) = \sum_i \psi_{\xi_i}^*(\mathbf{x}) c_{\xi_i}^\dagger \qquad \Psi(\mathbf{x}) = \sum_i \psi_{\xi_i}(\mathbf{x}) c_{\xi_i} \tag{35}$$

Look that creation/annihilation operators can be recovered integrating the field operators over all space.

$$c_{\xi_i}^\dagger = \int \Psi^\dagger(\mathbf{x})\psi_{\xi_i}(\mathbf{x})\mathrm{d}\mathbf{x} \qquad c_{\xi_i} = \int \Psi(\mathbf{x})\psi_{\xi_i}^*(\mathbf{x})\mathrm{d}\mathbf{x} \tag{36}$$

Finally this operators can evolve in time taking into account the Heisenberg picture.

$$\Psi(\mathbf{x}, t) = \mathrm{e}^{\imath\mathcal{H}t}\Psi(\mathbf{x})\mathrm{e}^{-\imath\mathcal{H}t} \tag{37}$$

Using the field operators we can write a new representation for one-body operators

$$F = \int \sum_{\mu,\nu} \psi_\mu^*(\mathbf{x}) f \psi_\nu(\mathbf{x}) c_\mu^\dagger c_\nu \mathrm{d}\mathbf{x} = \int \sum_\mu \left(\psi_\mu^*(\mathbf{x}) c_\mu^\dagger\right) f \sum_\nu \left(\psi_\nu(\mathbf{x}) c_\nu\right) \mathrm{d}\mathbf{x} = \int \Psi^\dagger(\mathbf{x}) f \Psi(\mathbf{x}) \mathrm{d}\mathbf{x} \tag{38}$$

and by extension two-body operators can also be rewritten.

$$G = \int \Psi^\dagger(\mathbf{x}_1)\Psi^\dagger(\mathbf{x}_2) g_{12} \Psi(\mathbf{x}_2)\Psi(\mathbf{x}_1) \mathrm{d}\mathbf{x}_1 \mathrm{d}\mathbf{x}_2 \tag{39}$$

1.5.1 Momentum space

Working with homogeneous systems should be useful use the annihilation/creation operators at momentum space. Compute them would require a Fourier transform and the corresponding anti-transform:

$$\Psi^\dagger(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}^\dagger \qquad \Psi(\mathbf{x}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}} \tag{40}$$

$$a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \int \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{x}} \Psi^\dagger(\mathbf{x}) \mathrm{d}\mathbf{x} \qquad a_{\mathbf{k}} = \frac{1}{\sqrt{N}} \int \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{x}} \Psi(\mathbf{x}) \mathrm{d}\mathbf{x} \tag{41}$$

[3] In Hilbert space basis change matrices are unitary, this is $D^\dagger = D^{-1}$.

[4] Wave-function tells us about the probability to find a particle on some state in some position meanwhile the inner product tells us about the probability to measure some observable eigenvalue associated to its eigenstate of a particle being in its own quantum state.

In case of discrete translation symmetry (lattice) momentum space operators can be defined

$$c_i^\dagger = \int \Psi^\dagger(\mathbf{x})\psi_i(\mathbf{x})\mathrm{d}\mathbf{x} = \int \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}^\dagger \psi_i(\mathbf{x})\mathrm{d}\mathbf{x} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}}^\dagger \tag{42a}$$

$$c_i = \int \Psi(\mathbf{x})\psi_i^*(\mathbf{x})\mathrm{d}\mathbf{x} = \int \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}} \psi_i^*(\mathbf{x})\mathrm{d}\mathbf{x} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}} \tag{42b}$$

Here $c_i^{(\dagger)}$ are the lattice site operator and $\psi_i(\mathbf{x}) \approx \delta(\mathbf{x}-\mathbf{R}_i)$. With this we can compute the anti-transform

$$a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}}\sum_i \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{R}_i} c_i^\dagger \qquad a_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_i \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{R}_i} c_i \tag{43}$$

The quantum operators can also be defined in momentum space. For one-body operators

$$F = \frac{1}{N}\int \sum_{\mathbf{k},\mathbf{k}'} \mathrm{e}^{\imath(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} a_{\mathbf{k}}^\dagger f(\mathbf{x}) a_{\mathbf{k}'}\mathrm{d}\mathbf{x} = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} f_{\mathbf{q}} \sum_{\mathbf{k}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}} \tag{44}$$

where after doing variable change $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ we have defined

$$f_{\mathbf{q}} = \frac{1}{\sqrt{N}}\int \mathrm{e}^{-\imath\mathbf{q}\cdot\mathbf{x}} f(\mathbf{x})\mathrm{d}\mathbf{x} \tag{45}$$

Similarly, for two-body operators

$$G = \frac{1}{N^2}\int\int \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \mathrm{e}^{\imath[(\mathbf{k}_3-\mathbf{k}_1)\cdot\mathbf{x}_1+(\mathbf{k}_4-\mathbf{k}_2)\cdot\mathbf{x}_2]} a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger g_{12} a_{\mathbf{k}_4} a_{\mathbf{k}_3}\mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_2 \tag{46}$$

For the case $g_{12} = g(\mathbf{x}_1 - \mathbf{x}_2) = g(\mathbf{r})$

$$G = \frac{1}{N^2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \int \mathrm{e}^{\imath(\mathbf{k}_3-\mathbf{k}_1)\cdot\mathbf{r}} g(\mathbf{r})\mathrm{d}\mathbf{r} \int \mathrm{e}^{\imath(\mathbf{k}_1+\mathbf{k}_4-\mathbf{k}_2-\mathbf{k}_3)\cdot\mathbf{x}_2} a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger a_{\mathbf{k}_4} a_{\mathbf{k}_3}\mathrm{d}\mathbf{x}_2 \tag{47}$$

and doing the variable change $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_3$ the second integral forces $\mathbf{k}_4 - \mathbf{k}_2 = \mathbf{q}$

$$G = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} g_{\mathbf{q}} \sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}} \tag{48}$$

1.5.2 Multiorbital lattice in momentum space

The general Hamiltonian for this model is

$$\mathcal{H} = \sum_{i,j}\sum_{\mu,\nu}\left[\delta_j^i \varepsilon_\nu^\mu - t_{j\nu}^{i\mu}\right] c_{i\mu}^\dagger c_{j\nu} + \sum_i \sum_{\mu,\nu,\lambda,\kappa} v_{\lambda\kappa}^{\mu\nu} c_{i\mu}^\dagger c_{i\nu}^\dagger c_{i\kappa} c_{i\lambda} \tag{49}$$

The quadratic part, $\mathcal{H}_0$, conformed by a local potential term and a hopping kinetic term, can be transformed into momentum space

$$\begin{aligned}
\mathcal{H}_0 &= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{i,j}\sum_{\mu,\nu} \mathrm{e}^{\imath(\mathbf{k}'\cdot\mathbf{R}_j - \mathbf{k}\cdot\mathbf{R}_i)}\left[\delta_j^i\varepsilon_\nu^\mu - t_{j\nu}^{i\mu}\right] a_{\mathbf{k}\mu}^\dagger a_{\mathbf{k}'\nu} \\
&= \frac{1}{N}\sum_{\mathbf{k},\mathbf{q}}\sum_{i,j}\sum_{\mu,\nu} \mathrm{e}^{-\imath(\mathbf{q}\cdot\mathbf{R}_j - \mathbf{k}\cdot\mathbf{r}_{ij})}\left[\delta_j^i\varepsilon_\nu^\mu - t_{j\nu}^{i\mu}\right] a_{\mathbf{k}\mu}^\dagger a_{\mathbf{k}-\mathbf{q}\nu} \\
&= \sum_{\mathbf{k}}\sum_{\mu,\nu} \epsilon_\nu^\mu(\mathbf{k}) a_{\mathbf{k}\mu}^\dagger a_{\mathbf{k}\nu}
\end{aligned} \tag{50}$$

Here we make the variable changes $\mathbf{r}_{ij} = \mathbf{R}_j - \mathbf{R}_i$ and $\mathbf{q} = \mathbf{k} - \mathbf{k}'$. Also, because of discrete translational symmetry the unique term of sum over $\mathbf{q}$ which is non-zero is $\mathbf{q} = 0$. Finally the momentum matrix element of the quadratic Hamiltonian is defined as

$$\epsilon_\nu^\mu(\mathbf{k}) = \varepsilon_\nu^\mu - \frac{1}{N}\sum_{i,j} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}_{ij}} t_{j\nu}^{i\mu} \tag{51}$$

The interaction part, $\mathcal{H}'$, which is purely local, is transformed like this

$$\begin{aligned}\mathcal{H}' &= \frac{1}{N^2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\sum_i\sum_{\mu,\nu,\lambda,\kappa} \mathrm{e}^{\imath(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{R}_i} v^{\mu\nu}_{\lambda\kappa} a^\dagger_{\mathbf{k}_1\mu} a^\dagger_{\mathbf{k}_2\nu} a_{\mathbf{k}_4\kappa} a_{\mathbf{k}_3\lambda} \\ &= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\mu,\nu,\lambda,\kappa} v^{\mu\nu}_{\lambda\kappa} a^\dagger_{\mathbf{k}+\mathbf{q}\mu} a^\dagger_{\mathbf{k}'-\mathbf{q}\nu} a_{\mathbf{k}'\kappa} a_{\mathbf{k}\lambda} \\ &= \sum_{\mathbf{q}} v^{\mu\nu}_{\lambda\kappa}(\mathbf{q}) \sum_{\mathbf{k},\mathbf{k}'}\sum_{\mu,\nu,\lambda,\kappa} a^\dagger_{\mathbf{k}+\mathbf{q}\mu} a^\dagger_{\mathbf{k}'-\mathbf{q}\nu} a_{\mathbf{k}'\kappa} a_{\mathbf{k}\lambda}\end{aligned} \tag{52}$$

where we can see that this interaction tensor is a constant on momentum space

$$v^{\mu\nu}_{\lambda\kappa}(\mathbf{q}) = \frac{v^{\mu\nu}_{\lambda\kappa}}{N} \tag{53}$$

2 Quantum Green's function

2.1 Classical Green's function

In a classical sense the Green's function $G(\mathbf{x})$ of some differential operator $\mathcal{L}$ is the potential created by a punctual source (represented by a Dirac's delta $\delta(\mathbf{x})$).

$$\mathcal{L}\left[G(\mathbf{x})\right] = \delta(\mathbf{x}) \tag{54}$$

The idea is that if you know a source $q(\mathbf{x})$ which creates a potential $V(\mathbf{x})$ and both are related by the same differential equation

$$\mathcal{L}\left[V(\mathbf{x})\right] = q(\mathbf{x}) \tag{55}$$

it is not necessary to solve this complicated differential equation. Look that one of the properties of the convolution[5] is that $(q * \delta)(\mathbf{x}) = q(\mathbf{x})$ so $V(\mathbf{x}) = (q * G)(\mathbf{x})$:

$$q(\mathbf{x}) = \int_{\mathcal{K}} q(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})\mathrm{d}\mathbf{y} = \int_{\mathcal{K}} q(\mathbf{y})\mathcal{L}\left[G(\mathbf{x}-\mathbf{y})\right]\mathrm{d}\mathbf{y} = \mathcal{L}\left[\int_{\mathcal{K}} q(\mathbf{y})G(\mathbf{x}-\mathbf{y})\mathrm{d}\mathbf{y}\right] = \mathcal{L}\left[V(\mathbf{x})\right] \tag{56}$$

2.2 Green's function expansion and Dyson equation

In quantum mechanics we deal with the Schrödinger equation.

$$\imath\partial_t\Psi(\mathbf{x},t) = \mathcal{H}\Psi(\mathbf{x},t) \tag{57}$$

This is a quite different case because the "source" and the "potential" are the same thing. In Dirac notation a spatial function can be written as $\Psi(\mathbf{x},t) = \langle\mathbf{x}|\Psi(t)\rangle$ using $|\mathbf{x}\rangle$ as a basis of a continuous Hilbert space, so recalling the time evolution and introducing the identity[6] operator:

$$\Psi(\mathbf{x},t) = \langle\mathbf{x}|\mathrm{e}^{-\imath\mathcal{H}(t-t')}|\Psi(t')\rangle = \int_{\mathbb{R}^3}\langle\mathbf{x}|\mathrm{e}^{-\imath\mathcal{H}(t-t')}|\mathbf{x}'\rangle\Psi(\mathbf{x}',t')\mathrm{d}\mathbf{x}' = \imath\int_{\mathbb{R}^3} G(\mathbf{x},\mathbf{x}';t-t')\Psi(\mathbf{x}',t')\mathrm{d}\mathbf{x}' \tag{58}$$

we have defined the quantum Green's function as a quantum propagator. In order to make explicit this interpretation as a propagator we introduce the causality by Heaviside function.

$$G(\mathbf{x},\mathbf{x}';t-t') = -\imath\Theta(t-t')\langle\mathbf{x}|\mathrm{e}^{-\imath\mathcal{H}(t-t')}|\mathbf{x}'\rangle \tag{59}$$

Now, taking into account

$$\Theta(t) = -\frac{1}{\imath 2\pi}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\imath\omega t}}{\omega+\imath\eta}\mathrm{d}\omega \tag{60}$$

[5] $(f*g)(\mathbf{x}) = \int_{\mathcal{K}} f(\mathbf{y})g(\mathbf{x}-\mathbf{y})\mathrm{d}\mathbf{y}$ being $\mathcal{K}$ all the vector space (real numbers, complex numbers, 3D space, space-time,...)

[6] For discrete space $\mathbb{I} = \sum_n |n\rangle\langle n|$ meanwhile for continuous space $\mathbb{I} = \int_{\mathbb{R}^3}|\mathbf{x}\rangle\langle\mathbf{x}|\mathrm{d}\mathbf{x}$

we can represent the Green's function in frequency space introducing the identity with the Hamiltonian eigenstates $|n\rangle$.

$$\begin{aligned} G(\mathbf{x},\mathbf{x}';t-t') &= -\frac{1}{\imath 2\pi}\int_{-\infty}^{\infty}\langle\mathbf{x}|\frac{\mathrm{e}^{-\imath(\omega+\mathcal{H})(t-t')}}{\omega+\imath\eta}|\mathbf{x}'\rangle\mathrm{d}\omega \\ &= -\frac{1}{\imath 2\pi}\int_{-\infty}^{\infty}\sum_n\frac{\langle\mathbf{x}|n\rangle\langle n|\mathbf{x}'\rangle}{\omega+\imath\eta}\mathrm{e}^{-\imath(\omega+\omega_n)(t-t')}\mathrm{d}\omega \end{aligned} \tag{61}$$

By a variable change and generalizing for all basis, not only spatial basis, we can take the Green's function in frequency space.

$$G_{\mu\nu}(\omega) = \sum_n\frac{\langle\mu|n\rangle\langle n|\nu\rangle}{\omega-\omega_n+\imath\eta} = \langle\mu|\frac{1}{\omega-\mathcal{H}+\imath\eta}|\nu\rangle \tag{62}$$

2.2.1 Dyson equation

Let split the Hamiltonian $\mathcal{H}=\mathcal{H}_0+\mathcal{W}$ being $\mathcal{W}$ some external field part. Look that we can identify two Green's operators.

$$G_0 = \frac{1}{\omega-\mathcal{H}_0+\imath\eta} \tag{63a}$$

$$G = \frac{1}{\omega-\mathcal{H}+\imath\eta} \tag{63b}$$

Taking profit of the following identity

$$\frac{1}{A-B} = \frac{1}{A}+\frac{1}{A}B\frac{1}{A-B} \tag{64}$$

we can see that

$$G = G_0+G_0\mathcal{W}G \tag{65}$$

which is the Dyson equation and can be expanded indefinitely.

$$\begin{aligned} G &= G_0+G_0\mathcal{W}G_0+G_0\mathcal{W}G_0\mathcal{W}G = \cdots = G_0\sum_{n=0}^{\infty}(\mathcal{W}G_0)^n \\ &= G_0+G_0\left[\mathcal{W}\sum_{n=0}^{\infty}(G_0\mathcal{W})^n\right]G_0 = G_0+G_0\tilde{\Sigma}G_0 \end{aligned} \tag{66}$$

Here we have find the improper (reducible) self-energy $\tilde{\Sigma}$.

2.3 Many-body finite temperature Green's function

Since now we have defined the Green's function for one-body zero temperature quantum physics. First of all, to generalize to a many-body we can follow the interpretation as a quantum propagator to define the zero temperature Green's function.

$$G_{\mu\nu}(t,t') = -\imath\Theta(t-t')\langle\Psi_0|c_\mu(t)c_\nu^\dagger(t')|\Psi_0\rangle+\imath\Theta(t'-t)\langle\Psi_0|c_\nu^\dagger(t')c_\mu(t)|\Psi_0\rangle = -\imath\langle\Psi_0|\mathcal{T}[c_\mu(t)c_\nu^\dagger(t')]|\Psi_0\rangle \tag{67}$$

Here $|\Psi_0\rangle$ is the ground state of the system and $\mathcal{T}$ is the time ordering operator which reorders the operators from greater time to lesser time respecting the commutation rules for bosons/fermions (in this case we thread with fermions). This last expression has two terms: the first one, for $t>t'$ creates a particle on ν state at time t' in the ground state and annihilates a particle on μ state in time t to finally projects the ground state to the result, and the second term, for $t<t'$ first annihilates at μ state at time t and then creates at ν state at time t'. This is we have the probability amplitude to propagate a particle from state ν to state μ and propagate a hole form state μ to state ν.

Now we have an intuitive idea for the interpretation of the Green's function in many-body quantum physics, but we have to take into account the thermal excitations that can put the system in an excited states. This is described by the thermal density matrix:

$$\varrho = \frac{1}{Z}\sum_n\mathrm{e}^{-\beta\omega_n}|\Psi_n\rangle\langle\Psi_n| \tag{68}$$

where $Z = \mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}}\right] = \sum_n \mathrm{e}^{-\beta\omega_n}$ is the partition function used to normalize, Ψ_n are the eigenstates of the Hamiltonian with eigenvalues ω_n and $\beta^{-1} = k_B T$ being k_B the Boltzmann constant and T the temperature. On this context the expected value of some operator $\mathcal{O}$ is defined as

$$\langle\mathcal{O}\rangle = \mathrm{tr}\left[\varrho\mathcal{O}\right] \tag{69}$$

Look that for $T \to 0$ (which is the same limit that $k_B T \ll \hbar\omega_1$) $Z = 1$ and $\langle\mathcal{O}\rangle = \langle\Psi_0|\mathcal{O}|\Psi_0\rangle$, so we can define the finite temperature Green's function.

$$G_{\mu\nu}(t,t') = -\imath\left\langle\mathcal{T}[c_\mu(t)c_\nu^\dagger(t')]\right\rangle = -\mathrm{tr}\left[\varrho\mathcal{T}[c_\mu(t)c_\nu^\dagger(t')]\right] = -\frac{\imath}{Z}\sum_n \mathrm{e}^{-\beta\omega_n}\langle\Psi_n|\mathcal{T}[c_\mu(t)c_\nu^\dagger(t')]|\Psi_n\rangle \tag{70}$$

We can split the two time order terms to define the greater Green's function (particle propagator) and lesser Green's function (hole propagator).

$$G_{\mu\nu}^{>}(t,t') = -\imath\left\langle c_\mu(t)c_\nu^\dagger(t')\right\rangle = -\frac{\imath}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\mathrm{e}^{\imath(\omega_n-\omega_m)(t-t')}\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle \tag{71a}$$

$$G_{\mu\nu}^{<}(t,t') = \imath\left\langle c_\nu^\dagger(t')c_\mu(t)\right\rangle = \frac{\imath}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\mathrm{e}^{\imath(\omega_m-\omega_n)(t-t')}\langle\Psi_n|c_\nu^\dagger|\Psi_m\rangle\langle\Psi_m|c_\mu|\Psi_n\rangle \tag{71b}$$

An interesting thing is that we have deduced that Green's function only depends on $t - t'$.

$$G(t,t') = \Theta(t-t')G^{>}(t,t') + \Theta(t'-t)G^{<}(t,t') \tag{72}$$

We can define also de retarded/advanced Green's function, $G^{r/a}(t,t') = \pm\Theta(\pm t \mp t')\left[G^{>}(t,t') - G^{<}(t,t')\right]$ since they have more information about spectral functions of the system.

$$G_{\mu\nu}^{r}(t,t') = -\imath\Theta(t-t')\left\langle\{c_\mu(t), c_\nu^\dagger(t')\}\right\rangle \tag{73a}$$

$$G_{\mu\nu}^{a}(t,t') = \imath\Theta(t'-t)\left\langle\{c_\mu(t), c_\nu^\dagger(t')\}\right\rangle \tag{73b}$$

Look that by definition

$$G^r - G^a = G^{>} - G^{<} \tag{74}$$

Now we can compute the Green's functions on frequency space. For greater/lesser it is trivial that it is a Dirac's delta.

$$G_{\mu\nu}^{>}(\omega) = -\frac{\imath 2\pi}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle\delta(\omega-\omega_m+\omega_n) \tag{75a}$$

$$G_{\mu\nu}^{<}(\omega) = \frac{\imath 2\pi}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\langle\Psi_n|c_\nu^\dagger|\Psi_m\rangle\langle\Psi_m|c_\mu|\Psi_n\rangle\delta(\omega-\omega_n+\omega_m) \tag{75b}$$

For the retarded/advanced functions is quite complicated due to the Heaviside's function, but we can proceed analogously as for the one-body zero temperature problem.

$$\begin{aligned} G_{\mu\nu}^{r}(\omega) &= \frac{1}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\left[\frac{\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle}{\omega-\omega_m+\omega_n+\imath\eta} + \frac{\langle\Psi_n|c_\nu^\dagger|\Psi_m\rangle\langle\Psi_m|c_\mu|\Psi_n\rangle}{\omega-\omega_n+\omega_m+\imath\eta}\right] \\ &= \frac{1}{Z}\sum_{m,n}\left(\mathrm{e}^{-\beta\omega_n}+\mathrm{e}^{-\beta\omega_m}\right)\frac{\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle}{\omega-\omega_m+\omega_n+\imath\eta} \end{aligned} \tag{76a}$$

$$\begin{aligned} G_{\mu\nu}^{a}(\omega) &= \frac{1}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\left[\frac{\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle}{\omega-\omega_m+\omega_n-\imath\eta} + \frac{\langle\Psi_n|c_\nu^\dagger|\Psi_m\rangle\langle\Psi_m|c_\mu|\Psi_n\rangle}{\omega-\omega_n+\omega_m-\imath\eta}\right] \\ &= \frac{1}{Z}\sum_{m,n}\left(\mathrm{e}^{-\beta\omega_n}+\mathrm{e}^{-\beta\omega_m}\right)\frac{\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle}{\omega-\omega_m+\omega_n-\imath\eta} \end{aligned} \tag{76b}$$

And finally, for the time-ordered Green's function:

$$G_{\mu\nu}(\omega) = \frac{1}{Z}\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\left[\frac{\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c_\nu^\dagger|\Psi_n\rangle}{\omega-\omega_m+\omega_n+\imath\eta} + \frac{\langle\Psi_n|c_\nu^\dagger|\Psi_m\rangle\langle\Psi_m|c_\mu|\Psi_n\rangle}{\omega-\omega_n+\omega_m-\imath\eta}\right] \tag{77}$$

Sometimes it is useful to define the following spectral function.

$$\begin{aligned} A_{\mu\nu}(\omega) &= \imath\left[G^{>}_{\mu\nu}(\omega) - G^{<}_{\mu\nu}(\omega)\right] = \frac{2\pi}{Z}\sum_{m,n}\left(\mathrm{e}^{-\beta\omega_n} + \mathrm{e}^{-\beta\omega_m}\right)\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c^\dagger_\nu|\Psi_n\rangle\delta(\omega-\omega_m+\omega_n) \\ &= \frac{2\pi}{Z}\left(1+\mathrm{e}^{-\beta\omega}\right)\sum_{m,n}\mathrm{e}^{-\beta\omega_n}\langle\Psi_n|c_\mu|\Psi_m\rangle\langle\Psi_m|c^\dagger_\nu|\Psi_n\rangle\delta(\omega-\omega_m+\omega_n) = \imath\left(1+\mathrm{e}^{-\beta\omega}\right)G^{>}_{\mu\nu}(\omega) \end{aligned} \tag{78}$$

So we can express greater/lesser Green's function proportional to spectral function.

$$G^{>}(\omega) = -\imath[1-f(\omega)]A(\omega) \tag{79a}$$

$$G^{<}(\omega) = \imath f(\omega)A(\omega) \tag{79b}$$

Here $f(\omega) = \left(1+\mathrm{e}^{\beta\omega}\right)^{-1}$ is the Fermi function. Look that greater/lesser Green's function manifest explicitly its behaviour as particle/hole propagator by the factor that is multiplying the spectral function, being the Fermi function the probability distribution for the particles and its opposite $1-f(\omega)$ the probability density for holes (the probability to propagate a particle is the same that the probability to find a hole and vice-versa). Then, the computation of the spectral function can be done taking into account Equation 74: $A(\omega) = \imath\left[G^r(\omega) - G^a(\omega)\right]$. Look that in frequency space $G^{a*}(\omega) = G^r(\omega)$:

$$A(\omega) = -2\Im\left[G^r(\omega)\right] \tag{80}$$

which recovers the expression with Dirac's delta by the limit

$$\lim_{\eta\to 0^+}\frac{1}{\omega+\imath\eta} = \mathcal{P}\frac{1}{\omega} - \imath\pi\delta(\omega) \tag{81}$$

but it would be useful to keep $\eta \gtrsim 0$ to broaden the spectral function. Now we can express the time-ordered Green's function with spectral function. We can use the definition of Equation 72 using the convolution theorem[7]. First of all, in the limit $\eta \to 0^+$ (broadening is already included in spectral function)

$$\mathcal{F}[\Theta(t)] = \imath\left[\mathcal{P}\frac{1}{\omega} - \imath\pi\delta(\omega)\right] \qquad \mathcal{F}[\Theta(-t)] = -\imath\left[\mathcal{P}\frac{1}{\omega} + \imath\pi\delta(\omega)\right] \tag{82}$$

so the Green's function:

$$\begin{aligned} G(\omega) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[(1-f(\sigma))A(\sigma)\left(\mathcal{P}\frac{1}{\omega-\sigma} - \imath\pi\delta(\omega-\sigma)\right) + f(\sigma)A(\sigma)\left(\mathcal{P}\frac{1}{\omega-\sigma} + \imath\pi\delta(\omega-\sigma)\right)\right]\mathrm{d}\sigma \\ &= \frac{1}{2\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{A(\sigma)}{\omega-\sigma}\mathrm{d}\sigma - \frac{\imath}{2}\tanh\left(\frac{\beta\omega}{2}\right)A(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\Im\left[G^r(\sigma)\right]}{\omega-\sigma}\mathrm{d}\sigma + \imath\tanh\left(\frac{\beta\omega}{2}\right)\Im\left[G^r(\omega)\right] \\ &= -\Re\left[G^r(\omega)\right] + \imath\tanh\left(\frac{\beta\omega}{2}\right)\Im\left[G^r(\omega)\right] \end{aligned} \tag{83}$$

On the real term look that since $G^r(\omega)$ has no poles at half-upper complex plane Kramers-Kronig relation apply.

2.3.1 The free propagator

The propagator of one free particle is the easiest example to solve. For this stablish a diagonal Hamiltonian

$$\mathcal{H}_0 = \sum_\mu \varepsilon_\mu c^\dagger_\mu c_\mu \tag{84}$$

where the computation of the time evolution of the annihilation operators is trivial

$$\partial_t c_\mu(t) = \imath\sum_\nu \varepsilon_\nu[c^\dagger_\nu c_\nu, c_\mu](t) = -\imath\varepsilon_\mu c_\mu(t) \tag{85}$$

giving us $c_\mu(t) = \mathrm{e}^{-\imath\epsilon_\mu t}c_\mu$. Now we can define and compute the free propagator.

$$\begin{aligned} G^0_\mu(t,t') &= -\imath\left\langle\mathcal{T}\left[c_\mu(t)c^\dagger_\mu(t')\right]\right\rangle \\ &= -\imath\mathrm{e}^{-\imath\varepsilon_\mu(t-t')}\left[\Theta(t-t')\left\langle c_\mu c^\dagger_\mu\right\rangle - \Theta(t'-t)\left\langle c^\dagger_\mu c_\mu\right\rangle\right] \end{aligned} \tag{86}$$

$$G^0_\mu(\omega) = \frac{1-f_\mu}{\omega-\varepsilon_\mu+\imath\eta} + \frac{f_\mu}{\omega-\varepsilon_\mu-\imath\eta} \tag{87}$$

Here f_μ is the probability to find an electron on state μ.

[7] $\mathcal{F}[f(t)g(t)] = \frac{1}{2\pi}F(\omega) * G(\omega)$ being $F(\omega) = \mathcal{F}[f(t)]$ and $G(\omega) = \mathcal{F}[g(t)]$.

2.4 Perturbation expansion

Since now we have computed the Green's function taking into account all the Hamiltonian, this means that we have been using the eigenstates of the total Hamiltonian being one of the things that we want to compute. To solve this we can split the Hamiltonian into two terms $\mathcal{H} = \mathcal{H}_0 + \mathcal{W}$ being $\mathcal{W}$ the part that describes the interaction with external field, phonons... In this situation it is useful to move to interaction picture. Let's start by defining the quantum states into the interaction picture

$$|\hat{\psi}(t)\rangle = \mathrm{e}^{\imath\mathcal{H}_0 t}|\psi(t)\rangle = \mathrm{e}^{\imath\mathcal{H}_0 t}\mathrm{e}^{-\imath\mathcal{H}t}|\psi\rangle \tag{88}$$

where you can see that $|\psi(t)\rangle$ and $|\psi\rangle$ are the same quantum state but in Schrödinger and Heisenberg pictures respectively. From this definition we can easily deduce how operators $\mathcal{O}$ evolve under interaction picture.

$$\hat{\mathcal{O}}(t) = \mathrm{e}^{\imath\mathcal{H}_0 t}\mathcal{O}\mathrm{e}^{-\imath\mathcal{H}_0 t} \tag{89}$$

Which is interesting is compute an operator that is able to evolve the interaction picture state from t' to t named $S(t,t')$.

$$\begin{aligned} |\hat{\psi}(t)\rangle &= S(t,t')|\hat{\psi}(t')\rangle \\ \mathrm{e}^{\imath\mathcal{H}_0 t}\mathrm{e}^{-\imath\mathcal{H}t}|\psi\rangle &= S(t,t')\mathrm{e}^{\imath\mathcal{H}_0 t'}\mathrm{e}^{-\imath\mathcal{H}t'}|\psi\rangle \end{aligned} \tag{90}$$

$$S(t,t') = \mathrm{e}^{\imath\mathcal{H}_0 t}\mathrm{e}^{-\imath\mathcal{H}(t-t')}\mathrm{e}^{-\imath\mathcal{H}_0 t'} \tag{91}$$

Look that this S operator obeys the following group property: $S(t,t'')S(t'',t') = S(t,t')$. We can also develop this operator in Taylor series to compute this operator. First we compute its time derivative

$$\partial_t S(t,t') = \imath\mathrm{e}^{\imath\mathcal{H}_0 t}(\mathcal{H}_0 - \mathcal{H})\mathrm{e}^{-\imath\mathcal{H}(t-t')}\mathrm{e}^{-\imath\mathcal{H}_0 t'} = -\imath\hat{\mathcal{W}}(t)S(t,t') \tag{92}$$

we can integrate the differential equation taking into account $S(t',t') = \mathbb{I}$

$$S(t,t') = \mathbb{I} - \imath\int_{t'}^{t}\hat{\mathcal{W}}(t_1)S(t_1,t')\mathrm{d}t_1 = \mathbb{I} - \imath\int_{t'}^{t}\hat{\mathcal{W}}(t_1)\mathrm{d}t_1 - \int_{t'}^{t}\hat{\mathcal{W}}(t_1)\left(\int_{t'}^{t_1}\hat{\mathcal{W}}(t_2)\mathrm{d}t_2\right)\mathrm{d}t_1 + \cdots \tag{93}$$

look that for every term there is $k!$ to reorder the time limits of the successive integrals

$$S(t,t') = \sum_{k=0}^{\infty}\frac{(-\imath)^k}{k!}\mathcal{T}\left[\left(\int_{t'}^{t}\hat{\mathcal{W}}(t'')\mathrm{d}t''\right)^k\right] = \mathcal{T}\left[\mathrm{e}^{-\imath\int_{t'}^{t}\hat{\mathcal{W}}(t'')\mathrm{d}t''}\right] \tag{94}$$

At this point let's define $|\Psi_0\rangle$ as the ground state of full Hamiltonian, $\mathcal{H}|\Psi_0\rangle = \omega_0|\Psi_0\rangle$, and $|\Phi_0\rangle$ as the ground state of the non-interactive part, $\mathcal{H}_0|\Phi_0\rangle = \varepsilon_0|\Phi_0\rangle$. By the Gell-Mann and Low theorem

$$|\Psi_0\rangle = S(0,-\infty)|\Phi_0\rangle \tag{95}$$

which means that if we evolve the non-interacting ground state in the interaction picture from a far enough moment it eventually reaches the exact ground state. This relation allows to define a perturbation scheme for the Green's function

$$G_{\mu\nu}(t,t') = -\imath\frac{\langle\Phi_0|\mathcal{T}\left[S(\infty,-\infty)c_\mu(t)c_\nu^\dagger(t')\right]|\Phi_0\rangle}{\langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle} \tag{96}$$

where we have add explicitly the normalization factor.

By an appropriate application of Wick's theorem every order of expansion of $\mathcal{T}\left[S(\infty,-\infty)c_\mu(t)c_\nu^\dagger(t')\right]$ can be separated into several diagrams which can be linked or unlinked. This allow us to write the numerator as a product between the sum of linked diagrams and the sum of the linked parts of the unlinked diagrams, but this second factor coincides with the denominator (good news because this diagrams often diverge) so we can expand the Green's function over all linked diagrams (Linked-Cluster theorem). To formulate this expansion let's define the free propagator using the quadratic/diagonalizable part of the Hamiltonian, $\mathcal{H}_0$

$$G_\mu^0(t,t') = -\imath\langle\Phi_0|\mathcal{T}\left[c_\mu(t)c_\mu^\dagger(t')\right]|\Phi_0\rangle \tag{97}$$

and look how interactions modify the propagator.

$$G_{\mu\nu}(t,t') = \delta_{\mu\nu}G_\mu^0(t,t') + \int_{-\infty}^{\infty}\mathrm{d}t_1\int_{-\infty}^{\infty}\mathrm{d}t_1' G_\mu^0(t,t_1)\tilde{\Sigma}_{\mu\nu}(t_1,t_1')G_\nu^0(t_1',t') \tag{98}$$

Here we have recovered the Dyson equation which in frequency space it is an algebraic equation (66). The improper self-energy can be reduced in several diagrams involving the proper (irreducible) self-energy:

$$\tilde{\Sigma} = \Sigma + \Sigma G^0 \tilde{\Sigma} \tag{99}$$

which is giving us the following form of the Dyson equation

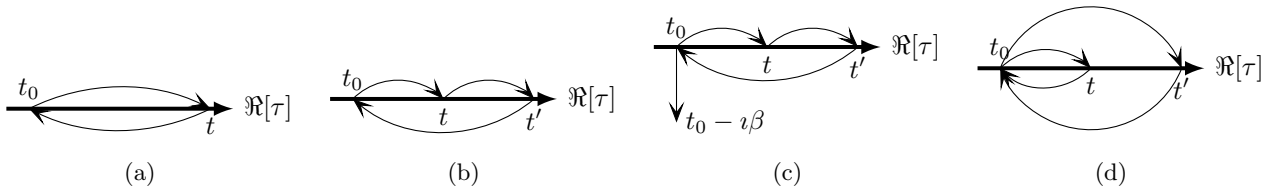
$$G = G^0 + G^0 \Sigma G \tag{100}$$

allowing to isolate the full propagator.

$$G = \frac{1}{(G^0)^{-1} - \Sigma} = \frac{1}{\omega - \mathcal{H}_0 - \Sigma} \tag{101}$$

At the end the main problem is to find a good approximation of the self-energy which is in general a complex number, so the broadening of the propagator is contained into the self-energy.

2.5 Non-equilibrium Green's function



(a) (b) (c) (d)

Figure 2: Contours Γ', Γ, Γ_v and $\Gamma_1 + \Gamma_1'$, (a,b,c,d respectively).

Since now we have worked with Green's functions for systems which return to initial state for large times but it is not necessary true. In non-equilibrium use asymptotic is not useful any more, but we can construct a theory equivalent to equilibrium theory.

Here we deal with a Hamiltonian

$$\mathcal{H}(t) = \mathcal{H}_b + \mathcal{W}(t) = \mathcal{H}_0 + \mathcal{H}_i + \mathcal{W}(t) \tag{102}$$

composed by the diagonalizable part $\mathcal{H}_0$, the non-diagonalizable part $\mathcal{H}_i$, and the external interaction $\mathcal{W}(t)$. For the density matrix and thermal expected value we will use $\mathcal{H}_b$

$$\varrho = \frac{1}{Z} \mathrm{e}^{-\beta \mathcal{H}_b} = \frac{1}{\mathrm{tr}\left[\mathrm{e}^{-\beta \mathcal{H}_b}\right]} \sum_n \mathrm{e}^{-\beta \mathcal{H}_b} |\Psi_n\rangle\langle\Psi_n| \tag{103}$$

$$\langle \mathcal{O}(t) \rangle = \mathrm{tr}\left[\varrho \mathcal{O}(t)\right] \tag{104}$$

considering that the thermodynamic degrees of freedom do not follow the variations of external interaction.

In general the time dependence is defined with the full Hamiltonian

$$\mathcal{O}(t) = \mathcal{T}\left[\mathrm{e}^{\imath \int^t \mathcal{H}(t')\mathrm{d}t'}\right] \mathcal{O} \mathcal{T}\left[\mathrm{e}^{-\imath \int^t \mathcal{H}(t')\mathrm{d}t'}\right] \tag{105}$$

but should be desired to use a simpler time evolution using the time independent part of the Hamiltonian

$$\hat{\mathcal{O}}(t) = \mathrm{e}^{\imath \mathcal{H}_b t} \mathcal{O} \mathrm{e}^{-\imath \mathcal{H}_b t} \tag{106}$$

or even the simplest with the quadratic term.

$$\tilde{\mathcal{O}}(t) = \mathrm{e}^{\imath \mathcal{H}_0 t} \mathcal{O} \mathrm{e}^{-\imath \mathcal{H}_0 t} \tag{107}$$

To illustrate this let's move from full Hamiltonian time dependence to time-independent Hamiltonian time dependence. Analogously to interaction picture:

$$\mathcal{O}(t) = \mathcal{T}\left[\mathrm{e}^{\imath \int_{t_0}^t \hat{\mathcal{W}}(t')\mathrm{d}t'}\right] \hat{\mathcal{O}}(t) \mathcal{T}\left[\mathrm{e}^{-\imath \int_{t_0}^t \hat{\mathcal{W}}(t')\mathrm{d}t'}\right] = V_b^\dagger(t_0, t) \hat{\mathcal{O}}(t) V_b(t_0, t) \tag{108}$$

Now, if we define the contour ordered operator $\mathcal{T}_{\Gamma'}$ and being Γ' the contour on complex plane defined in Fig.2a we can use the following result where apply the contour ordered over an integral exponential over $\hat{\mathcal{W}}(t)$ and $\hat{\mathcal{O}}(t)$ to recover $\mathcal{O}(t)$.

$$\begin{aligned}
\mathcal{O}(t) &= \mathcal{T}_{\Gamma'}\left[\mathrm{e}^{-\imath\int_{\Gamma'}\hat{\mathcal{W}}(t)\mathrm{d}\tau}\hat{\mathcal{O}}(t)\right] = \sum_{n=0}^{\infty}\frac{(-\imath)^n}{n!}\int_{\Gamma'}\mathrm{d}\tau_1\cdots\int_{\Gamma'}\mathrm{d}\tau_n\mathcal{T}_{\Gamma'}\left[\hat{\mathcal{W}}(\tau_1)\cdots\hat{\mathcal{W}}(\tau_n)\hat{\mathcal{O}}(t)\right] \\
&= \sum_{n=0}^{\infty}\frac{(-\imath)^n}{n!}\sum_{m=0}^{n}\binom{n}{m}\int_{\leftarrow}\mathrm{d}\tau_{m+1}\cdots\int_{\leftarrow}\mathrm{d}\tau_n\mathcal{T}_{\leftarrow}\left[\hat{\mathcal{W}}(\tau_{m+1})\cdots\hat{\mathcal{W}}(\tau_n)\right]\hat{\mathcal{O}}(t) \\
&\qquad\times\int_{\rightarrow}\mathrm{d}\tau_1\cdots\int_{\rightarrow}\mathrm{d}\tau_m\mathcal{T}_{\rightarrow}\left[\hat{\mathcal{W}}(\tau_1)\cdots\hat{\mathcal{W}}(\tau_m)\right] \\
&= \sum_{k=0}^{\infty}\frac{(-\imath)^k}{k!}\int_{\leftarrow}\mathrm{d}\tau_1\cdots\int_{\leftarrow}\mathrm{d}\tau_k\mathcal{T}_{\leftarrow}\left[\hat{\mathcal{W}}(\tau_1)\cdots\hat{\mathcal{W}}(\tau_k)\right]\hat{\mathcal{O}}(t) \\
&\times\sum_{m=0}^{\infty}\frac{(-\imath)^m}{m!}\int_{\rightarrow}\mathrm{d}\tau_1\cdots\int_{\rightarrow}\mathrm{d}\tau_m\mathcal{T}_{\rightarrow}\left[\hat{\mathcal{W}}(\tau_1)\cdots\hat{\mathcal{W}}(\tau_m)\right] = V_b^{\dagger}(t_0,t)\hat{\mathcal{O}}(t)V_b(t_0,t)
\end{aligned} \tag{109}$$

To do this development we have splitted the contour between the part that goes from t_0 to t ($\leftarrow$ or forward) and the part that goes from t to t_0 ($\rightarrow$ or backward). Then we have take into account that for the n-th term of the sumation there are $\binom{n}{m}$ ways to combine forward and backward integrals. Finally the introduction of sum index $k = n - m$ was necessary to separate the sums.

Now we can define the contour ordered Green's function using the contour Γ defined in Fig.2b.

$$G_{\mu\nu}(t,t') = -\imath\left\langle\mathcal{T}_{\Gamma}\left[c_\mu(t)c_\nu^{\dagger}(t')\right]\right\rangle \tag{110}$$

Notice that we can use Eq (109) to rewrite the Green's function

$$G_{\mu\nu}(t,t') = -\imath\left\langle\mathcal{T}_{\Gamma}\left[S_\Gamma\hat{c}_\mu(t)\hat{c}_\nu^{\dagger}(t')\right]\right\rangle \tag{111}$$

being

$$S_\Gamma = \mathrm{e}^{-\imath\int_\Gamma\hat{\mathcal{W}}(\tau)\mathrm{d}\tau} \tag{112}$$

At this point we construct a Green's function which statistics and temporal evolutions depends on $\mathcal{H}_b$ that includes the interaction term but we still a step forward by defining the following operators.

$$S'_\Gamma = \mathrm{e}^{-\imath\int_\Gamma\tilde{\mathcal{W}}(\tau)\mathrm{d}\tau} \tag{113}$$

$$S^i_{\Gamma_v} = \mathrm{e}^{-\imath\int_{\Gamma_v}\tilde{\mathcal{H}}_i(\tau)\mathrm{d}\tau} \tag{114}$$

Here Γ_v is the contour defined in Fig.2c. After doing all necessary transformations Green's function is expressed with time dependences and statistics only dependent on $\mathcal{H}_0$.

$$G_{\mu\nu}(t,t') = -\imath\frac{\left\langle\mathcal{T}_{\Gamma_v}\left[S^i_{\Gamma_v}S'_\Gamma\tilde{c}_\mu(t)\tilde{c}_\nu^{\dagger}(t')\right]\right\rangle_0}{\left\langle\mathcal{T}_{\Gamma_v}\left[S^i_{\Gamma_v}S'_\Gamma\right]\right\rangle_0} \tag{115}$$

Now we have introduced the non-interacting expected value.

$$\left\langle\mathcal{O}(t)\right\rangle_0 = \mathrm{tr}\left[\varrho_0\mathcal{O}(t)\right] \tag{116}$$

$$\varrho_0 = \frac{1}{Z_0}\mathrm{e}^{-\beta\mathcal{H}_0}\quad Z_0 = \mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}_0}\right] \tag{117}$$

On this new expression of Green's function the use of a quadratic density matrix allows the application of the Wick's theorem and therefore the use of a diagrammatic expansion. As in the equilibrium case only the linked diagrams contribute to the Green's function. The use of linked diagrams allow us to recover de Dyson equation

$$G_{\mu\nu}(t,t') = \delta_{\mu\nu}G^0_\mu(t,t') + \int_{\Gamma_v}G^0_\mu(t,\tau)U_\mu(\tau)G_{\mu\nu}(\tau,t')\mathrm{d}\tau + \int_{\Gamma_v}\int_{\Gamma_v}G^0_\mu(t,\tau_1)\Sigma_{\mu\lambda}(\tau_1,\tau_2)G_{\lambda\nu}(\tau_2,t')\mathrm{d}\tau_2\mathrm{d}\tau_1 \tag{118}$$

where we have added a term related with external field interacton mediated by a one-body external potential $U(\tau)$. Before go on let's talk about Γ_v contour which have a contribution related to part that goes from t_0 to $t_0 - \imath\beta$. This part vanishes in the limit $t_0 \to \infty$ (so $\Gamma_v = \Gamma$) which is considered only when the transient regime is not relevant on the problem. Since this point we will consider it.

2.5.1 Analytic continuation and Langreth theorem

Dyson equation defined before involve contour integrals which are impractical for calculations, so we need to perform some analytical continuation to get real time integrals. For this it will be useful to recover the lesser, greater, retarded and advanced functions and also define the causal and anti-causal functions $G^{c/\bar{c}}(t,t')$:

$$G^{c}_{\mu\nu}(t,t') = -\imath \left\langle \mathcal{T}\left[c_\mu(t)c^\dagger_\nu(t')\right]\right\rangle = -\imath\Theta(t-t')\left\langle c_\mu(t)c^\dagger_\nu(t')\right\rangle + \imath\Theta(t'-t)\left\langle c^\dagger_\nu(t')c_\mu(t)\right\rangle \tag{119a}$$

$$G^{\bar{c}}_{\mu\nu}(t,t') = -\imath \left\langle \bar{\mathcal{T}}\left[c_\mu(t)c^\dagger_\nu(t')\right]\right\rangle = -\imath\Theta(t'-t)\left\langle c_\mu(t)c^\dagger_\nu(t')\right\rangle + \imath\Theta(t-t')\left\langle c^\dagger_\nu(t')c_\mu(t)\right\rangle \tag{119b}$$

Look that apart that already known relation $G^{>} - G^{<} = G^{r} - G^{a}$ we can find that $G^{>} + G^{<} = G^{c} + G^{\bar{c}}$ having only four independent functions. Look that, in the limit $t_0 \to -\infty$, we can split $\Gamma = \Gamma_f + \Gamma_b$ being "forward" the part that goes from $-\infty$ to the greatest time and "backward" the part where returns to $-\infty$[8]. This makes that contour ordered function is equal to some of these new functions under particular contour definitions.

$$G(t,t') = \begin{cases} G^{c}(t,t') & t,t' \in \Gamma_f \\ G^{\bar{c}}(t,t') & t,t' \in \Gamma_b \\ G^{>}(t,t') & t \in \Gamma_b, t' \in \Gamma_f \\ G^{<}(t,t') & t \in \Gamma_f, t' \in \Gamma_b \end{cases} \tag{120}$$

Now we can derive the Langreth theorem. If we take an integral along Γ contour

$$C(t,t') = \int_\Gamma A(t,\tau)B(\tau,t')\mathrm{d}\tau \tag{121}$$

and we deform Γ making a new contour $\Gamma_1 + \Gamma_1'$ where Γ_1 is a Γ' contour type between t_0 and t, and Γ_1' is a Γ' contour type between t_0 and t' (Fig.2d) we can define for example, the lesser function (equal to contour-ordered function under the contour conditions of Eq (120)) as

$$C^{<}(t,t') = \int_{\Gamma_1} A(t,\tau)B^{<}(\tau,t')\mathrm{d}\tau + \int_{\Gamma_1'} A^{<}(t,\tau)B(\tau,t')\mathrm{d}\tau \tag{122}$$

where the introduction of $A^<$ and $B^<$ on the correspondent term is because in Γ_1' and Γ_1 contours respectively is accomplished the condition for contour-ordered function being equal to lesser function. Now let an inspection of the first term

$$\begin{aligned} \int_{\Gamma_1} A(t,\tau)B^{<}(\tau,t')\mathrm{d}\tau &= \int_{-\infty}^{t} A^{>}(t,t_1)B^{<}(t_1,t')\mathrm{d}t_1 + \int_{t}^{-\infty} A^{<}(t,t_1)B(t_1,t')\mathrm{d}t_1 \\ &= \int_{-\infty}^{\infty} A^{r}(t,t_1)B^{<}(t_1,t')\mathrm{d}t_1 \end{aligned} \tag{123}$$

and analogously in the second term B^a emerge.

$$C^{<}(t,t') = \int_{-\infty}^{\infty} \left[A^{r}(t,t_1)B^{<}(t_1,t') + A^{<}(t,t_1)B^{a}(t_1,t')\right]\mathrm{d}t_1 \tag{124}$$

The same analysis can be done for greater functions and the result is the same changing only $<$ by $>$. Also this result can be generalized by products of n factors $C = A_1 \cdots A_n$:

$$C^{<} = A_1^r \cdots A_n^< + \cdots + A_1^r \cdots A_{i-1}^r A_i^< A_{i+1}^a \cdots A_n^a + \cdots + A_1^< \cdots A_n^a \tag{125}$$

Often is useful work with the retarded functions.

$$C^{r}(t,t') = \Theta(t-t')\left[C^{>}(t,t') - C^{<}(t,t')\right] = \int_{t'}^{t} A^{r}(t,t_1)B^{r}(t_1,t')\mathrm{d}t_1 \tag{126}$$

In a diagrammatic expansion of several terms some structures like $C(\tau,\tau') = A(\tau,\tau')B(\tau,\tau')$ and $D(\tau,\tau') = A(\tau,\tau')B(\tau',\tau)$ will appear being τ,τ' contour variables. By the same analysis one can get the lesser/greater and retarded functions.

$$C^{<}(t,t') = A^{<}(t,t')B^{<}(t,t') \tag{127a}$$

$$D^{<}(t,t') = A^{<}(t,t')B^{>}(t',t) \tag{127b}$$

$$C^{r}(t,t') = A^{<}(t,t')B^{r}(t,t') + A^{r}(t,t')B^{<}(t,t') + A^{r}(t,t')B^{r}(t,t') \tag{127c}$$

$$D^{r}(t,t') = A^{r}(t,t')B^{<}(t',t) + A^{<}(t,t')B^{a}(t',t) \tag{127d}$$

[8] t and t' can belong to both parts since we can deform the contour into the complex plane.

2.6 Kinetic equations

On this part we will use matricial expression of integral equations, as for example Dyson equation

$$\begin{aligned} G &= \mathfrak{G} + \mathfrak{G}UG + \mathfrak{G}\Sigma G \\ G &= \mathfrak{G} + GU\mathfrak{G} + G\Sigma\mathfrak{G} \end{aligned} \tag{128}$$

where the second alternative form is given by developing improper self-energy from left instead of right. Here the free propagator has been written using $\mathfrak{G}$ instead of G^0 for a more comfortable superscript notation.

2.6.1 Kadanoff-Baym formulation

First of all take a Hamiltonian without external potential ($U = 0$), then it is clear

$$\begin{aligned} \mathfrak{G}^{-1}G &= 1 + \Sigma G \\ G\mathfrak{G}^{-1} &= 1 + G\Sigma \end{aligned} \tag{129}$$

so by introducing this potential this equations are simply transformed

$$\begin{aligned} \left(\mathfrak{G}^{-1} - U\right) G &= 1 + \Sigma G \\ G\left(\mathfrak{G}^{-1} - U\right) &= 1 + G\Sigma \end{aligned} \tag{130}$$

We want to develop some equations for lesser functions so we can use Eq (125) taking into account that deltas will vanish because we need times being in different branches on the contours. By some algebra and using

$$\begin{aligned} C^r &= \frac{1}{2}(C^r + C^a) + \frac{1}{2}(C^r - C^a) \\ C^a &= \frac{1}{2}(C^r + C^a) - \frac{1}{2}(C^r - C^a) \end{aligned} \tag{131}$$

we get

$$[\mathfrak{G}^{-1} - U, G^<] - \frac{1}{2}[\Sigma^r + \Sigma^a, G^<] + \frac{1}{2}[G^r + G^a, \Sigma^<] = \frac{1}{2}\{\Sigma^r - \Sigma^a, G^<\} - \frac{1}{2}\{G^r - G^a, \Sigma^<\} \tag{132}$$

Now let's recall the spectral function $A = \imath(G^> - G^<) = 2\Im[G^r]$ and the fact of Eq (74) and define $C^m = (C^r + C^a)/2$ and an analogue of spectral function for self-energy $\Gamma = \imath(\Sigma^> - \Sigma^<) = 2\Im[\Sigma^r]$

$$[\mathfrak{G}^{-1} - U, G^<] - [\Sigma^m, G^<] + [G^m, \Sigma^<] = \frac{1}{2\imath}\{\Gamma, G^<\} - \frac{1}{2\imath}\{A, \Sigma^<\} = \frac{1}{2}\{\Sigma^>, G^<\} - \frac{1}{2}\{G^>, \Sigma^<\} \tag{133}$$

This is the generalized Kandoff-Bayn equation (GKB) and also can be derived for the greater functions

$$[\mathfrak{G}^{-1} - U, G^>] - [\Sigma^m, G^>] + [G^m, \Sigma^>] = \frac{1}{2\imath}\{\Gamma, G^>\} - \frac{1}{2\imath}\{A, \Sigma^>\} = \frac{1}{2}\{\Sigma^>, G^<\} - \frac{1}{2}\{G^>, \Sigma^<\} \tag{134}$$

If we subtract these two GKB

$$[\mathfrak{G}^{-1} - U - \Sigma^m, A] + [G^m, \Gamma] = 0 \tag{135}$$

which is an equation for non-equilibrium spectral function.

GKB has the form of a differential equation with the corresponding boundary conditions G^m, Σ^m which need to be solved independently with Dyson equation. This can envolve some complications depending on the problem.

2.6.2 Keldysh formulation

Using the Langreth theorem we can generate an integral equation for $G^<$, named Keldysh equation. Let's start with Dyson equation

$$G^< = \mathfrak{G}^< + \mathfrak{G}^r\Sigma^rG^< + \mathfrak{G}^r\Sigma^<G^a + \mathfrak{G}^<\Sigma^aG^a \tag{136}$$

Look that if we iterate over $G^<$ we can finally get the following expression.

$$G^< = (1 + G^r\Sigma^r)\,\mathfrak{G}^<\,(1 + \Sigma^aG^a) + G^r\Sigma^<G^a \tag{137}$$

The equation for the greater function is equivalent.

$$G^> = (1 + G^r\Sigma^r)\,\mathfrak{G}^>\,(1 + \Sigma^aG^a) + G^r\Sigma^>G^a \tag{138}$$

This Keldysh equation is not more that integral form of GKB.

2.7 Imaginary-time (Matsubara) Green's functions

As we will see later sometimes it is convenient to use the imaginary time branch, $t = t_0 - \imath\tau$ of the contour. In this branch we define the Matsubara Green's function (take the case $\tau > \tau'$):

$$\begin{aligned} G^M(\tau,\tau') &= -\left\langle \mathcal{T}_\tau[c(\tau)c^\dagger(\tau')]\right\rangle = -\frac{1}{Z}\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}}\mathrm{e}^{\tau\mathcal{H}}c\mathrm{e}^{-\tau\mathcal{H}}\mathrm{e}^{\tau'\mathcal{H}}c^\dagger\mathrm{e}^{-\tau'\mathcal{H}}\right] \\ &= -\frac{1}{Z}\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}}\mathrm{e}^{(\tau-\tau')\mathcal{H}}c\mathrm{e}^{-(\tau-\tau')\mathcal{H}}c^\dagger\right] = G^M(\tau-\tau') \end{aligned} \tag{139}$$

Here we have defined the imaginary-time order operator $\mathcal{T}_\tau$. Also we have used the cyclic property of the trace and the fact that every Hamiltonian is imaginary-time independent to show that Matsubara Green's function only depends to time difference. Also notice that in frequency representation factors like $\mathrm{e}^{-(\beta-\tau+\tau')\omega_n}$ will appear making it only converge for $|\tau-\tau'| < \beta$. If we want to extend this function outside of this range:

$$\begin{aligned} G^M(\tau+\beta) &= -\frac{1}{Z}\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}}\mathrm{e}^{(\tau+\beta)\mathcal{H}}c\mathrm{e}^{-(\tau+\beta)\mathcal{H}}c^\dagger\right] = -\frac{1}{Z}\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}}c^\dagger c(\tau)\right] \\ &= \frac{1}{Z}\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}}\mathcal{T}_\tau(c(\tau)c^\dagger)\right] = -G^M(\tau) \end{aligned} \tag{140}$$

where the minus sign is added because we are dealing with fermionic systems. Look that we found that Matsubara Green's function is periodic with a period 2β, so it can be developed in Fourier series:

$$G^M(n) = \frac{1}{2}\int_{-\beta}^{\beta}\mathrm{e}^{\imath n\pi\tau/\beta}G^M(\tau)\mathrm{d}\tau = \frac{1-\mathrm{e}^{-\imath n\pi}}{2}\int_0^\beta \mathrm{e}^{\imath n\pi\tau/\beta}G^M(\tau)\mathrm{d}\tau \tag{141a}$$

$$G^M(\tau) = \frac{1}{\beta}\sum_n \mathrm{e}^{-\imath n\pi\tau/\beta}G^M(n) \tag{141b}$$

The anti-periodicity property makes that only odd n values work for fermions.

$$G^M(\imath\omega_n) = \int_0^\beta \mathrm{e}^{\imath\omega_n\tau}G^M(\tau)\mathrm{d}\tau \qquad \omega_n = (2n+1)\frac{\pi}{\beta} \tag{142a}$$

$$G^M(\tau) = \frac{1}{\beta}\sum_n \mathrm{e}^{-\imath\omega_n\tau}G^M(\imath\omega_n) \tag{142b}$$

The Matsubara Green's function can be expanded with Hamiltonian eigenstates as other Green's function in equilibrium theory[9]

$$G^M(\tau) = -\frac{1}{Z}\sum_{m,n}\mathrm{e}^{-\beta\varepsilon_n}\mathrm{e}^{(\varepsilon_n-\varepsilon_m)\tau}\langle\Psi_n|c|\Psi_m\rangle\langle\Psi_m|c^\dagger|\Psi_n\rangle \tag{143}$$

and now we can compute its frequency representation:

$$\begin{aligned} G^M(\imath\omega_k) &= -\frac{1}{Z}\sum_{n,m}\mathrm{e}^{-\beta\varepsilon_n}\int_0^\beta \mathrm{e}^{(\imath\omega_k+\varepsilon_n-\varepsilon_m)\tau}\langle\Psi_n|c|\Psi_m\rangle\langle\Psi_m|c^\dagger|\Psi_n\rangle \\ &= -\frac{1}{Z}\sum_{m,n}\left(\mathrm{e}^{-\beta\varepsilon_n}+\mathrm{e}^{-\beta\varepsilon_m}\right)\frac{\langle\Psi_n|c|\Psi_m\rangle\langle\Psi_m|c^\dagger|\Psi_n\rangle}{\imath\omega_k+\varepsilon_n-\varepsilon_m} \end{aligned} \tag{144}$$

This looks very similar to retarded equilibrium Green's function. We can define an analytical continuation on the complex plane

$$G(z) = -\frac{1}{Z}\sum_{m,n}\left(\mathrm{e}^{-\beta\varepsilon_n}+\mathrm{e}^{-\beta\varepsilon_m}\right)\frac{\langle\Psi_n|c|\Psi_m\rangle\langle\Psi_m|c^\dagger|\Psi_n\rangle}{z+\varepsilon_n-\varepsilon_m} \tag{145}$$

such that for $z = \imath\omega_k$ we recover the Matsubara Green's function and for $z = \omega + \imath\eta$ we recover the retarded equilibrium Green's function. This allow us to compute the Matsubara from retarded-equilibrium and vice-versa.

2.7.1 Analytical continuation

After the computation of the Matsubara Green's function you have a point set (y_i, x_i). This can be approximated with a non-linear model $f(x_i,\beta)$ where β is a vector containing all the parameters of the model. To fit the

[9] Work with Matsubara Green's function is like work in equilibrium since Hamiltonian is always imaginary-time independent.

points with the model we are using the least squares technique. This consists in to minimize the sum of the squares of the error at every point $r_i = y_i - f(x_i, \beta)$.

$$S = \sum_{i=1}^{n} r_i^2 \tag{146}$$

$$\frac{\partial S}{\partial \beta_j} = 2 \sum_{i=1}^{n} r_i \frac{\partial r_i}{\partial \beta_j} = 0 \tag{147}$$

This is done by an iterative process, $\beta = \beta^k$ with $k \to \infty$ (this superscript k is an iteration index) and $\beta^{k+1} = \beta^k + \Delta\beta$. This $\Delta\beta$ can be computed by a linearisation of the model

$$f(x_i, \beta) \simeq f(x_i, \beta^k) + \sum_{j=1}^{m} J_{ij} \Delta\beta_j \tag{148}$$

where we defined the Jacobian matrix

$$J_{ij} = \left. \frac{\partial f(x_i, \beta)}{\partial \beta_j} \right|_{\beta=\beta^k} = -\frac{\partial r_i}{\partial \beta_j}. \tag{149}$$

With this we can redefine local error

$$r_i = y_i - f(x_i, \beta^k) + f(x_i, \beta^k) - f(x_i, \beta) \simeq \Delta y_i - \sum_{s=1}^{m} J_{is} \Delta\beta_s \tag{150}$$

to find the minimum of the error function

$$\frac{\partial S}{\partial \beta_j} = -2 \sum_{i=1}^{n} J_{ij} \left[\Delta y_i - \sum_{s=1}^{m} J_{is} \Delta\beta_s \right] = 0 \tag{151}$$

which expressed in matrix notation we can find the following condition

$$J^T J \Delta\beta = J^T \Delta \mathbf{y}. \tag{152}$$

Now we can compute $\Delta\beta$ in function of the data set and the model computed with the k-th iteration parameters since the matrix $J^T J$ is a squared matrix, so it is invertible.

The model chosen is Padé approximation

$$R(x) = \frac{P(x)}{Q(x)} = \frac{\sum_{i=0}^{m} a_i x^i}{1 + \sum_{j=1}^{n} b_j x^j} \tag{153}$$

which is the better approximation of order $m + n$ for a function. Notice that because of the behaviour of Matsubara Green's function, which tends to 0 for $|z| \to \infty$ it would be convenient that $n > m$. If we define $\beta = (a_0, ..., a_m, b_1, ..., b_n)$, so $\beta_j = a_j$ for $j = 0, ..., m$ and $\beta_j = b_{j-m}$ for $j = m + 1, ..., m + n$, the Jacobian can be easily computed

$$J_{ij} = \begin{cases} \dfrac{1}{Q(x_i)} x_i^j & j = 0, ..., m \\ -\dfrac{R(x_i)}{Q(x_i)} x_i^{j-m} & j = m+1, ..., m+n \end{cases}. \tag{154}$$

Finally only an initial guess is needed. First of all a_m and b_m should be non-zero to capture maximum degree of polynomials and also take a look that non of your x_i is a zero of $Q(x)$.

2.7.2 Products in frequency space

It will be useful to analyse how direct and convolution products act in frequency space in periodic functions as Matsubara components of contour functions. First of all let's define the convolution:

$$C(\tau) = \int_0^\beta A(\tau') B(\tau - \tau') \mathrm{d}\tau' \tag{155}$$

and compute the transform:

$$\begin{aligned} C(\imath\omega_k) &= \int_0^\beta \mathrm{e}^{\imath\omega_k\tau}\left[\int_0^\beta A(\tau')B(\tau-\tau')\mathrm{d}\tau'\right]\mathrm{d}\tau = \int_0^\beta \mathrm{e}^{\imath\omega_k\tau'}A(\tau')\left[\int_{-\tau'}^{\beta-\tau'}\mathrm{e}^{\imath\omega_k\sigma}B(\sigma)\mathrm{d}\sigma\right]\mathrm{d}\tau' \\ &= \int_0^\beta \mathrm{e}^{\imath\omega_k\tau'}A(\tau')\left[\int_0^{\beta-\tau'}\mathrm{e}^{\imath\omega_k\sigma}B(\sigma)\mathrm{d}\sigma - \mathrm{e}^{-\imath\omega_k\beta}\int_{\beta-\tau'}^{\beta}\mathrm{e}^{\imath\omega_k\sigma'}B(\sigma')\mathrm{d}\sigma'\right]\mathrm{d}\tau' \\ &= A(\imath\omega_k)B(\imath\omega_k) \end{aligned} \tag{156}$$

Here we have used the variable changes $\sigma = \tau - \tau'$ and $\sigma' = \sigma + \beta$ and the fact that $\mathrm{e}^{\pm\imath\omega_k\beta} = -1\ \forall k = 2n+1 : n \in \mathbb{Z}$. We can see how we recover the convolution theorem.

Now let's see how to transform products like $C(\tau) = A(\tau)B(\tau)$. First let's define the convolution on frequency space:

$$[A * B](\imath\omega_k) = \sum_m A(\imath\omega_m)B(\imath\omega_k - \imath\omega_m) \tag{157}$$

and go to imaginary-time space where we will recover $C(\tau)$:

$$C(\tau) = \frac{1}{\beta^2}\sum_k [A*B](\imath\omega_k)\mathrm{e}^{-\imath\omega_k\tau} = \frac{1}{\beta^2}\sum_m A(\imath\omega_m)\mathrm{e}^{-\imath\omega_m\tau}\sum_n B(\imath\omega_n)\mathrm{e}^{-\imath\omega_n\tau} = A(\tau)B(\tau) \tag{158}$$

In this derivation we have used $\omega_n = \omega_k - \omega_m$. At the end we can see that we also recover the convolution theorem.

$$C(\imath\omega_k) = \frac{1}{\beta}[A*B](\imath\omega_k) = \frac{1}{\beta}\sum_m A(\imath\omega_m)B(\imath\omega_k - \imath\omega_m) \tag{159}$$

2.8 Keldysh formalism

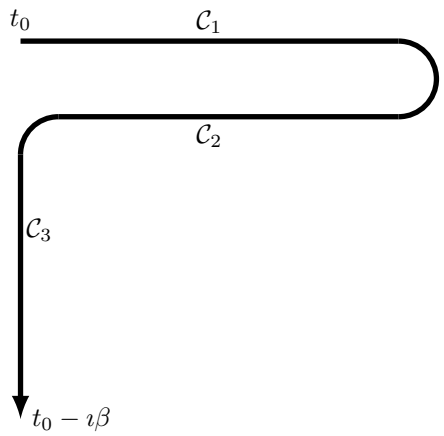


Figure 3: Keldysh contour divided into three branches being $\mathcal{C}_1$ and $\mathcal{C}_2$ into the real axis and $\mathcal{C}_3$ into the imaginary axis.

The non-equilibrium Green's function $G_{\mu\nu}(t,t') = -\imath\left\langle \mathcal{T}_\mathcal{C}[c_\mu(t), c_\nu^\dagger(t')]\right\rangle$ can be divided into nine components $G^{ij}_{\mu\nu}(t,t')$ such that $G_{\mu\nu}(t,t') = G^{ij}_{\mu\nu}(t,t')$ if $t \in \mathcal{C}_i, t' \in \mathcal{C}_j$. The components with a time argument on the imaginary branch, $t = t_0 - \imath\tau$ (or $t' = t_0 - \imath\tau'$) will be labeled only with τ (or τ'). Now look that the largest real-time argument can be traslated from $\mathcal{C}_1$ to $\mathcal{C}_2$ and viceversa giving us some redundances.

$$G^{11}(t,t') = G^{12}(t,t') \qquad \text{if} \quad t' \geq t \tag{160a}$$
$$G^{11}(t,t') = G^{21}(t,t') \qquad \text{if} \quad t' < t \tag{160b}$$
$$G^{22}(t,t') = G^{12}(t,t') \qquad \text{if} \quad t' \leq t \tag{160c}$$
$$G^{22}(t,t') = G^{21}(t,t') \qquad \text{if} \quad t' > t \tag{160d}$$
$$G^{13}(t,\tau') = G^{23}(t,\tau') \tag{160e}$$
$$G^{31}(\tau,t') = G^{32}(\tau,t') \tag{160f}$$

This equations restrict to only six linearly independent physical components defined as retarded, advanced, Keldish, left-mixing, right-mixing and Matsubara components[10]:

$$G^R_{\mu\nu}(t,t') = \frac{1}{2}\left(G^{11} - G^{12} + G^{21} - G^{22}\right) = -\imath\Theta(t-t')\left\langle\{c_\mu(t), c^\dagger_\nu(t')\}\right\rangle \tag{161a}$$

$$G^A_{\mu\nu}(t,t') = \frac{1}{2}\left(G^{11} + G^{12} - G^{21} - G^{22}\right) = \imath\Theta(t'-t)\left\langle\{c_\mu(t), c^\dagger_\nu(t')\}\right\rangle \tag{161b}$$

$$G^K_{\mu\nu}(t,t') = \frac{1}{2}\left(G^{11} + G^{12} + G^{21} + G^{22}\right) = -\imath\left\langle[c_\mu(t), c^\dagger_\nu(t')]\right\rangle \tag{161c}$$

$$G^\rceil_{\mu\nu}(t,\tau') = \frac{1}{2}\left(G^{13} + G^{23}\right) = \imath\left\langle c^\dagger_\nu(\tau')c_\mu(t)\right\rangle \tag{161d}$$

$$G^\lceil_{\mu\nu}(\tau,t') = \frac{1}{2}\left(G^{31} + G^{32}\right) = -\imath\left\langle c_\mu(\tau)c^\dagger_\nu(t')\right\rangle \tag{161e}$$

$$G^M_{\mu\nu}(\tau,\tau') = -\imath G^{33} = -\left\langle\mathcal{T}_\tau[c_\mu(\tau)c^\dagger_\nu(\tau')]\right\rangle \tag{161f}$$

Alternatively we can define two more components defined in the real-time axis, lesser and greater.

$$G^<_{\mu\nu}(t,t') = G^{12} = \imath\left\langle c^\dagger_\nu(t')c_\mu(t)\right\rangle \tag{162a}$$

$$G^>_{\mu\nu}(t,t') = G^{21} = -\imath\left\langle c_\mu(t)c^\dagger_\nu(t')\right\rangle \tag{162b}$$

If we analyze the complex conjugate of the physical components we can add more restrictions to the linear independence[11].

$$(G^{<,>,K}_{\mu\nu})^*(t,t') = -G^{<,>,K}_{\nu\mu}(t',t) \tag{163a}$$

$$(G^R_{\mu\nu})^*(t,t') = G^A_{\nu\mu}(t',t) \tag{163b}$$

$$(G^\rceil_{\mu\nu})^*(t,\tau') = G^\lceil_{\nu\mu}(\beta-\tau',t) \tag{163c}$$

$$(G^M_{\mu\nu})^*(\tau-\tau') = G^M_{\nu\mu}(\tau-\tau') \tag{163d}$$

Look that Hamiltonian is imaginary-time independent, so Matsubara component has translational symmetry, $G^M_{\mu\nu}(\tau,\tau') = G^M_{\mu\nu}(\tau-\tau')$, in consequence it is also hermitian. Thanks to this hermitian relations we can stablish a minimal set to solve Dyson equations: $\{G^R, G^<, G^\rceil, G^M\}$.

2.8.1 Initial conditions

One can see that by definition Matsubara component can be used to compute the initial conditions for the other components (related by the fact which will be seen after that Matsubara compoonent describes the equilibrium state). Look that for example the limit $\tau - \tau' \to 0^-$, so $\tau < \tau'$. In this case $G^M_{\mu\nu}(0^-) = \left\langle c^\dagger_\nu c_\mu\right\rangle = \imath G^<_{\mu\nu}(0,0)$. Also, by imaginary-time translational symmetry G^M can be related with left/right-mixed components when real-time is zero.

$$G^>(0,0) = \imath G^M(0^+) \tag{164a}$$

$$G^<(0,0) = \imath G^M(0^-) = -\imath G^M(\beta - 0^+) \tag{164b}$$

$$G^\rceil(0,\tau') = \imath G^M(-\tau') = -\imath G^M(\beta-\tau') \tag{164c}$$

$$G^\lceil(\tau,0) = \imath G^M(\tau) \tag{164d}$$

2.8.2 Revision of Langreth thorem

With all of this new components introduced Langreth theorem can be rederived into this new rules. First start with the contour product $C(t,t') = \imath A(t,t')B(t',t)$:

$$C^R(t,t') = \imath A^R(t,t')B^<(t',t) + \imath A^<(t,t')B^A(t',t) \tag{165a}$$

$$C^{\gtrless}(t,t') = \imath A^{\gtrless}(t,t')B^{\lesseqgtr}(t',t) \tag{165b}$$

$$C^\rceil(t,\tau') = \imath A^\rceil(t,\tau')B^\lceil(\tau',t) \tag{165c}$$

$$C^M(\tau) = A^M(\tau)B^M(-\tau) \tag{165d}$$

[10] Retarded and advanced are already known from previous sections.

[11] To perform the hermitian conjugate of a fermionic operator defined on imaginary-time axis take into account the KMS boundary conditions: $G(t,-\imath\tau') = -G(t,-\imath(\tau'+\beta))$ and $G(\tau,t') = -G(-\imath(\tau+\beta),t')$ (in fermion case). This can be derived taking into account the cyclic property of the trace.

Now let's decompose the product $C(t,t') = \imath A(t,t')B(t,t')$

$$C^R(t,t') = \imath A^<(t,t')B^R(t,t') + \imath A^R(t,t')B^>(t,t') \tag{166a}$$
$$C^{\gtrless}(t,t') = \imath A^{\gtrless}(t,t')B^{\gtrless}(t,t') \tag{166b}$$
$$C^{\rceil}(t,\tau') = \imath A^{\rceil}(t,\tau')B^{\rceil}(t,\tau') \tag{166c}$$
$$C^M(\tau) = A^M(\tau)B^M(\tau) \tag{166d}$$

Also we can deduce the rules for the convolution $C(t,t') = [A*B](t,t') = \int_{\mathcal{C}} A(t,t_1)B(t_1,t')\mathrm{d}t_1$:

$$C^R(t,t') = \int_{t'}^{t} A^R(t,t_1)B^R(t_1,t')\mathrm{d}t_1 \tag{167a}$$
$$C^{\gtrless}(t,t') = \int_0^t A^R(t,t_1)B^{\gtrless}(t_1,t')\mathrm{d}t_1 + \int_0^{t'} A^{\gtrless}(t,t_1)B^A(t_1,t')\mathrm{d}t_1 - \imath\int_0^\beta A^{\rceil}(t,\tau_1)B^{\lceil}(\tau_1,t')\mathrm{d}\tau_1 \tag{167b}$$
$$C^{\rceil}(t,\tau') = \int_0^t A^R(t,t_1)B^{\rceil}(t_1,\tau')\mathrm{d}t_1 + \int_0^\beta A^{\rceil}(t,\tau_1)B^M(\tau_1-\tau)\mathrm{d}\tau_1 \tag{167c}$$
$$C^M(\tau) = \int_0^\beta A^M(\tau-\tau_1)B^M(\tau_1)\mathrm{d}\tau_1 \tag{167d}$$

2.9 Self-energy approximations

It was shown by Baym that the macroscopic conservation laws imposes that $\Sigma(q,q')$ (here $q = (\mathbf{x},t)$ to brief notation) is obtained from a functional $\Phi[G]$

$$\Sigma(q,q') = \frac{\delta\Phi}{\delta G(q',q)} \tag{168}$$

By this property the self-energy can be well approximated.

2.9.1 Hartree-Fock approximation

The first order diagrams of the self energy are giving us a function which is singular, this is proportional to $\delta_{\mathcal{C}}(t,t')$ (defined as contour delta which is only non-zero for $t = t'$ and both time arguments at the same branch), so $\Sigma^{HF}(q,q') = \delta_{\mathcal{C}}(t,t')\Sigma^{HF}(\mathbf{x},\mathbf{x}',t)$. From the variational definition we can find

$$\Sigma^{HF}(\mathbf{x},\mathbf{x}',t) = \imath G^<(\mathbf{x},t;\mathbf{x}',t)v(\mathbf{x},\mathbf{x}') - \imath\delta(\mathbf{x}-\mathbf{x}')\int v(\mathbf{x},\mathbf{y})G^<(\mathbf{y},t;\mathbf{y},t)\mathrm{d}\mathbf{y} \tag{169}$$

We can replace the field operators on Green's functions by creation/annihilation ones

$$\Sigma^{HF}(\mathbf{x},\mathbf{x}',t) = \imath\sum_{\lambda,\kappa} G^<_{\lambda\kappa}(t,t)\psi_\lambda(\mathbf{x})\psi^*_\kappa(\mathbf{x}')v(\mathbf{x},\mathbf{x}') - \imath\delta(\mathbf{x}-\mathbf{x}')\sum_{\lambda,\kappa} G^<_{\lambda\kappa}(t,t)\int\psi_\lambda(\mathbf{y})\psi^*_\kappa(\mathbf{y})v(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y} \tag{170}$$

and finally get the matricial expression for self-energy

$$\begin{aligned}\Sigma^{HF}_{\mu\nu}(t) &= \imath\sum_{\lambda,\kappa} G^<_{\lambda\kappa}(t,t)\left[\int\int\psi_\lambda(\mathbf{x})\psi^*_\kappa(\mathbf{x}')v(\mathbf{x},\mathbf{x}')\psi^*_\mu(\mathbf{x})\psi_\nu(\mathbf{x}')\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\right.\\ &\left.\quad - \int\int\psi_\lambda(\mathbf{y})\psi^*_\kappa(\mathbf{y})v(\mathbf{x},\mathbf{y})\psi^*_\mu(\mathbf{x})\psi_\nu(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y}\right]\\ &= \imath\sum_{\lambda,\kappa} G^<_{\lambda\kappa}(t,t)\left[v^{\mu\kappa}_{\lambda\nu} - v^{\mu\kappa}_{\nu\lambda}\right]\end{aligned} \tag{171}$$

where v is the e-e coulomb operator so the final expression is in fact a self-interaction term.

This time-local self-energy component should be added to Hamiltonian to get an effective time-dependent Hamiltonian and get separated the correlated-time part of self-energy (second order and beyond) which can be decomposed into contour components. But before we need to get the initial condition for the Hartree-Fock self-energy. Recalling the initial conditions:

$$\Sigma^{HF}_{\mu\nu}(0) = \imath\sum_{\lambda,\kappa} G^<_{\lambda\kappa}(0,0)\left[v^{\mu\kappa}_{\lambda\nu} - v^{\mu\kappa}_{\nu\lambda}\right] = \sum_{\lambda,\kappa}\lim_{\tau\to0^+} G^M_{\lambda\kappa}(\beta-\tau)\left[v^{\mu\kappa}_{\lambda\nu} - v^{\mu\kappa}_{\nu\lambda}\right] \tag{172}$$

The initial condition for time-local self-energy is related with Matsubara Green's function at β which can be recovered knowing the Matsubara component on frequency space, giving us a self-consistent scheme to derive this initial condition.

$$\Sigma^{HF}_{\mu\nu}(0) = -\frac{1}{\beta}\lim_{\tau\to 0^+}\sum_k\sum_{\lambda,\kappa}(1+\imath\omega_k\tau)G^M_{\lambda\kappa}(\imath\omega_k)\left[v^{\mu\kappa}_{\lambda\nu} - v^{\mu\kappa}_{\nu\lambda}\right] \tag{173}$$

2.9.2 Second Born approximation

This approximation consists into add two second order diagrams into the self-energy: $\Sigma(q,q') = \Sigma^{HF}(q,q') + \Sigma^{(2a)}(q,q') + \Sigma^{(2b)}(q,q')$

$$\Sigma^{(2a)}(q,q') = G(q,q')\int\int v(q,q_1)G(q_1,q_2)G(q_2,q_1)v(q_2,q')\mathrm{d}q_1\mathrm{d}q_2 \tag{174a}$$

$$\Sigma^{(2b)}(q,q') = -\int\int G(q,q_1)v(q,q_2)G(q_1,q_2)G(q_2,q')v(q_1,q')\mathrm{d}q_1\mathrm{d}q_2 \tag{174b}$$

Here $v(q,q') = \delta_{\mathcal{C}}(t,t')v(\mathbf{x},\mathbf{x}')$ is the local time coulomb interaction. As for the HF approximation we can recover the expression for orbital basis:

$$\Sigma^{(2a)}_{\mu\nu}(t,t') = \imath\sum_{\lambda,\kappa}\sum_{\alpha,\beta}\sum_{\xi,\chi}G_{\lambda\kappa}(t,t')v^{\mu\chi}_{\lambda\alpha}P^{\alpha\xi}_{\chi\beta}(t,t')v^{\beta\kappa}_{\xi\nu} \tag{175a}$$

$$\Sigma^{(2b)}_{\mu\nu}(t,t') = -\imath\sum_{\lambda,\kappa}\sum_{\alpha,\beta}\sum_{\xi,\chi}v^{\mu\beta}_{\lambda\xi}v^{\kappa\chi}_{\alpha\nu}P^{\lambda\alpha}_{\beta\kappa}(t,t')G_{\xi\chi}(t,t') \tag{175b}$$

2.9.3 GW approximation

In this approximation the non-singular part of the self-energy is given by a screened interaction:

$$W(q,q') = v(q,q') + \int\int v(q,q_1)P(q_1,q_2)W(q_2,q')\mathrm{d}q_1\mathrm{d}q_2 \tag{176}$$

This is the coulombic potential dressed by the polarizability of the system. This polarizability is represented with the irreducible polarization $P(q,q') = -\imath G(q,q')G(q',q)$ and it is trivial that for small polarizabilities screened interaction becomes the bare coulombic interaction. The screened interaction has a singular term, so for numerical purposes it should be more useful to define $\tilde{W} = W - v$:

$$\tilde{W}(q,q') = \int\int v(q,q_1)P(q_1,q_2)v(q_2,q')\mathrm{d}q_1\mathrm{d}q_2 + \int\int v(q,q_1)P(q_1,q_2)\tilde{W}(q_2,q')\mathrm{d}q_1\mathrm{d}q_2 \tag{177}$$

For the expression in orbital basis let's first define the irreducible polarization components:

$$P^{\lambda\kappa}_{\mu\nu}(t,t') = -\imath G_{\lambda\nu}(t,t')G_{\kappa\mu}(t',t) \tag{178}$$

which comes from the expansion of the Green's functions on orbital basis. Then the screened interaction on orbital basis shuold be defined as:

$$W^{\mu\nu}_{\lambda\kappa}(t,t') = \int\int \psi^*_\mu(\mathbf{x})\psi^*_\nu(\mathbf{x}')W(q,q')\psi_\lambda(\mathbf{x})\psi_\kappa(\mathbf{x}')\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \tag{179}$$

and its equation

$$\begin{aligned}
\tilde{W}^{\mu\nu}_{\lambda\kappa}(t,t') &= \sum_{\alpha,\beta,\xi,\chi}\int\int\int\int \psi^*_\mu(\mathbf{x})\psi_\lambda(\mathbf{x})v(q,q_1)\psi^*_\alpha(\mathbf{x}_1)\psi_\xi(\mathbf{x}_1)P^{\alpha\beta}_{\xi\chi}(t_1,t_2)\psi^*_\beta(\mathbf{x}_2)\psi_\chi(\mathbf{x}_2)W(q_2,q') \\
&\qquad\qquad \times\psi^*_\nu(\mathbf{x}')\psi_\kappa(\mathbf{x}')\mathrm{d}q_1\mathrm{d}q_2\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \\
&= \sum_{\alpha,\beta,\xi,\chi}v^{\mu\alpha}_{\lambda\xi}\int_{\mathcal{C}}P^{\xi\chi}_{\alpha\beta}(t,t_2)\left[\tilde{W}^{\beta\nu}_{\chi\kappa}(t_2,t') + \delta_{\mathcal{C}}(t_2,t')v^{\beta\nu}_{\chi\kappa}\right]\mathrm{d}t_2 \\
&= \sum_{\alpha,\beta,\xi,\chi}v^{\mu\alpha}_{\lambda\xi}P^{\xi\chi}_{\alpha\beta}(t,t')v^{\beta\nu}_{\chi\kappa} + \sum_{\alpha,\xi}v^{\mu\alpha}_{\lambda\xi}X^{\xi\nu}_{\alpha\kappa}(t,t')
\end{aligned} \tag{180}$$

Here we have defined the convolution product between irreducible polarization and time-correlated screened interaction as $X(t,t')$.

Finally we can define the time-correlated part of the self energy, Σ, as:

$$\begin{aligned}\Sigma(q,q') &= \imath G(q,q')\tilde{W}(q,q')\\ \Sigma_{\mu\nu}(t,t') &= \imath\sum_{\lambda,\kappa} G_{\lambda\kappa}(t,t')\tilde{W}^{\mu\kappa}_{\lambda\nu}(t,t')\end{aligned} \tag{181}$$

which fulfils the following initial conditions:

$$\tilde{W}^{<}(0,0) = \imath\tilde{W}^{M}(0^{-}) \tag{182a}$$

$$\tilde{W}^{\rceil}(0,\tau) = -\imath\tilde{W}^{M}(\beta-\tau) \tag{182b}$$

Compute the Matsubara component is a very important problem since it solves the equilibrium problem by analytical continuation and it establishes the initial conditions for the non-equilibrium problem. Also the solution becomes simple since by imaginary-time translational symmetry it can be solved in Matsubara-frequency space, where imaginary-time convolution integrals become algebraic products.

Let's find the irreducible polarization in frequency space. Since $P^M(\tau) = \imath G^M(\tau)G^M(-\tau)$ it will be a convolution product, so we should find how $G(-\tau)$ is expressed in frequency space:

$$\int_0^\beta \mathrm{e}^{\imath\omega_k\tau}G^M(-\tau)\mathrm{d}\tau = -\mathrm{e}^{\imath\omega_k\beta}\int_0^\beta \mathrm{e}^{\imath(-\omega_k)\sigma}G^M(\sigma)(-\mathrm{d}\sigma) = -G^M(-\imath\omega_k) \tag{183}$$

where we have used $\sigma = \beta - \tau$. Now we can find the irreducible polarization in frequency space:

$$P^M(\imath\omega_k) = -\frac{\imath}{\beta}\sum_m G^M(\imath\omega_k - \imath\omega_m)G^M(-\imath\omega_m) \tag{184}$$

Now we can easily find the X-function and the screened interaction since they are defined as a convolution.

$$X^M(\imath\omega_k) = P^M(\imath\omega_k)\tilde{W}^M(\imath\omega_k) = -\frac{\imath}{\beta}\sum_m G^M(\imath\omega_k - \imath\omega_m)G^M(-\imath\omega_m)\tilde{W}^M(\imath\omega_k) \tag{185}$$

$$\tilde{W}^M(\imath\omega_k) = vP^M(\imath\omega_k)v + vX^M(\imath\omega_k) = \frac{vP^M(\imath\omega_k)v}{1-vP^M(\imath\omega_k)} = \frac{v}{\left[vP^M(\imath\omega_k)\right]^{-1}-1} \tag{186}$$

And finally the correlated self-energy:

$$\Sigma^M(\imath\omega_k) = -\frac{\imath}{\beta}\sum_m G^M(\imath\omega_m)\tilde{W}^M(\imath\omega_k - \imath\omega_m) = -\frac{\imath}{\beta}\sum_m \frac{G^M(\imath\omega_k - \imath\omega_m)v}{\left[\frac{v}{\imath\beta}\sum_n G^M(\imath\omega_m - \imath\omega_n)G^M(-\imath\omega_n)\right]^{-1}-1} \tag{187}$$

In this expression we can see clearly the nature of the self-energy as a functional of Green's function.

2.10 Dyson equation and KB formulation

As we saw, from perturbative expantion we can take the Dyson equation which can be presented into two forms depending if the expansion of the improper self-energy is done from right or from left.

$$G_{\mu\nu}(t,t') = G^0_{\mu\nu}(t,t') + \int_{\mathcal{C}}\int_{\mathcal{C}} G^0_{\mu\lambda}(t,t_1)\Sigma_{\lambda\kappa}(t_1,t_2)G_{\kappa\nu}(t_2,t')\mathrm{d}t_1\mathrm{d}t_2 \tag{188a}$$

$$G_{\mu\nu}(t,t') = G^0_{\mu\nu}(t,t') + \int_{\mathcal{C}}\int_{\mathcal{C}} G_{\mu\lambda}(t,t_1)\Sigma_{\lambda\kappa}(t_1,t_2)G^0_{\kappa\nu}(t_2,t')\mathrm{d}t_1\mathrm{d}t_2 \tag{188b}$$

Here the non-interactive propagator evolves by the action of non-interaxtive (or quadratic) hamiltonian $\mathcal{H}_0 = \sum_{\mu\nu}\varepsilon^\mu_\nu(t)c^\dagger_\mu c_\nu$:

$$G^0_{\mu\nu}(t,t') = -\imath\left\langle\mathcal{T}_{\mathcal{C}}\tilde{c}_\mu(t)\tilde{c}^\dagger_\nu(t')\right\rangle \tag{189}$$

where $\tilde{c}(t) = \mathrm{e}^{\imath\mathcal{H}_0 t}c\mathrm{e}^{-\imath\mathcal{H}_0 t}$. Now recalling the fact that $[c^\dagger_\mu c_\nu, c_\lambda] = -\delta_{\mu\lambda}c_\nu$, $[c^\dagger_\mu c_\nu, c^\dagger_\lambda] = \delta_{\nu\lambda}c^\dagger_\mu$ and $\partial_t c(t) = \imath[\mathcal{H}, c](t)$ we can compute the derivatives of the non-interactive Green's function:

$$\imath\partial_t G^0_{\lambda\kappa}(t,t') = \sum_\nu \varepsilon^\lambda_\nu(t)G^0_{\nu\kappa}(t,t') + \delta_{\mathcal{C}}(t,t')\delta_{\lambda\kappa} \tag{190a}$$

$$-\imath\partial_{t'} G^0_{\lambda\kappa}(t,t') = \sum_\mu \varepsilon^\mu_\kappa(t)G^0_{\lambda\mu}(t,t') + \delta_{\mathcal{C}}(t,t')\delta_{\lambda\kappa} \tag{190b}$$

where the contour delta term comes from the implicit $\Theta_{\mathcal{C}}(t,t')$ on time-order operator[12]. Now we can compute the derivatives of the Green's function.

$$\imath\partial_t G_{\mu\nu}(t,t') - \sum_\beta \varepsilon^\mu_\beta(t) G_{\beta\nu}(t,t') - \int_{\mathcal{C}} \Sigma_{\mu\kappa}(t,t_2) G_{\kappa\nu}(t_2,t')\mathrm{d}t_2 = \delta_{\mathcal{C}}(t,t')\delta_{\mu\nu} \tag{191a}$$

$$-\imath\partial_{t'} G_{\mu\nu}(t,t') - \sum_\alpha \varepsilon^\alpha_\nu(t) G_{\mu\alpha}(t,t') - \int_{\mathcal{C}} G_{\mu\lambda}(t,t_1) \Sigma_{\lambda\nu}(t_1,t')\mathrm{d}t_1 = \delta_{\mathcal{C}}(t,t')\delta_{\mu\nu} \tag{191b}$$

This is the Kadanoff-Baym formulation of Dyson equation which is not more than an integro-differential form of Dyson equation. To avoid orbital indices we can use matrix notation and the left-derivative operator $\overleftarrow{\partial}$.

$$\left[\imath\partial_t - \varepsilon(t)\right] G(t,t') - \int_{\mathcal{C}} \Sigma(t,t_2) G(t_2,t')\mathrm{d}t_2 = \delta_{\mathcal{C}}(t,t') \tag{192a}$$

$$G(t,t')\left[-\imath\overleftarrow{\partial}_{t'} - \varepsilon(t)\right] - \int_{\mathcal{C}} G(t,t_1)\Sigma(t_1,t')\mathrm{d}t_1 = \delta_{\mathcal{C}}(t,t') \tag{192b}$$

2.11 Numerical approach to KB

By a correct application of the Langreth theorem and the time limits for the different components of the Green's function we can write Kadanoff-Baym equations (we will ignore the orbital subscripts)

$$\left[\imath\partial_t - \epsilon(t)\right] G^R(t,t') - \int_{t'}^{t} \Sigma^R(t,t_1) G^R(t_1,t')\mathrm{d}t_1 = \delta(t-t') \tag{193a}$$

$$\left[\imath\partial_t - \epsilon(t)\right] G^<(t,t') - \int_{0}^{t} \Sigma^R(t,t_1) G^<(t_1,t')\mathrm{d}t_1 = Q^<(t,t') \tag{193b}$$

$$\left[\imath\partial_t - \epsilon(t)\right] G^\rceil(t,\tau') - \int_{0}^{t} \Sigma^R(t,t_1) G^\rceil(t_1,\tau')\mathrm{d}t_1 = Q^\rceil(t,\tau') \tag{193c}$$

$$\left[-\partial_\tau - \epsilon(0^-)\right] G^M(\tau) - \int_0^\beta \Sigma^M(\tau-\tau_1) G^M(\tau_1)\mathrm{d}\tau_1 = \delta(\tau) \tag{193d}$$

and the conjugate version

$$G^R(t,t')\left[-\imath\overleftarrow{\partial}_{t'} - \epsilon(t')\right] - \int_{t'}^{t} G^R(t,t_1)\Sigma^R(t_1,t')\mathrm{d}t_1 = \delta(t-t') \tag{194a}$$

$$G^<(t,t')\left[-\imath\overleftarrow{\partial}_{t'} - \epsilon(t')\right] - \int_{0}^{t'} G^<(t,t_1)\Sigma^A(t_1,t')\mathrm{d}t_1 = \bar{Q}^<(t,t') \tag{194b}$$

$$G^\rceil(t,\tau')\left[-\imath\overleftarrow{\partial}_{t'} - \epsilon(t')\right] - \int_{0}^{\beta} G^\rceil(t,\tau_1)\Sigma^M(\tau_1-\tau')\mathrm{d}\tau_1 = \bar{Q}^\rceil(t,\tau') \tag{194c}$$

$$G^M(\tau)\left[\overleftarrow{\partial}_\tau - \epsilon(0^+)\right] - \int_0^\beta \Sigma^M(\tau-\tau_1) G^M(\tau)\mathrm{d}\tau_1 = \delta(\tau) \tag{194d}$$

where $\varepsilon(t)$ are the hamiltonian matrix elements (both, time-dependent and time-independent) and the $Q(t,t')$, $\bar{Q}(t,t')$ functions

$$Q^<(t,t') = \int_0^{t'} \Sigma^<(t,t_1) G^A(t_1,t')\mathrm{d}t_1 - \imath\int_0^\beta \Sigma^\rceil(t,\tau_1) G^\lceil(\tau_1,t')\mathrm{d}\tau_1 \tag{195a}$$

$$Q^\rceil(t,\tau') = \int_0^\beta \Sigma^\rceil(t,\tau_1) G^M(\tau_1-\tau')\mathrm{d}\tau_1 \tag{195b}$$

$$\bar{Q}^<(t,t') = \int_0^{t} G^R(t,t_1) \Sigma^<(t_1,t')\mathrm{d}t_1 - \imath\int_0^\beta G^\rceil(t,\tau_1)\Sigma^\lceil(\tau_1,t')\mathrm{d}\tau_1 \tag{195c}$$

$$\bar{Q}^\rceil(t,\tau') = \int_0^{t} G^R(t,t_1) \Sigma^\rceil(t_1,\tau')\mathrm{d}t_1 \tag{195d}$$

One should pay attention to the equation for the Matsubara component, since Hamiltonian is imaginary-time independent we can make the Fourier series (by the periodic property of Matsubara component, $G^M(\tau+\beta) = -G^M(\tau)$ in the fermion case)

$$G^M(\imath\omega_n) = \frac{1}{\imath\omega_n - h(0^-) - \Sigma^M(\imath\omega_n)} \tag{196}$$

[12] $\partial_t\Theta_{\mathcal{C}}(t,t') = \delta_{\mathcal{C}}(t,t')$ and $\partial_{t'}\Theta_{\mathcal{C}}(t,t') = -\delta_{\mathcal{C}}(t,t')$

resulting on the initial equilibrium state, so the other three equations can be solved by increasing time successively. This equations can be identified as Volterra integro-differential equations

$$\left(\frac{\mathrm{d}}{\mathrm{d}s}+p(s)\right)y(s)+\int_0^s K(s,u)y(u)\mathrm{d}u=q(s) \tag{197}$$

At the end lesser, retarded and left mixed components represent a set of coupled Volterra equations where we can use the Matsubara component as the initial condition. Instead we may need other components to complete the equations them can be obtained from hermitian relations.

Retarded function For the retarded Green's function we can use as initial condition $G^R_{\mu\nu}(t,t)=-\imath\delta^\mu_\nu$ since $\left\langle\{c_\mu(t),c^\dagger_\nu(t)\}\right\rangle=\delta^\mu_\nu$. For the causality property $G^R(t,t')=0$ if $t'>t$ so we can use $G^R(t'+s,t')=y(s)$ to solve the Volterra equation. Then by the use of $\imath\epsilon(t'+s)=p(s)$, $\imath\Sigma^R(t'+s,t'+u)=K(s,u)$ (so $t_1\to t'+u$) and $-\imath\delta(s)=q(s)$ we can recover VIDE.

Left-mixed function The initial condition for the left-mixed Green's funciton is completely determined by Matsubara Green's function, $G^\rceil(0,\tau')=-\imath G^M(\beta-\tau')$, so to recover VIDE we only need to use $G^\rceil(s,\tau')=y(s)$, $\imath\epsilon(s)=p(s)$, $\imath\Sigma^R(s,u)=K(s,u)$ and $-\imath Q^\rceil(s,\tau')=q(s)$.

Lesser function For the initial condition we can use the left-mixed component $G^<_{\mu\nu}(0,t')=(G^\rceil_{\nu\mu})^*(t',0)$ and then recover VIDE in the same way as the left-mixed component: $G^<(s,t')=y(s)$, $\imath\epsilon(s)=p(s)$, $\imath\Sigma^R(s,u)=K(s,u)$ and $-\imath Q^<(s,t')=q(s)$.

2.11.1 Initial condition in time domain

Numerically the solution of the Matsubara component in frequency domain implies a truncation since the Fourier anti-transform is an infinite sum over all Matsubara frequencies. For this reason should be more convenient to work at time domain. First of all we have to solve the non-interactive Matsubara Green's function, $g^M(\tau)$ which obeys

$$\left[-\partial_\tau-\epsilon\right]g^M(\tau)=\delta(\tau) \tag{198}$$

being the Dyson equation for imaginary time branch with null self-energy. Easily we can see that it's expression in frequency space is

$$g^M(\imath\omega_k)=\frac{1}{\imath\omega_k-\epsilon} \tag{199}$$

which can be compared with the solution of the Dyson equation

$$g^M(\tau)=f(\epsilon)\mathrm{e}^{-\epsilon\tau} \tag{200}$$

in order to find $g^M(0)=f(\epsilon)$. Look that this solution has been taken for an homogeneus equation and $f(\epsilon)$ should be taken with initial condition. In this case there is no directly an initial condition, insead we can see that only for $\tau=0$ the Dyson equation is inhomogeneus. This inhomogeneity is taken by the Fourier transform

$$g^M(\imath\omega_k)=\int_0^\beta f(\epsilon)\mathrm{e}^{(\imath\omega_k-\epsilon)\tau}\mathrm{d}\tau=f(\epsilon)\frac{\mathrm{e}^{(\imath\omega_k-\epsilon)\tau}}{\imath\omega_k-\epsilon}\bigg|_{\tau=0}^{\tau=\beta}=f(\epsilon)g^M(\imath\omega_k)\left[\xi\mathrm{e}^{-\epsilon\beta}-1\right] \tag{201}$$

having finally an expression for $f(\epsilon)=[\xi\mathrm{e}^{-\epsilon\beta}-1]^{-1}$.

$$g^M(\tau)=\frac{\mathrm{e}^{-\epsilon\tau}}{\xi\mathrm{e}^{-\epsilon\beta}-1} \tag{202}$$

2.11.2 Storage of the minimal set (NESSi)

To perform a numerical solution of the Green's functions we need to divide the Keldysh contour into small time slices. The real axis is divided on N_t+1 sliced with width h defining $t_n=nh$ with $n=0,...,N_t$. For the imaginary time branch it is performed in the similar way with $\tau_m=m\eta$ for $m=0,...,N_\tau$ with the particularity that this branch is restricted to $0<\tau<\beta$ so $\tau_0=0^+$ and $\tau_{N_\tau}=\beta^-$.

Every contour function $C(t,t')$ (Green's function, self energy...) is stored in a time step $T[C]_n$ with $n = 0,...,N_t$ except for Matsubara component which is defined in $n=-1$ since its time argument is in the imaginary branch (only one by time translational symmetry).

$$(T[C]_n)^R_j = C^R(nh, jh) \qquad j = 0,...,n \tag{203a}$$
$$(T[C]_n)^<_j = C^<(jh, nh) \qquad j = 0,...,n \tag{203b}$$
$$(T[C]_n)^\rceil_m = C^\rceil(nh, m\eta) \qquad m = 0,...,N_\tau \tag{203c}$$
$$(T[C]_{-1})^M_m = C^M(m\eta) \qquad m = 0,...,N_\tau \tag{203d}$$

Look that by definition for the retarded component it is only necessary store the part where $t \geq t'$. Then, by the hermitian relations and the equality $C^> - C^< = C^R - C^A$ for the lesser component is only necessary to store the part where $t \leq t'$.

2.12 Energy and Galitskii-Migdal formula

The energy of a quantum system is the expected value of the Hamiltonian. In our case we can split the hamiltonian into three terms

$$\mathcal{H}(t) = \sum_{\mu,\nu} \varepsilon^\mu_\nu(t) c^\dagger_\mu c_\nu + \sum_{\mu,\nu} h^\mu_\nu c^\dagger_\mu c_\nu + \sum_{\mu,\nu,\lambda,\kappa} v^{\mu\nu}_{\lambda\kappa} c^\dagger_\mu c^\dagger_\nu c_\kappa c_\lambda. \tag{204}$$

The first term represents the kinetic time dependent part, the second is the potential energy and the third is the e-e interaction. The expected value of the quadratic parts is related to lesser Green's function since $\langle c^\dagger_\mu(t) c_\nu(t)\rangle = \xi\imath (G^\nu_\mu)^<(t,t)$, so in absence of interactions

$$E_0 = E_{kin}(t) + E_{pot}(t) = \xi\imath \sum_{\mu,\nu} (\varepsilon(t) + h)^\mu_\nu \, (G^\nu_\mu)^<(t,t) \tag{205}$$

To compute the expected value of interaction hamiltonian we will make an analogy with Dyson equation. Recalling the derivative of a creation operator, $\partial_t c_\alpha(t) = -[\mathcal{H}, c_\alpha](t)$, and the commutation operations that will be used

$$[c^\dagger_\mu c_\nu, c_\alpha] = -\delta^\alpha_\mu c_\nu \tag{206a}$$
$$\begin{aligned}[c^\dagger_\mu c^\dagger_\nu c_\kappa c_\lambda] &= \left(\delta^\alpha_\nu c^\dagger_\mu c_\alpha - \delta^\alpha_\mu c^\dagger_\nu\right) c_\kappa c_\lambda \\ &= \left(\delta^\alpha_\nu c^\dagger_\mu - \delta^\alpha_\mu c_\alpha c^\dagger_\nu\right) c_\kappa c_\lambda\end{aligned} \tag{206b}$$

then, deriving a contour Green's function

$$\begin{aligned}
-\imath\partial_t G^\alpha_\beta(t,t') &= \delta_\mathcal{C}(t,t')\delta^\alpha_\beta + \sum_\nu [\varepsilon(t)+h]^\alpha_\nu \, G^\nu_\beta(t,t') \\
&- \frac{\imath}{2} \sum_{\mu,\nu,\lambda,\kappa} v^{\mu\nu}_{\lambda\kappa} \left\langle \mathcal{T}_\mathcal{C} \left[\delta^\alpha_\nu c^\dagger_\mu(t) c_\alpha(t) - \delta^\alpha_\mu c^\dagger_\nu(t)\right] c_\kappa(t) c_\lambda(t) c_\beta(t')\right\rangle \\
&- \frac{\imath}{2} \sum_{\mu,\nu,\lambda,\kappa} v^{\mu\nu}_{\lambda\kappa} \left\langle \mathcal{T}_\mathcal{C} \left[\delta^\alpha_\nu c^\dagger_\mu(t) - \delta^\alpha_\mu c_\alpha(t) c^\dagger_\nu(t)\right] c_\kappa(t) c_\lambda(t) c_\beta(t')\right\rangle \\
&= \delta_\mathcal{C}(t,t')\delta^\alpha_\beta + \sum_\nu [\varepsilon(t)+h]^\alpha_\nu \, G^\nu_\beta(t,t') \\
&- \frac{\imath}{2} \sum_{\mu,\nu,\lambda,\kappa} v^{\mu\nu}_{\lambda\kappa} \left\langle \mathcal{T}_\mathcal{C} \left[\delta^\alpha_\mu \delta^\alpha_\nu - 2\delta^\alpha_\mu c^\dagger_\nu(t)\right] c_\kappa(t) c_\lambda(t) c_\beta(t')\right\rangle \\
&= \delta_\mathcal{C}(t,t')\delta^\alpha_\beta + \sum_\nu [\varepsilon(t)+h]^\alpha_\nu \, G^\nu_\beta(t,t') + \imath \sum_{\nu,\lambda,\kappa} v^{\alpha\nu}_{\lambda\kappa} \left\langle \mathcal{T}_\mathcal{C} c^\dagger_\nu(t) c_\kappa(t) c_\lambda(t) c^\dagger_\beta(t')\right\rangle.
\end{aligned} \tag{207}$$

Here, in a first place we split the interaction term into the two halfs with the two possible combinations of the commutator. Then, with the last line we change the indices μ and ν and we use the property $v^{\nu\mu}_{\lambda\kappa} = -v^{\mu\nu}_{\lambda\kappa}$ to add both terms. The term related with $\delta^\alpha_\mu\delta^\alpha_\nu$ is excluded by Pauli's principle. In analogy with Dyson equation in Kdanoff-Baym form

$$[G * \Sigma]^\alpha_\beta(t,t') = \imath \sum_{\nu,\lambda,\kappa} v^{\alpha\nu}_{\lambda\kappa} \left\langle \mathcal{T}_\mathcal{C} c^\dagger_\nu(t) c_\kappa(t) c_\lambda(t) c^\dagger_\beta(t')\right\rangle. \tag{208}$$

If we make the expected value of interaction hamiltonian we can see that is the trace of lesser component of $G * \Sigma$

$$\begin{aligned} E_{int}(t) &= -\imath \sum_{\mu} ([G*\Sigma]^{\mu}_{\mu})^{<}(t,t) \\ &= -\imath \sum_{\mu,\nu} \left[\int_0^t (G^{\mu}_{\nu})^{R}(t,t_1)(\Sigma^{\nu}_{\mu})^{<}(t_1,t)dt_1 + \int_0^t (G^{\mu}_{\nu})^{<}(t,t_1)(\Sigma^{\nu}_{\mu})^{A}(t_1,t)dt_1 \right. \\ &\left. -\imath \int_0^{\beta} (G^{\mu}_{\nu})^{\rceil}(t,\tau_1)(\Sigma^{\nu}_{\mu})^{\lceil}(\tau_1,t)d\tau_1 \right] \end{aligned} \tag{209}$$

and the total energy of the system $E = E_{kin}(t) + E_{pot}(t) + E_{int}(t)$.

3 Jahn-Teller mixed states on an electromagnetic field with second quantization for electrons

3.1 Crystal field

In an octahedrical crystal field d electrons energy levels are splitted according the irreducible representations of O_h group into e_g and t_{2g} orbitals. The t_{2g} shell is a 3-fold degenerated representation which orbitals correspond to the following combinations of spherical harmonics, Y_{lm}.

$$\zeta = \frac{\imath}{\sqrt{2}} [Y_{2,+1} + Y_{2,-1}] \qquad \sim \sqrt{3}yz \tag{210a}$$

$$\eta = -\frac{1}{\sqrt{2}} [Y_{2,+1} - Y_{2,-1}] \qquad \sim \sqrt{3}xz \tag{210b}$$

$$\tau = -\frac{\imath}{\sqrt{2}} [Y_{2,+2} - Y_{2,-2}] \qquad \sim \sqrt{3}xy \tag{210c}$$

On the other hand the e_g orbitals are expressed in the following way.

$$u = Y_{2,0} \qquad \sim \frac{1}{2}(3z^2 - r^2) \tag{211a}$$

$$v = \frac{1}{\sqrt{2}} [Y_{2,+2} + Y_{2,-2}] \qquad \sim \frac{\sqrt{3}}{2}(x^2 - y^2) \tag{211b}$$

It is well known that the energy $t_{2g} - e_g$ gap is $10Dq$[13]. An electron on t_{2g} shell is stabilized with $-4Dq$ but an electron in e_g shell is excited with $6Dq$.

$$\mathcal{H}_{CF} = \sum_i \sum_{\sigma=\uparrow,\downarrow} Dq \left[6 \sum_{\mu \in e_g} c^{\dagger}_{i\mu\sigma} c_{i\mu\sigma} - 4 \sum_{\mu \in t_{2g}} c^{\dagger}_{i\mu\sigma} c_{i\mu\sigma} \right] \tag{212}$$

3.2 Coulombic interactions

Inside the atomic shell electrons interact between them by coulombic potential,

$$V_C = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = e^2 \sum_{k=0}^{\infty} \frac{r_<^k}{r_>^{k+1}} \frac{4\pi}{2k+1} \sum_{q=-k}^{k} (-1)^q Y_{k,q}(\theta_1,\varphi_1) Y_{k,-q}(\theta_2,\varphi_2) \tag{213}$$

which is decomposed with Legendre polynomials where $r_< = \min(r_1, r_2)$ and $r_> = \max(r_1, r_2)$.

This is clearly a two body operator, so the matrix element is expressed in the following way.

$$\langle l_a m_a, l_b m_b | r_{12}^{-1} | l_c m_c, l_d m_d \rangle = \delta^{m_c+m_d}_{m_a+m_b} (-1)^{m_a - m_c} \sum_k c^k(l_a, m_a; l_c, m_c) c^k(l_b, m_b; l_d, m_d) F^k(l_a, l_b, l_c, l_d) \tag{214}$$

$$F^k(l_a, l_b, l_c, l_d) = \int_0^{\infty} r_1^2 \int_0^{\infty} r_2^2 \frac{r_<^k}{r_>^{k+1}} R_{l_a}(r_1) R_{l_b}(r_2) R_{l_c}(r_1) R_{l_d}(r_2) \mathrm{d}r_1 \mathrm{d}r_2 \tag{215}$$

$$c^k(l, m; l', m') = \sqrt{\frac{4\pi}{2k+1}} \int_0^{\pi} \sin\theta \int_0^{2\pi} Y^*_{l,m}(\theta,\varphi) Y_{l',m'}(\theta,\varphi) Y_{k,m-m'}(\theta,\varphi) \mathrm{d}\theta \mathrm{d}\varphi \tag{216}$$

[13] Dq is the differential of quanta.

On this integrals, for the case $l_a = l_b = l_c = l_d = 2$ only $k = 0, 2, 4$ are kept. F^0, F^2, F^4 can be substituted with $F_0 = F^0$, $F_2 = F^2/49$ and $F_4 = F^4/441$ which are used to construct the Racah parameters:

$$A = F_0 - 49F_4 \tag{217a}$$
$$B = F_2 - 5F_4 \tag{217b}$$
$$C = 35F_4 \tag{217c}$$

The integral $c^0(2, m; 2, m') = \delta_m^{m'}$ meanwhile the other two can be expressed matricially such that $\langle m|c^k|m'\rangle = c^k(2, m; 2, m')$ with the basis $\{+2, +1, 0, -1, -2\}$.

$$c^2 = \begin{pmatrix} -2 & \sqrt{6} & -2 & 0 & 0 \\ -\sqrt{6} & 1 & 1 & -\sqrt{6} & 0 \\ -2 & -1 & 2 & -1 & -2 \\ 0 & -\sqrt{6} & 1 & 1 & -\sqrt{6} \\ 0 & 0 & -2 & \sqrt{6} & -2 \end{pmatrix} \tag{218a}$$

$$c^4 = \begin{pmatrix} 1 & -\sqrt{5} & \sqrt{15} & -\sqrt{35} & \sqrt{70} \\ \sqrt{5} & -4 & \sqrt{30} & -\sqrt{40} & \sqrt{35} \\ \sqrt{15} & -\sqrt{30} & 6 & -\sqrt{30} & \sqrt{15} \\ \sqrt{35} & -\sqrt{40} & \sqrt{30} & -4 & \sqrt{5} \\ \sqrt{70} & -\sqrt{35} & \sqrt{15} & -\sqrt{5} & 1 \end{pmatrix} \tag{218b}$$

The hamiltonian of this interaction is expressed as

$$\mathcal{H}_{ee} = \frac{e^2}{2} \sum_i \sum_{\sigma,\sigma'} \sum_{\mu,\nu} \sum_{\lambda,\kappa} \langle \mu\nu|r_{12}^{-1}|\lambda\kappa\rangle c_{i\mu\sigma}^\dagger c_{i\nu\sigma'}^\dagger c_{i\kappa\sigma'} c_{i\lambda\sigma} \tag{219}$$

Our orbital basis is not expressed in spherical harmonics, so the matrix elements have to be computed taking into account $|\mu\rangle = \sum_m a_m |m\rangle$.

$$\langle \mu\nu|r_{12}^{-1}|\lambda\kappa\rangle = \sum_{m,n} \sum_{p,q} a_m^* b_n^* f_p g_q \langle mn|r_{12}^{-1}|pq\rangle \tag{220}$$

3.3 Jahn-Teller effect

The presence of d electrons induces E_g kind distortions on octahedrical complexes. This has two distortion modes:

$$Q_3 = 2Z - X - Y = \varrho \cos\vartheta \tag{221}$$
$$Q_2 = \sqrt{3}(X - Y) = \varrho \sin\vartheta \tag{222}$$

which can be combined by changing the angle ϑ: $Q = Q_3 + Q_2$. The anharmonic modes of a crystal favors tetragonal elongations, corresponding to $\vartheta = n2\pi/3$ being this elongations at z, x, y axis for $n = 0, 1, 2$ respectively. Using the vibronic constant we can construct this hamiltonian term.

$$\begin{aligned} \mathcal{H}_{JT} = \sum_i \sum_\sigma \Bigg[& \frac{F_E + 2G_E}{2} \sum_{\mu \in e_g} c_{i\mu\sigma}^\dagger c_{i\mu\sigma} + \frac{F_T}{2} \sum_{\mu \in t_{2g}} c_{i\mu\sigma}^\dagger c_{i\mu\sigma} \\ & -(F_E \cos\vartheta + G_E \cos 2\vartheta) \left(c_{iu\sigma}^\dagger c_{iu\sigma} - c_{iv\sigma}^\dagger c_{iv\sigma} \right) + (F_E \sin\vartheta - G_E \sin 2\vartheta) \left(c_{iu\sigma}^\dagger c_{iv\sigma} + c.c. \right) \\ & -\frac{F_T}{2} \left((\cos\vartheta - \sqrt{3}\sin\vartheta) c_{i\zeta\sigma}^\dagger c_{i\zeta\sigma} + (\cos\vartheta + \sqrt{3}\sin\vartheta) c_{i\eta\sigma}^\dagger c_{i\eta\sigma} - 2\cos\vartheta c_{i\tau\sigma}^\dagger c_{i\tau\sigma} \right) \Bigg] \end{aligned} \tag{223}$$

3.4 Spin-orbit coupling

The spin-orbit coupling operator is simply $\xi_{SO} \mathbf{l} \cdot \mathbf{s}$. In our orbital basis, $\{\zeta, \eta, \tau, u, v\}$ the orbiital angular momentum (OAL) matrices are:

$$\mathbf{l} = \begin{pmatrix} 0 & 0 & 0 & -\imath\sqrt{3} & -\imath \\ 0 & 0 & -\imath & 0 & 0 \\ 0 & \imath & 0 & 0 & 0 \\ \imath\sqrt{3} & 0 & 0 & 0 & 0 \\ \imath & 0 & 0 & 0 & 0 \end{pmatrix} \hat{x} + \begin{pmatrix} 0 & 0 & \imath & 0 & 0 \\ 0 & 0 & 0 & \imath\sqrt{3} & -\imath \\ -\imath & 0 & 0 & 0 & 0 \\ 0 & -\imath\sqrt{3} & 0 & 0 & 0 \\ 0 & \imath & 0 & 0 & 0 \end{pmatrix} \hat{y} + \begin{pmatrix} 0 & \imath & 0 & 0 & 0 \\ -\imath & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \imath 2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\imath 2 & 0 & 0 \end{pmatrix} \hat{z} \tag{224}$$

meanwhile the expression of the spin matrices is developed on the following section. The term of the hamiltonian is simply computed.

$$\mathcal{H}_{SO} = \xi_{SO} \sum_i \sum_{\sigma,\sigma'} \sum_{\mu,\nu \in d} \langle \mu | \mathbf{l} | \nu \rangle \cdot \langle \sigma | \mathbf{s} | \sigma' \rangle c^\dagger_{i\mu\sigma} c_{i\nu\sigma'} \tag{225}$$

3.4.1 Spin rotation

Spin can be forced to be quantized to any direction $\hat{n} = (\cos\alpha \sin\beta, \sin\alpha \sin\beta, \cos\beta)$ by the action of the magnetic field. When it is quantized in z direction the spin operator is expressed with Pauli matrices: $\sigma/2$. It is more confortable to use spin labels, $\uparrow$ and $\downarrow$, in the direction where spin is quantized, so the matrices have to be transformed by $2s_\alpha = \mathcal{R}^\dagger \sigma_\alpha \mathcal{R}$ with $\alpha = x, y, z$. This $\mathcal{R}$ is the rotor that $\mathcal{R}\hat{z}\mathcal{R}^\dagger = \hat{n}$:

$$\mathcal{R}(\alpha, \beta) = \mathrm{e}^{-\imath\alpha \frac{\sigma_z}{2}} \mathrm{e}^{-\imath\beta \frac{\sigma_y}{2}} \tag{226}$$

This can be easily computed using the following:

$$\mathrm{e}^{-\imath\chi\sigma_\alpha} = \sum_{k=0}^{\infty} \frac{(-\imath\chi)^k}{k!} \sigma_\alpha^k = \sum_{m=0}^{\infty} (-1)^m \frac{\chi^{2m}}{(2m)!} \mathbb{I} - \imath \sum_{m=0}^{\infty} (-1)^m \frac{\chi^{2m+1}}{(2m+1)!} \sigma_\alpha = \mathbb{I} \cos\chi - \imath\sigma_\alpha \sin\chi \tag{227}$$

so the rotor is expanded as follows:

$$\mathcal{R}(\alpha, \beta) = \mathbb{I} \cos\frac{\alpha}{2} \cos\frac{\beta}{2} + \imath \left[\sigma_x \sin\frac{\alpha}{2} \sin\frac{\beta}{2} - \sigma_y \cos\frac{\alpha}{2} \sin\frac{\beta}{2} - \sigma_z \sin\frac{\alpha}{2} \cos\frac{\beta}{2} \right] \tag{228a}$$

$$\mathcal{R}^\dagger(\alpha, \beta) = \mathbb{I} \cos\frac{\alpha}{2} \cos\frac{\beta}{2} - \imath \left[\sigma_x \sin\frac{\alpha}{2} \sin\frac{\beta}{2} - \sigma_y \cos\frac{\alpha}{2} \sin\frac{\beta}{2} - \sigma_z \sin\frac{\alpha}{2} \cos\frac{\beta}{2} \right] \tag{228b}$$

where we have used the following property related to Pauli matrices: $\sigma_i \sigma_j = \delta_{ij} + \imath\epsilon_{ijk}\sigma_k$ being ϵ_{ijk} the Levi-Civitta symbol.

Now we can compute the rotated spin matrices. It will be usefull to derive $\sigma_i\sigma_j\sigma_k = (\delta_{ij} + \imath\epsilon_{ijl}\sigma_l)\sigma_k = \delta_{ij}\sigma_k - \epsilon_{ijl}\epsilon_{lkm}\sigma_m + \imath\epsilon_{ijk} = \delta_{jk}\sigma_i - \delta_{ik}\sigma_j + \delta_{ij}\sigma_k + \imath\epsilon_{ijk}$

$$\begin{aligned}
2s_\alpha &= \mathcal{R}^\dagger(\alpha,\beta)\sigma_\alpha\mathcal{R}(\alpha,\beta) \\
&= \mathcal{R}^\dagger(\alpha,\beta) \left\{ \sigma_\alpha \cos\frac{\alpha}{2}\cos\frac{\beta}{2} + \imath \left[\sigma_\alpha\sigma_x \sin\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_\alpha\sigma_y \cos\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_\alpha\sigma_z \sin\frac{\alpha}{2}\cos\frac{\beta}{2} \right] \right\} \\
&= \cos\frac{\alpha}{2}\cos\frac{\beta}{2} \left\{ \sigma_\alpha \cos\frac{\alpha}{2}\cos\frac{\beta}{2} + \imath \left[\sigma_\alpha\sigma_x \sin\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_\alpha\sigma_y \cos\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_\alpha\sigma_z \sin\frac{\alpha}{2}\cos\frac{\beta}{2} \right] \right\} - \\
&\quad - \imath \sin\frac{\alpha}{2}\sin\frac{\beta}{2} \left\{ \sigma_x\sigma_\alpha \cos\frac{\alpha}{2}\cos\frac{\beta}{2} + \imath \left[\sigma_x\sigma_\alpha\sigma_x \sin\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_x\sigma_\alpha\sigma_y \cos\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_x\sigma_\alpha\sigma_z \sin\frac{\alpha}{2}\cos\frac{\beta}{2} \right] \right\} + \\
&\quad + \imath \cos\frac{\alpha}{2}\sin\frac{\beta}{2} \left\{ \sigma_y\sigma_\alpha \cos\frac{\alpha}{2}\cos\frac{\beta}{2} + \imath \left[\sigma_y\sigma_\alpha\sigma_x \sin\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_y\sigma_\alpha\sigma_y \cos\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_y\sigma_\alpha\sigma_z \sin\frac{\alpha}{2}\cos\frac{\beta}{2} \right] \right\} + \\
&\quad + \imath \sin\frac{\alpha}{2}\cos\frac{\beta}{2} \left\{ \sigma_z\sigma_\alpha \cos\frac{\alpha}{2}\cos\frac{\beta}{2} + \imath \left[\sigma_z\sigma_\alpha\sigma_x \sin\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_z\sigma_\alpha\sigma_y \cos\frac{\alpha}{2}\sin\frac{\beta}{2} - \sigma_z\sigma_\alpha\sigma_z \sin\frac{\alpha}{2}\cos\frac{\beta}{2} \right] \right\}
\end{aligned} \tag{229}$$

With this general expression we can take the three components of the operator.

$$2s_x = \sigma_x \cos\alpha\cos\beta - \sigma_y \sin\alpha + \sigma_z \cos\alpha \sin\beta \tag{230a}$$

$$2s_y = \sigma_x \sin\alpha\cos\beta + \sigma_y \cos\alpha + \sigma_z \sin\alpha\sin\beta \tag{230b}$$

$$2s_z = -\sigma_x \sin\beta + \sigma_z \cos\beta \tag{230c}$$

Look that now $\hat{n} \cdot \mathbf{s} = \sigma_z/2$

3.5 Ligant-TM hopping

There is the possibility that an electron is leaving the ligand to jump to a TM neighbour site. On this situation we have a p-kind hole in ligand site which is created by destroying an electron on this site with $c_{a\alpha\sigma}$ being a the ligand site and $\alpha = x, y, z$. When a hole is created the ligand site is excited with the transfer charge energy.

$$\mathcal{H}_{lig} = \Delta_{CT} \sum_a \sum_\sigma \sum_\alpha c_{a\alpha\sigma} c^\dagger_{a\alpha\sigma} \tag{231}$$

When this electron is destroyed on ligand site an electron has to be put on a TM site at the same time by electromagnetic induced hopping.

$$\mathcal{W}_{\hat{\epsilon}} = \sum_{a,i}\sum_{\sigma}\sum_{\alpha,\mu} t^{\mu}_{q_{ia}\hat{\epsilon}\alpha} c^{\dagger}_{i\mu\sigma} c_{a\alpha\sigma} + c.c. \tag{232}$$

Here $\hat{\epsilon}$ is the polarization vector of the electric field, q_{ij} is the direction between the two neighour sites x, y, z (if i and j are not nieghbour $t^{\mu}_{q_{ia}\hat{\epsilon}\alpha} = 0$) and $t^{\mu}_{q_{ia}\hat{\epsilon}\alpha}$ is the Slater-Koster overlaping integral.

$$t^{\mu}_{q_{ia}\hat{\epsilon}\alpha} = -\imath \int \psi_{\mu}(\mathbf{r}) \nabla \phi_{\alpha}(\mathbf{r} \pm a\hat{e}_{q_{ia}}) \mathrm{d}^3\mathbf{r} \tag{233}$$

Note that for the ligands there are also some internal terms as e-e correlations and SOC, but they can be neglected since we are interested on the physics on energy ranges below charge-transfer energy and those terms only affect if one electron is annihilated from the ligand (six electrons on the p shell results on a non-degenerated ^1S atomic term).

The charge transfer states ($|\Phi\rangle$ and let ligand at $\mathbf{R}_k$) are considered virtual, so we should use perturbation theory to expand the state with an electron at orbital μ in the position $\mathbf{R}_i$ corresponding to a TM atom. Taking into account that the relevant hamiltonian term is $\frac{e}{m}\imath\mathbf{A}(t)\cdot\nabla$

$$|\Psi\rangle \to |\Psi\rangle - \frac{\langle\Phi|\mathcal{H}|\Psi\rangle}{\Delta_{CT}}|\Phi\rangle = |\Psi\rangle - \frac{e}{m}\frac{\langle\Phi|-\imath\nabla|\Psi\rangle\cdot\mathbf{A}(t)}{\Delta_{CT}}|\Phi\rangle = |\Psi\rangle - \frac{e}{m}\frac{\mathbf{t}^{w}_{\mu}(\mathbf{R}_{ki})\cdot\mathbf{A}(t)}{\Delta_{CT}}|\Phi\rangle \tag{234}$$

Now guess an state $|\Psi'\rangle$ being an state with an electron on a TM atom at orbital ν at site $\mathbf{R}_j$ connected by site i with the ligand at site k

$$\frac{e}{m}\imath\mathbf{A}(t)\langle\Psi|\nabla|\Psi'\rangle = -\left(\frac{e}{m}\right)^2 \frac{2}{\Delta_{CT}} \left(\mathbf{t}^{\mu}_{w}(\mathbf{R}_{ik})\cdot\mathbf{A}(t)\right)\left(\mathbf{t}^{w}_{\nu}(\mathbf{R}_{kj})\cdot\mathbf{A}(t)\right) = -\left(\frac{e}{m}\right)^2 \frac{2}{\Delta_{CT}}\alpha^{\mu\nu}_{ij}(t) \tag{235}$$

3.6 Density current operator

In QFT the gauge invariant kinetic energy under electromagnetic fild is described with

$$\mathcal{H}_{kin} = \frac{1}{2m}\int \Psi^{\dagger}(\mathbf{x})\left[-\imath\nabla + e\mathbf{A}\right]^2 \Psi(\mathbf{x})\mathrm{d}\mathbf{x} \tag{236}$$

and the current density is related with the variations of the Hamiltonian with the vector potential

$$\mathbf{j}(\mathbf{x},t) = -\frac{\delta\mathcal{H}}{\delta\mathbf{A}(\mathbf{x},t)} = \frac{\imath e}{2m}\left[\Psi^{\dagger}(\mathbf{x})\left(\nabla\Psi(\mathbf{x})\right) - \left(\nabla\Psi^{\dagger}(\mathbf{x})\right)\Psi(\mathbf{x})\right] - \frac{e^2}{m}n(\mathbf{x},t)\mathbf{A}(\mathbf{x},t) \tag{237}$$

being the first term the paramagnetic current and the second the diamagnetic currend: $\mathbf{j} = \mathbf{j}_p + \mathbf{j}_d$. Also with variations we can define the conductivity

$$\sigma^{\alpha}_{\beta}(t,t') = \frac{\delta\langle j^{\alpha}(t)\rangle}{\delta E^{\beta}(t')} \tag{238}$$

and the susceptibility

$$\chi^{\alpha}_{\beta}(t,t') = \frac{\delta\langle j^{\alpha}(t)\rangle}{\delta A^{\beta}(t')} \tag{239}$$

which are related by

$$\sigma^{\alpha}_{\beta}(t,t') = \Theta(t-t')\int_{t'}^{t}\chi^{\alpha}_{\beta}(t,t_1)\mathrm{d}t_1 \tag{240}$$

since $\mathbf{E}(t) = -\partial_t\mathbf{A}(t)$.

$$\begin{aligned}\int_{-\infty}^{t}\mathrm{d}t'\frac{\delta\langle j^{\alpha}(t)\rangle}{\delta A^{\beta}(t')}\delta A^{\beta}(t') &= \lim_{\lambda\to 0}\frac{\langle j^{\alpha}(t)\rangle\left[A^{\beta}(t')+\lambda\delta A^{\beta}(t')\right] - \langle j^{\alpha}(t)\rangle\left[A^{\beta}(t')\right]}{\lambda} \\ &= -\int_{-\infty}^{t}\mathrm{d}t'\sigma^{\alpha}_{\beta}(t,t')\partial_{t'}\delta A^{\beta}(t') = \int_{-\infty}^{t}\mathrm{d}t'\left[\partial_{t'}\sigma^{\alpha}_{\beta}(t,t')\right]\delta A^{\beta}(t') \\ &= \int_{-\infty}^{t}\mathrm{d}t'\chi^{\alpha}_{\beta}(t,t')\delta A^{\beta}(t')\end{aligned} \tag{241}$$

Then, by recovering the Kubo formula

$$\left\langle j_p^\alpha(t)\right\rangle = \imath\int_{t'}^{t}\left\langle[j_p^\alpha(\mathbf{x},t),\mathbf{j}_p(\mathbf{x}',t')]\right\rangle\cdot\mathbf{A}(t')\mathrm{d}\mathbf{x}'\mathrm{d}t' \tag{242}$$

so we can define the Keldysh susceptibility as

$$\tilde{\chi}_\beta^\alpha(t,t') = \imath\left\langle\mathcal{T}_\mathcal{C} j_p^\alpha(\mathbf{x},t)j_p^\beta(\mathbf{x}',t')\right\rangle - \frac{e^2}{m}\left\langle n(\mathbf{x},t)\right\rangle\delta_\beta^\alpha\delta_\mathcal{C}(t,t') \tag{243}$$

such that $(\tilde{\chi}_\beta^\alpha)^R = \chi_\beta^\alpha$.

If we take the expression for density current we can relate it with the Green's function. We can start with the diamagnetic current

$$\left\langle\mathbf{j}_d(t)\right\rangle = -\frac{e^2}{m}\mathbf{A}(t)\int\mathrm{d}\mathbf{x}\left\langle\Psi^\dagger(\mathbf{x},t)\Psi(\mathbf{x},t)\right\rangle = -\frac{e^2}{m}\mathbf{A}(t)\sum_\mu\left\langle c_\mu^\dagger(t)c_\mu(t)\right\rangle = -\imath\xi\frac{e^2}{m}\mathbf{A}(t)\sum_\mu(G_\mu^\mu)^<(t,t) \tag{244}$$

For the paramagnetic term let's be more quiet

$$\begin{aligned}
\left\langle\Psi^\dagger(\mathbf{x})\left(\nabla\Psi(\mathbf{x})\right)\right\rangle &= \int\mathrm{d}\mathbf{x}\sum_{\mu,\nu}\psi_\nu^*(\mathbf{x})\nabla\psi_\mu(\mathbf{x})\left\langle c_\nu^\dagger(t)c_\mu(t)\right\rangle \\
&\approx -\xi\sum_{\substack{\mu,\nu\\ i,j,\sigma}}(G_{j\nu\sigma}^{i\mu\sigma})^<(t,t)\int\mathrm{d}\mathbf{x}\sum_{w,k}\left[\psi_\nu^*(\mathbf{x}-\mathbf{R}_j) - \frac{e}{m}\frac{\mathbf{t}_w^\nu(\mathbf{R}_{jk})\cdot\mathbf{A}(t)}{\Delta_{CT}}\phi_{p_w}^*(\mathbf{x}-\mathbf{R}_k)\right] \\
&\times(-\imath\nabla)\left[\psi_\mu(\mathbf{x}-\mathbf{R}_i) - \frac{e}{m}\frac{\mathbf{t}_\mu^w(\mathbf{R}_{ki})\cdot\mathbf{A}(t)}{\Delta_{CT}}\phi_{p_w}(\mathbf{x}-\mathbf{R}_k)\right] \\
&= \frac{e}{m}\frac{\xi}{\Delta_{CT}}\sum_{\substack{\mu,\nu\\ i,j,\sigma}}(G_{j\nu\sigma}^{i\mu\sigma})^<(t,t) \\
&\times\sum_{w,k}\left[\mathbf{t}_w^\nu(\mathbf{R}_{jk})\left(\mathbf{t}_\mu^w(\mathbf{R}_{ki})\cdot\mathbf{A}(t)\right) + \left(\mathbf{t}_w^\nu(\mathbf{R}_{jk})\cdot\mathbf{A}(t)\right)\mathbf{t}_\mu^w(\mathbf{R}_{ki})\right] \\
&= \frac{e}{m}\frac{\xi}{\Delta_{CT}}\sum_{\substack{\mu,\nu\\ i,j,\sigma}}\frac{\delta\alpha_{ji}^{\nu\mu}(t)}{\delta\mathbf{A}(t)}(G_{j\nu\sigma}^{i\mu\sigma})^<(t,t)
\end{aligned} \tag{245}$$

$$\begin{aligned}
\left\langle\left(\nabla\Psi^\dagger(\mathbf{x})\right)\Psi(\mathbf{x})\right\rangle &= \int\mathrm{d}\mathbf{x}\sum_{\mu,\nu}\psi_\nu(\mathbf{x})\nabla\psi_\mu^*(\mathbf{x})\left\langle c_\mu^\dagger(t)c_\nu(t)\right\rangle \\
&= -\xi\sum_{\substack{\mu,\nu\\ i,j,\sigma}}\left[(G_{j\nu\sigma}^{i\mu\sigma})^<(t,t)\int\mathrm{d}\mathbf{x}\psi_\nu^*(\mathbf{x}-\mathbf{R}_j)(-\imath\nabla)\psi_\mu(\mathbf{x}-\mathbf{R}_i)\right]^* = \left\langle\Psi^\dagger(\mathbf{x})\left(\nabla\Psi(\mathbf{x})\right)\right\rangle^*
\end{aligned} \tag{246}$$

$$\left\langle\mathbf{j}_p(t)\right\rangle = -\left(\frac{e}{m}\right)^2\frac{\xi}{\Delta_{CT}}\sum_{\substack{\mu,\nu\\ i,j,\sigma}}\Im\left[\beta_{ji}^{\nu\mu}(t)(G_{j\nu\sigma}^{i\mu\sigma})^<(t,t)\right] \tag{247}$$

3.6.1 From current correlation

On this derivation we will explore the term of the susceptibility related with the correpation of the paramagnetic current.

$$
\begin{aligned}
(\tilde{\chi}_p)^\alpha_\beta(t,t') &= \imath \left\langle \mathcal{T}_\mathcal{C} j_p^\alpha(\mathbf{x},t) j_p^\beta(\mathbf{x}',t') \right\rangle \\
&= -\imath \left(\frac{e}{2m}\right)^2 \left\{ \left\langle \mathcal{T}_\mathcal{C} \Psi^\dagger(\mathbf{x},t) \left(\partial_\alpha \Psi(\mathbf{x},t)\right) \Psi^\dagger(\mathbf{x}',t') \left(\partial_\beta \Psi(\mathbf{x}',t')\right) \right\rangle \right. \\
&\quad - \left\langle \mathcal{T}_\mathcal{C} \Psi^\dagger(\mathbf{x},t) \left(\partial_\alpha \Psi(\mathbf{x},t)\right) \left(\partial_\beta \Psi^\dagger(\mathbf{x}',t')\right) \Psi(\mathbf{x}',t') \right\rangle \\
&\quad - \left\langle \mathcal{T}_\mathcal{C} \left(\partial_\alpha \Psi^\dagger(\mathbf{x},t)\right) \Psi(\mathbf{x},t) \Psi^\dagger(\mathbf{x}',t') \left(\partial_\beta \Psi(\mathbf{x}',t')\right) \right\rangle \\
&\quad \left. + \left\langle \mathcal{T}_\mathcal{C} \left(\partial_\alpha \Psi^\dagger(\mathbf{x},t)\right) \Psi(\mathbf{x},t) \left(\partial_\beta \Psi^\dagger(\mathbf{x}',t')\right) \Psi(\mathbf{x}',t') \right\rangle \right\} \\
&= -\imath \left(\frac{e}{2m}\right)^2 \sum_{\substack{\mu,\nu \\ \lambda,\kappa}} \int\int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \left\{ \left(\psi^*_\mu(\mathbf{x}) \partial_\alpha \psi_\nu(\mathbf{x})\right) \left(\psi^*_\lambda(\mathbf{x}') \partial_\beta \psi_\kappa(\mathbf{x}')\right) \right. \\
&\quad - \left(\psi^*_\mu(\mathbf{x}) \partial_\alpha \psi_\nu(\mathbf{x})\right) \left(\psi_\kappa(\mathbf{x}') \partial_\beta \psi^*_\lambda(\mathbf{x}')\right) \\
&\quad - \left(\psi_\nu(\mathbf{x}) \partial_\alpha \psi^*_\mu(\mathbf{x})\right) \left(\psi^*_\lambda(\mathbf{x}') \partial_\beta \psi_\kappa(\mathbf{x}')\right) \\
&\quad \left. + \left(\psi_\nu(\mathbf{x}) \partial_\alpha \psi^*_\mu(\mathbf{x})\right) \left(\psi_\kappa(\mathbf{x}') \partial_\beta \psi^*_\lambda(\mathbf{x}')\right) \right\} \left\langle \mathcal{T}_\mathcal{C} c^\dagger_\mu(t) c_\nu(t) c^\dagger_\lambda(t') c_\kappa(t') \right\rangle \\
&= \frac{\imath}{4} \left(\frac{e}{m}\right)^3 \sum_{\substack{\mu,\nu,\lambda,\kappa \\ i,j,k,l}} \Re\left\{ \frac{\delta \alpha^{\mu\nu}_{ij}(t)}{\delta A_\alpha(t)} \right\} \Re\left\{ \frac{\delta \alpha^{\lambda\kappa}_{kl}(t')}{\delta A_\beta(t')} \right\} \left\langle \mathcal{T}_\mathcal{C} c^\dagger_\mu(t) c_\nu(t) c^\dagger_\lambda(t') c_\kappa(t') \right\rangle \\
&= -\frac{\imath}{4} \left(\frac{e}{m}\right)^3 \sum_{\substack{\mu,\nu,\lambda,\kappa \\ i,j,k,l}} \Re\left\{ \frac{\delta \alpha^{\mu\nu}_{ij}(t)}{\delta A_\alpha(t)} \right\} \Re\left\{ \frac{\delta \alpha^{\lambda\kappa}_{kl}(t')}{\delta A_\beta(t')} \right\} \left[G^\nu_\mu(t,t) G^\kappa_\lambda(t',t') + \xi G^\nu_\lambda(t,t') G^\kappa_\mu(t',t) \right]
\end{aligned}
\tag{248}
$$

Where we have taken into account that

$$
\int \mathrm{d}\mathbf{x} \psi^*_\nu(\mathbf{x}) \nabla \psi_\mu(\mathbf{x}) = \frac{e}{\imath m} \frac{\delta \alpha^{\nu\mu}_{ji}(t)}{\delta \mathbf{A}(t)} \tag{249a}
$$

$$
\int \mathrm{d}\mathbf{x} \psi_\nu(\mathbf{x}) \nabla \psi^*_\mu(\mathbf{x}) = \frac{\imath e}{m} \frac{\delta \alpha^{\mu\nu}_{ij}(t)}{\delta \mathbf{A}(t)} \tag{249b}
$$

In the retarded component the first term vanish since it will become into $[G^{11}(t,t) + G^{22}(t,t)][G^{11}(t',t') - G^{22}(t',t')]$, so the final expression is

$$
\begin{aligned}
\chi^\alpha_\beta(t,t') &= -\frac{\imath\xi}{4} \left(\frac{e}{m}\right)^3 \sum_{\substack{\mu,\nu,\lambda,\kappa \\ i,j,k,l}} \Re\left\{ \frac{\delta \alpha^{\mu\nu}_{ij}(t)}{\delta A_\alpha(t)} \right\} \Re\left\{ \frac{\delta \alpha^{\lambda\kappa}_{kl}(t')}{\delta A_\beta(t')} \right\} \left[(G^\nu_\lambda)^R(t,t') (G^\kappa_\mu)^<(t',t) \right. \\
&\quad \left. + (G^\nu_\lambda)^<(t,t') (G^\kappa_\mu)^A(t',t) \right] \\
&= -\frac{\imath\xi}{4} \left(\frac{e}{m}\right)^3 \sum_{\substack{\mu,\nu,\lambda,\kappa \\ i,j,k,l}} \Re\left\{ \frac{\delta \alpha^{\mu\nu}_{ij}(t)}{\delta A_\alpha(t)} \right\} \Re\left\{ \frac{\delta \alpha^{\lambda\kappa}_{kl}(t')}{\delta A_\beta(t')} \right\} \left[(G^\nu_\lambda)^R(t,t') (G^\kappa_\mu)^<(t',t) \right. \\
&\quad \left. - \left\{ (G^\mu_\kappa)^R(t,t') (G^\lambda_\nu)^<(t',t) \right\}^* \right] \\
&= \frac{\xi}{4} \left(\frac{e}{m}\right)^3 \sum_{\substack{\mu,\nu,\lambda,\kappa \\ i,j,k,l}} \Re\left\{ \frac{\delta \alpha^{\mu\nu}_{ij}(t)}{\delta A_\alpha(t)} \right\} \Re\left\{ \frac{\delta \alpha^{\lambda\kappa}_{kl}(t')}{\delta A_\beta(t')} \right\} \Im\left[(G^\nu_\lambda)^R(t,t') (G^\kappa_\mu)^<(t',t) \right]
\end{aligned}
\tag{250}
$$

3.6.2 From variational calculus

Now, in order to take the susceptibility we need to know $\delta G^<(t,t)/\delta \mathbf{A}(t')$. For this we can recall the Dyson equation

$$
G^\mu_\nu(t,t') = \mathfrak{G}^\mu_\nu(t,t') + \sum_{\lambda,\kappa} \int_\mathcal{C} \int_\mathcal{C} \mathrm{d}t_1 \mathrm{d}t_2 \mathfrak{G}^\mu_\lambda(t,t_1) \Sigma^\lambda_\kappa(t_1,t_2) G^\kappa_\nu(t_2,t') \tag{251}
$$

and the differential equation for the free propagator

$$
\sum_\lambda \left[\imath \delta^\mu_\lambda \partial_t - \epsilon^\mu_\lambda(t)\right] \mathfrak{G}^\lambda_\nu(t,t') = \delta_\mathcal{C}(t,t') \delta^\mu_\nu \tag{252}
$$

For simplicity we can define

$$(\mathfrak{G}^{-1})^{\mu}_{\nu}(t,t') = \delta_{\mathcal{C}}(t,t')\left[\imath\delta^{\mu}_{\nu}\partial_t - \epsilon^{\mu}_{\nu}(t)\right] \tag{253}$$

and apply it from left to Dyson equation

$$\sum_{\lambda}\int_{\mathcal{C}} \mathrm{d}t_1 \Lambda^{\mu}_{\lambda}(t,t_1)G^{\lambda}_{\nu}(t_1,t') = \delta_{\mathcal{C}}(t,t')\delta^{\mu}_{\nu} \tag{254}$$

where $\Lambda(t,t') = \mathfrak{G}^{-1}(t,t') - \Sigma(t,t')$. Now we can apply the product rule to get the functional variation of the two sites of the equation

$$\sum_{\lambda}\int_{\mathcal{C}} \mathrm{d}t_1 \delta\Lambda^{\mu}_{\lambda}(t,t_1)G^{\lambda}_{\nu}(t_1,t') + \sum_{\lambda}\int_{\mathcal{C}} \mathrm{d}t_1 \Lambda^{\mu}_{\lambda}(t,t_1)\delta G^{\lambda}_{\nu}(t_1,t') = 0 \tag{255}$$

and finally apply the Green's function by left as convolution we can get δG:

$$\delta G^{\mu}_{\nu}(t,t') = -\sum_{\lambda,\kappa}\int_{\mathcal{C}}\int_{\mathcal{C}} \mathrm{d}t_1\mathrm{d}t_2 G^{\mu}_{\lambda}(t,t_1)\delta\Lambda^{\lambda}_{\kappa}(t_1,t_2)G^{\kappa}_{\nu}(t_2,t') \tag{256}$$

4 Many d-electrons on crystal field with Green's functions

For this problem we will take into account only the following partial Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{CF} + V_C \tag{257}$$

This Hamiltonian is time independent, so can be solved in the Matsubara branch or alternatively the equilibrium retarded function can be computed and perform the analytical continuation to imaginary-frequency axis.

5 Numerical approximations

5.1 Polynomial interpolation

Consider an array y_j for $j = 0, ..., k$ which represents a set of samples taken at $t_j = jh$ being h the time-step. This array can be approximated to a polynomial of order k:

$$\mathcal{P}^{(k)}(t) = \sum_{r,l=0}^{k} h^{-r}t^r P^{(k)}_{rl} y_l \tag{258}$$

Look that to match $\mathcal{P}^{(k)}(jh) = y_j$ $P^{(k)} = M^{-1}$ such that $M_{rl} = l^r$. With this interpolation we can compute the derivative of the polynomial as an approximation of $\dot{y}(t)$ at every $t = mh$.

$$\left.\frac{\mathrm{d}y}{\mathrm{d}t}\right|_{t=mh} \approx \frac{1}{h}\sum_{l=0}^{k}\sum_{r=1}^{k} r m^{r-1} P^{(k)}_{rl} y_l = \frac{1}{h}\sum_{l=0}^{k} D^{(k)}_{ml} y_l \tag{259}$$

The integration can be approximated also using the polynomial.

$$\int_{nh}^{mh} y(t)\mathrm{d}t \approx h\sum_{r,l=0}^{k}\frac{m^{r+1}-n^{r+1}}{r+1}P^{(k)}_{rl}y_l = h\sum_{l=0}^{k} I^{(k)}_{nml} y_l \tag{260}$$

Now consider a set of samples with $j = 0, ..., n$ with $n > k$. We can approximate the derivative at $y = nh$ to order k with the backward differentiation. Just construct a polynomial with samples $y_n, y_{n-1}, ..., y_{n-k}$:

$$\left.\frac{\mathrm{d}y}{\mathrm{d}t}\right|_{t=nh} \approx -\frac{\mathrm{d}\mathcal{P}^{(k)}}{\mathrm{d}t} = -\frac{1}{h}\sum_{l=0}^{k} D^{(k)}_{0l} y_{n-l} = \frac{1}{h}\sum_{l=0}^{k} a^{(k)}_{l} y_{n-l} \tag{261}$$

Applying the discrete criterion for $0^0 = 1$ we can see that $a^{(k)}_l = -D^{(k)}_{0l} = -P^{(k)}_{1l}$.

With this array of $n+1$ samples we can approximate the integral from $t = 0$ to mh at order k:

$$\mathcal{I}_m = \int_0^{mh} y(t)\mathrm{d}t \approx h\sum_{l=0}^{\max(k,m)} w^{(k)}_{ml} y_l \tag{262}$$

- $k \geq m$:
  At this starting point we can use the polynomial integration formula with a polynomial generated with $y_0, ..., y_k$.

$$\mathcal{I}_m = h \sum_{l=0}^{k} I_{0ml}^{(k)} y_l = h \sum_{l=0}^{k} s_{ml}^{(k)} y_l \tag{263}$$

- $k < m$:
  From this point we can use the backward differentiation taking into account that $\dot{\mathcal{I}}(t) = y(t)$.

$$y_m = \frac{1}{h} \sum_{l=0}^{k} a_l^{(k)} \mathcal{I}_{m-l} \tag{264}$$

$$\mathcal{I}_m = \frac{1}{a_0^{(k)}} \left[h y_m - \sum_{l=1}^{k} a_l^{(k)} \mathcal{I}_{m-l} \right] \tag{265}$$

With all of this we have a matrix equation $S\mathbf{y} = A\mathcal{I}$ from where we can take the integration weights $w_{ml}^{(k)}$ making only the matrix product $A^{-1}S$.

$$A = \frac{1}{h} \begin{pmatrix} h & 0 & \cdots & & & \\ \vdots & \ddots & & & & \\ 0 & \cdots & h & & & \\ 0 & a_k^{(k)} & \cdots & a_0^{(k)} & 0 & \cdots \\ \vdots & & \ddots & & \ddots & \\ 0 & \cdots & 0 & a_k^{(k)} & \cdots & a_0^{(k)} \end{pmatrix} \tag{266a}$$

$$S = \begin{pmatrix} h s_{00}^{(k)} & \cdots & h s_{0k}^{(k)} & 0 & \cdots & \\ \vdots & & \vdots & & \vdots & \\ h s_{k0}^{(k)} & \cdots & h s_{kk}^{(k)} & 0 & \cdots & \\ & & & 1 & 0 & \cdots \\ & & & 0 & \ddots & \vdots \\ & & & \vdots & & \end{pmatrix} \tag{266b}$$

In general convolutions can be computed with the integration wrights, but if the integration range is less than interpolation order an analytic expansion is needed. This can be achieved with polynomials $\mathcal{P}^{(k)}[y_0, ..., y_k]$. Finally we can compute numerically the convolutions with:

$$\begin{aligned} x(t) &= \int_0^{mh} y(t-t') z(t') \mathrm{d}t' = \int_0^{mh} \mathrm{d}t' \sum_{r,l=0}^{k} h^{-r} (t-t')^r P_{rl}^{(k)} y_l \sum_{a,b=0}^{k} h^{-a} t'^a P_{ab}^{(k)} z_b \\ &= h \sum_{l,b=0}^{k} y_l z_b \sum_{r,a=0}^{k} P_{rl}^{(k)} P_{ab}^{(k)} \int_0^m \mathrm{d}s (m-s)^r s^a = h \sum_{l,b=0}^{k} R_{mlb} y_l z_b \end{aligned} \tag{267}$$

where $t = mh$ and $t' = sh$. Now we can compute the convolution weights:

$$\begin{aligned} R_{mlb} &= \sum_{r,a=0}^{k} P_{rl}^{(k)} P_{ab}^{(k)} \int_0^m \mathrm{d}s (m-s)^r s^a = \sum_{r,a=0}^{k} P_{rl}^{(k)} P_{ab}^{(k)} \int_0^m \mathrm{d}s \sum_{q=0}^{r} \binom{r}{q} (-1)^q s^{a+q} m^{r-q} \\ &= \sum_{r,a=0}^{k} \sum_{q=0}^{r} \binom{r}{q} (-1)^q P_{rl}^{(k)} P_{ab}^{(k)} \frac{m^{a+r+1}}{a+q+1} \end{aligned} \tag{268}$$

5.2 Numerical convolutions

5.2.1 Matsubara

In Matsubara branch we can find convolutions like

$$C^M(\tau) = \int_0^{\beta} A^M(\tau - \tau') B^M(\tau') \mathrm{d}\tau' \tag{269}$$

which is convenient to separate by the periodic behaviour of the Matsubara functions.

$$C_1^M(mh_\tau) = \int_0^{mh_\tau} A^M(mh_\tau - \tau')B(\tau')\mathrm{d}\tau' \tag{270a}$$

$$C_2^M(mh_\tau) = \int_{mh_\tau}^{\beta} A_M(mh_\tau - \tau')B(\tau')\mathrm{d}\tau' = \int_0^{\beta - mh_\tau} \xi A^M(mh_\tau + \tau'')B^M(\beta - \tau'')\mathrm{d}\tau'' \tag{270b}$$

In the first part we can separate two cases taking into account if the integration range is bigger or shorter than interpolation order, k.

$$(C_1^M)_m \approx \begin{cases} h_\tau \sum_{j,l=0}^{k} R_{mjl} A_j^M B_l^M & m \leq k \\ h_\tau \sum_{l=0}^{m} w_{ml} A_{m-l}^M B_l^M & m > k \end{cases} \tag{271}$$

For the second part we can make an analogous approximation.

$$(C_2^M)_m \approx \begin{cases} h_\tau \sum_{\substack{j,l=0 \\ N_\tau - m}}^{k} R_{N_\tau - m,jl} \xi A_{N_\tau - j}^M B_{N_\tau - l}^M & m \geq N_\tau - k \\ h_\tau \sum_{l=0} w_{N_\tau - m,l} \xi A_{m+l}^M B_{N_\tau - l}^M & m < N_\tau - k \end{cases} \tag{272}$$

On this part, for case than k is larger than integration rate $(N_\tau - k)h_\tau \leq mh_\tau \leq N_\tau h_\tau$ and the convolution, from the point of view of B^M is done from β to $\beta - mh$.

5.2.2 Left-mixed

For this component the first part

$$C_1^\rceil(nh, mh_\tau) = \int_0^{nh} A^R(nh, t')B^\rceil(t', mh_\tau)\mathrm{d}t' \tag{273}$$

is computed with VIDE and VIE, so we focus into the parts involving Matsubara branch.

$$C_2^\rceil(nh, mh_\tau) = \int_0^{mh_\tau} A^\rceil(nh, \tau')B^M(\tau' - mh_\tau)\mathrm{d}\tau' = \int_0^{mh_\tau} \xi A^\rceil(nh, mh_\tau - \tau'')B^M(\beta - \tau'')\mathrm{d}\tau'' \tag{274}$$

$$C_3^\rceil(nh, mh_\tau) = \int_{mh_\tau}^{\beta} A^\rceil(nh, \tau')B^M(\tau' - mh_\tau)\mathrm{d}\tau' = \int_0^{\beta - mh_\tau} A^\rceil(nh, \tau'' + mh_\tau)B^M(\tau'')\mathrm{d}\tau'' \tag{275}$$

As in Matsubara component every part can be sepparated in cases.

$$(C_2^\rceil)_{nm} \approx \begin{cases} h_\tau \sum_{j,l=0}^{k} R_{mjl} \xi A_{nl}^\rceil B_{N_\tau - j}^M & m \leq k \\ h_\tau \sum_{l=0}^{m} w_{ml} \xi A_{n,m-l}^\rceil B_{N_\tau - l}^M & m > k \end{cases} \tag{276}$$

$$(C_3^\rceil)_{nm} \approx \begin{cases} h_\tau \sum_{j,l=0}^{k} R_{N_\tau - m,jl} A_{n,N_\tau - l}^\rceil B_j^M & m \geq N_\tau - k \\ h_\tau \sum_{\substack{l=0 \\ N-m}} w_{N_\tau - m,l} A_{n,m+l}^\rceil B_l^M & m < N_\tau - k \end{cases} \tag{277}$$

5.3 Volterra integro-differential equation (VIDE)

In general the a VIDE can be expressed as:

$$\dot{y}(t) + p(t)y(t) + \int_0^t K(t, s)y(s)\mathrm{d}s = q(t) \tag{278}$$

with a known initial condition $y(0) = y_0$. This can be reformulated with numerical approximations of k-th order:

- Bootstrapping:
  To compute the first k time-steps we can use

$$\frac{1}{h}\sum_{l=0}^{k} D_{ml}^{(k)} y_l + p_m y_m + h\sum_{l=0}^{k} s_{ml}^{(k)} K_{ml} y_l = q_m \tag{279}$$

  for $m \leq k$. Knowing our initial condition it is reduced to a matrix equation.

$$\begin{pmatrix} M_{11} & \cdots & M_{1k} \\ \vdots & \ddots & \vdots \\ M_{k1} & \cdots & M_{kk} \end{pmatrix} \begin{pmatrix} y_1 \\ \vdots \\ y_k \end{pmatrix} = \begin{pmatrix} q_1 - M_{10} y_0 \\ \vdots \\ q_k - M_{k0} y_0 \end{pmatrix} \tag{280}$$

$$M_{ml} = \frac{1}{h} D_{ml}^{(k)} + p_l \delta_{ml} + h s_{ml}^{(k)} K_{ml} \tag{281}$$

- Time-stepping:
  Now, for $m > k$ we can use the backward differentiation.

$$\frac{1}{h}\sum_{l=0}^{k} a_l^{(k)} y_{m-l} + p_m y_m + h\sum_{l=0}^{m} w_{ml}^{(k)} K_{ml} y_l = q_m \tag{282}$$

$$y_m = \left[h^{-1} a_0^{(k)} + p_m + h w_{mm}^{(k)} K_{mm}\right]^{-1} \left[q_m - h^{-1}\sum_{l=1}^{k} a_l^{(k)} y_{m-l} - h\sum_{l=0}^{m-1} w_{ml}^{(k)} K_{ml} y_l\right] \tag{283}$$

5.4 Volterra integral equation (VIE)

VIE is an equation that forgets the derivative part:

$$y(t) + \int_0^t K(t,s) y(s) \mathrm{d}s = q(t) \tag{284}$$

also with an initial condition $y(0) = y_0$.

- Bootstrapping
  We can compute the steps $m \leq k$:

$$y_m + h\sum_{l=0}^{k} s_{ml}^{(k)} K_{ml} y_l = q_m \tag{285}$$

  which can be reduced to a matrix equation.

$$\begin{pmatrix} M_{11} & \cdots & M_{1k} \\ \vdots & \ddots & \vdots \\ M_{k1} & \cdots & M_{kk} \end{pmatrix} \begin{pmatrix} y_1 \\ \vdots \\ y_k \end{pmatrix} = \begin{pmatrix} q_1 - M_{10} y_0 \\ \vdots \\ q_k - M_{k0} y_0 \end{pmatrix} \tag{286}$$

$$M_{ml} = \delta_{ml} + h s_{ml}^{(k)} K_{ml} \tag{287}$$

- Time-stepping
  This time, in absence of derivative, backward differentiation is not necessary.

$$y_m + h\sum_{l=0}^{m} w_{ml}^{(k)} K_{ml} y_l = q_m \tag{288}$$

$$y_m = \left[1 + h w_{mm}^{(k)} K_{mm}\right]^{-1} \left[q_m - h\sum_{l=0}^{m-1} w_{ml}^{(k)} K_{ml} y_l\right] \tag{289}$$

A Tensor inverse

Let two interactions in its tensor form such that

$$S_{kn}^{im} W_{ml}^{nj} = \delta_{kl}^{ij} = \begin{cases} 1 & \text{if } i = l \text{ and } j = k \\ 0 & \text{otherwise} \end{cases} \tag{290}$$

where δ^{ij}_{kl} is a generalized Kronecker delta (look that $\delta^{im}_{kn}W^{nj}_{ml} = W^{ij}_{kl}$ and $W^{im}_{kn}\delta^{nj}_{ml} = W^{ij}_{kl}$). If this is accomplished we can define S as the inverse of W, $S = W^{-1}$. In order to compute this inverse we can vectorize S and δ:

$$\delta^{ij}_{kl} \to d[p] \qquad p = iN^3 + jN^2 + kN + l \tag{291a}$$

$$S^{im}_{kn} \to s[q] \qquad q = iN^3 + mN^2 + kN + n \tag{291b}$$

where N is the number of orbital basis, and define the following linear application:

$$d[p] = M[p,q]s[q] \tag{292}$$

Here $M[p,q]$ encodes the elements of W:

$$M[p,q] = \begin{cases} W^{nj}_{ml} & \text{if } i_p = i_q \text{ and } k_p = k_q \\ 0 & \text{otherwise} \end{cases} \tag{293}$$

where i_p refers the tensor index i linked to vector index p. The linear application defines a set of N^4 equations of N^4 variables which can be decoupled into N^2 sets of N^2 equations of N^2 variables since for a particular choice of i, k indices all elements of W are encoded. This means that we just should take, for example, $i = k = 0$, so:

$$p' = jN^2 + l \tag{294a}$$

$$q' = mN^2 + n \tag{294b}$$

then construct the sumbatrix $M[p', q']$ and compute its inverse where $M^{-1}[q', p']$ will correspond to elements of S taking into account the tensor notation $S^{im}_{kn} = \delta^{ij}_{kl}S^{lm}_{jn}$.

B Green's functions basis

Green's functions kind objects are defined with field operators

$$G(\mathbf{x}, t; \mathbf{x}', t') = -\imath \left\langle \mathcal{T}_\mathcal{C} \Psi(\mathbf{x}, t)\Psi^\dagger(\mathbf{x}', t') \right\rangle \tag{295}$$

but if we recall the basis change of field operators

$$G(\mathbf{x}, t; \mathbf{x}', t') = -\imath \sum_{i,j}\sum_{\mu,\nu} \left\langle \mathcal{T}_\mathcal{C} c_{i\mu}(t)c^\dagger_{j\nu}(t') \right\rangle \psi_{i\mu}(\mathbf{x})\psi^*_{j\nu}\mathbf{x}' = \sum_{i,j}\sum_{\mu,\nu} G^\mu_\nu(i,j;t,t')\psi_{i\mu}(\mathbf{x})\psi^*_{j\nu}(\mathbf{x}') \tag{296}$$

we can define the matrix elements of the Green's function using orbitals (Greek indices) and lattice sites (Latin indices). They behave independently. Now we can define the Green's function in momentum space using $\mathbf{r}_{ij} = \mathbf{R}_j - \mathbf{R}_i$

$$G^\mu_\nu(i,j;t,t') = -\frac{\imath}{N}\sum_{\mathbf{k},\mathbf{k}'} \mathrm{e}^{\imath(\mathbf{k}\cdot\mathbf{R}_i - \mathbf{k}'\cdot\mathbf{R}_j)} \left\langle \mathcal{T}_\mathcal{C} a_{\mathbf{k}\mu}(t)a^\dagger_{\mathbf{k}'\nu}(t') \right\rangle = -\frac{\imath}{N}\sum_{\mathbf{k},\mathbf{q}} \mathrm{e}^{-\imath(\mathbf{k}\cdot\mathbf{r}_{ij} + \mathbf{q}\cdot\mathbf{R}_j)} \left\langle \mathcal{T}_\mathcal{C} a_{\mathbf{k}\mu}(t)a^\dagger_{\mathbf{k}-\mathbf{q}\nu}(t') \right\rangle \tag{297}$$

Look that by discrete translational symmetry the sum over $\mathbf{q}$ can only conserve the term with v$\mathbf{q} = 0$ so we can define the momentum space Green's functions as

$$G^\mu_\nu(\mathbf{k}; t, t') = -\imath \left\langle \mathcal{T}_\mathcal{C} a_{\mathbf{k}\mu}(t)a^\dagger_{\mathbf{k}\nu}(t') \right\rangle \tag{298}$$

with the following transformation

$$G^\mu_\nu(i,j;t,t') = \frac{1}{N}\sum_{\mathbf{k}} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{r}_{ij}} G^\mu_\nu(\mathbf{k};t,t') \tag{299}$$

$$G^\mu_\nu(\mathbf{k};t,t') = \frac{1}{N}\sum_{i,j} \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}_{ij}} G^\mu_\nu(i,j;t,t') \tag{300}$$

which account for other objects like self-energy.

Interaction-like objects, like polarization bubbles can be quite difficult, so let's derive from real space to lattice-orbital space

$$P(\mathbf{x}, t; \mathbf{x}', t') = -\imath \sum_{i,j}\sum_{\mu,\nu,\lambda,\kappa} G^\mu_\kappa(i,j;t,t')G^\nu_\lambda(j,i;t',t)\psi_{i\mu}(\mathbf{x})\psi_{j\nu}(\mathbf{x}')\psi^*_{i\lambda}(\mathbf{x})\psi^*_{j\kappa}(\mathbf{x}') \tag{301}$$

recalling that a lattice wave function is approximated to a Dirac delta, so same position argument belongs to the same lattice site but not necessarily to the same orbital.

$$P^{\mu\nu}_{\lambda\kappa}(i,j;t,t') = -\imath G^{\mu}_{\kappa}(i,j;t,t')G^{\nu}_{\lambda}(j,i;t',t) \tag{302}$$

This product can be performed in momentum space

$$P^{\mu\nu}_{\lambda\kappa}(i,j;t,t') = -\imath \sum_{\mathbf{k},\mathbf{k}'} \mathrm{e}^{\imath(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_{ij}} G^{\mu}_{\kappa}(\mathbf{k};t,t')G^{\nu}_{\lambda}(\mathbf{k}',t',t) = -\imath \sum_{\mathbf{k},\mathbf{q}} \mathrm{e}^{-\imath\mathbf{q}\cdot\mathbf{r}_{ij}} G^{\mu}_{\kappa}(\mathbf{k}+\mathbf{q};t,t')G^{\nu}_{\lambda}(\mathbf{k},t',t) \tag{303}$$

where gain the variable change $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ is done, so we can define the polarization bubble in momentum space

$$P^{\mu\nu}_{\lambda\kappa}(\mathbf{q};t,t') = -\imath \sum_{\mathbf{k}} G^{\mu}_{\kappa}(\mathbf{k}+\mathbf{q};t,t')G^{\nu}_{\lambda}(\mathbf{k};t',t) \tag{304}$$

with the following transformation

$$P^{\mu\nu}_{\lambda\kappa}(i,j;t,t') = \sum_{\mathbf{q}} \mathrm{e}^{-\imath\mathbf{q}\cdot\mathbf{r}_{ij}} P^{\mu\nu}_{\lambda\kappa}(\mathbf{q};t,t') \tag{305}$$

$$P^{\mu\nu}_{\lambda\kappa}(\mathbf{q};t,t') = \frac{1}{N}\sum_{\mathbf{q}} \mathrm{e}^{\imath\mathbf{q}\cdot\mathbf{r}_{ij}} P^{\mu\nu}_{\lambda\kappa}(i,j;t,t') \tag{306}$$

The other kind of bubble is the self energy in GW approximation

$$\Sigma(\mathbf{x},t;\mathbf{x}',t') = \imath G(\mathbf{x},t;\mathbf{x}',t')\tilde{W}(\mathbf{x},t;\mathbf{x}',t') = \imath \sum_{i,j}\sum_{\lambda,\kappa} G^{\lambda}_{\kappa}(i,j;t,t')\bar{W}(\mathbf{x},t;\mathbf{x}',t')\psi_{i\lambda}(\mathbf{x})\psi^{*}_{j\kappa}(\mathbf{x}') \tag{307}$$

$$\Sigma^{\mu}_{\nu}(i,j;t,t') = \int\int \Sigma(\mathbf{x},t;\mathbf{x}',t')\psi^{*}_{i\mu}(\mathbf{x})\psi_{j\nu}(\mathbf{x}')\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' = \imath \sum_{\lambda,\kappa} G^{\lambda}_{\kappa}(i,j;t,t')\tilde{W}^{\mu\kappa}_{\lambda\nu}(i,j;t,t') \tag{308}$$

Now just apply the Fourier transform

$$\Sigma^{\mu}_{\nu}(i,j;t,t') = \imath \sum_{\mathbf{q},\mathbf{q}'}\sum_{\lambda,\kappa} \mathrm{e}^{-\imath(\mathbf{q}+\mathbf{q}')\cdot\mathbf{r}_{ij}} G^{\lambda}_{\kappa}(\mathbf{q};t,t')\tilde{W}^{\mu\kappa}_{\lambda\nu}(\mathbf{q}';t,t') \tag{309}$$

by a variable change $\mathbf{q}+\mathbf{q}' = \mathbf{k}$ we can define the self-energy

$$\Sigma^{\mu}_{\nu}(\mathbf{k};t,t') = \imath \sum_{\mathbf{q}}\sum_{\lambda,\kappa} G^{\lambda}_{\kappa}(\mathbf{k}-\mathbf{q};t,t')\tilde{W}^{\mu\kappa}_{\lambda\nu}(\mathbf{q};t,t') \tag{310}$$

with the same transformation as P.

For those cases that a convolution is performed

$$\begin{aligned} C(\mathbf{x},t;\mathbf{x}',t') &= \int\int A(\mathbf{x},t;\mathbf{x}_1,t_1)B(\mathbf{x}_1,t_1;\mathbf{x}',t')\mathrm{d}\mathbf{x}_1\mathrm{d}t_1 \\ &= \sum_{i,j,l}\int\int A(i,l;t,t_1)B(l,j;t_1,t')\psi_i(\mathbf{x})\psi^{*}_{l}(\mathbf{x}_1)\psi_l(\mathbf{x}_1)\psi^{*}_{j}(\mathbf{x}')\mathrm{d}\mathbf{x}_1\mathrm{d}t_1 \\ &= \sum_{i,j,l}\int A(i,l;t,t_1)B(l,j;t_1,t')\psi_i(\mathbf{x})\psi^{*}_{j}(\mathbf{x}')\mathrm{d}t_1 \end{aligned} \tag{311}$$

$$\begin{aligned} C(i,j;t,t') &= \sum_{l}\int A(i,l;t,t_1)B(l,j;t_1,t')\mathrm{d}t_1 = \sum_{\mathbf{k},\mathbf{k}'}\sum_{l} \mathrm{e}^{-\imath(\mathbf{k}\cdot\mathbf{r}_{il}+\mathbf{k}'\cdot\mathbf{r}_{lj})}\int A(\mathbf{k};t,t_1)B(\mathbf{k}';t_1,t')\mathrm{d}t_1 \\ &= \sum_{\mathbf{k},\mathbf{k}'} \mathrm{e}^{\imath(\mathbf{k}\cdot\mathbf{R}_i-\mathbf{k}'\cdot\mathbf{R}_j)}\sum_{l}\mathrm{e}^{-\imath(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_l}\int A(\mathbf{k};t,t_1)B(\mathbf{k}';t_1,t')\mathrm{d}t_1 \\ &= \sum_{\mathbf{k}} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{r}_{ij}}\int A(\mathbf{k};t,t_1)B(\mathbf{k};t_1,t')\mathrm{d}t_1 = \sum_{\mathbf{k}} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{r}_{ij}} C(\mathbf{k};t,t') \end{aligned} \tag{312}$$

$$C(\mathbf{k};t,t') = \int A(\mathbf{k};t,t_1)B(\mathbf{k};t_1,t')\mathrm{d}t_1 \tag{313}$$

C Electric field and vector potential

An electromagnetic pulse is described with an oscillating function of frequency ω enveloped with some function, normally a gaussian distribution with deviation σ

$$\mathbf{E}(t) = \mathbf{E}_0 \mathrm{e}^{-\frac{t^2}{2\sigma^2}} \sin(\omega t + \varphi) = \Im\left[\bar{\mathbf{E}}_0 \mathrm{e}^{-\frac{t^2}{2\sigma^2}} \mathrm{e}^{\imath\omega t}\right] \tag{314}$$

where $\bar{\mathbf{E}}_0 = \mathbf{E}_0 \mathrm{e}^{\imath\varphi}$. By definition $\mathbf{E}(t) = -\partial_t \mathbf{A}(t)$, so

$$\mathbf{A}(t) = \int_{-\infty}^{t} \mathbf{E}(t')\mathrm{d}t'. \tag{315}$$

The integral of a gaussian is known as error function

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{e}^{-t^2} \mathrm{d}t \tag{316}$$

but the electric field is not strictly a gaussian but it can be arranged like that. The argument on the exponential is a second degree polynomial with complex coefficients $p(t)$, so $\bar{\mathbf{E}}(\mathbf{t}) = \bar{\mathbf{E}}_0 \mathrm{e}^{-p(t)}$

$$p(t) = \frac{1}{2\sigma^2} t^2 - \imath\omega t = \frac{1}{2\sigma^2} t^2 - \imath\omega t + k^2 - k^2 = \left(\frac{1}{\sqrt{2}\sigma} t - k\right)^2 - k^2$$

if we look into the linear term on t

$$\frac{\sqrt{2}k}{\sigma} = \imath\omega \implies k = \imath\frac{\sigma\omega}{\sqrt{2}}.$$

Now, by a variable change $u(t') = \dfrac{1}{\sqrt{2}\sigma} t' - \imath\dfrac{\sigma\omega}{\sqrt{2}}$ so $\mathrm{d}u = \dfrac{\mathrm{d}t'}{\sqrt{2}\sigma}$ the vector potential can be solved

$$\begin{aligned}
\mathbf{A}(t) &= \Im\left\{\bar{\mathbf{E}}_0 \mathrm{e}^{-\frac{\sigma^2\omega^2}{2}} \sqrt{2}\sigma \left[\int_{-\infty}^{0} \mathrm{e}^{-u^2}\mathrm{d}u + \int_0^{\frac{1}{\sqrt{2}\sigma}t - \imath\frac{\sigma\omega}{\sqrt{2}}} \mathrm{e}^{-u^2}\mathrm{d}u\right]\right\} \\
&= \mathbf{E}_0 \sigma \sqrt{\frac{\pi}{2}} \mathrm{e}^{-\frac{\sigma^2\omega^2}{2}} \Im\left\{\mathrm{e}^{\imath\varphi}\left[1 + \mathrm{erf}\left(\frac{1}{\sqrt{2}\sigma}t - \imath\frac{\sigma\omega}{\sqrt{2}}\right)\right]\right\} \\
&= \mathbf{E}_0 \sigma \sqrt{\frac{\pi}{2}} \mathrm{e}^{-\frac{\sigma^2\omega^2}{2}} \left\{[1 + f(t)]\sin\varphi + g(t)\cos\varphi\right\}
\end{aligned} \tag{317}$$

where we have defined for shortness

$$\mathrm{erf}\left(\frac{1}{\sqrt{2}\sigma}t - \imath\frac{\sigma\omega}{\sqrt{2}}\right) = f(t) + \imath g(t) \tag{318}$$

In the limit of $t \to \infty$ instead the electric field is 0 there can be a constant vector potential. At this limit the error function goes to 1

$$\mathbf{A}(\infty) = \mathbf{E}_0 \sqrt{2\pi}\sigma \mathrm{e}^{-\frac{\sigma^2\omega^2}{2}} \sin\varphi \tag{319}$$

We can see that there is a remainder vector potential for transient effects. In other case if we define an adiabatical switched electric field

$$\mathbf{E}(t) = \mathrm{e}^{-\eta|t|} \Im\left\{\bar{\mathbf{E}}_0 \mathrm{e}^{\imath\omega t}\right\} \tag{320}$$

we can compute the vector potential at infinite

$$\mathbf{A}(\infty) = \Im\left\{\bar{\mathbf{E}}_0 \left[\int_{-\infty}^{0} \mathrm{e}^{(\eta+\imath\omega)t}\mathrm{d}t + \int_0^{\infty} \mathrm{e}^{-(\eta-\imath\omega)t}\mathrm{d}t\right]\right\} = \Im\left\{\bar{\mathbf{E}}_0 \left[\frac{1}{\eta+\imath\omega} + \frac{1}{\eta-\imath\omega}\right]\right\} = 2\bar{\mathbf{E}}_0 \frac{\eta\sin\varphi}{\eta^2+\omega^2} \tag{321}$$

Since in adiabatical switching $\eta \to 0$ this transient effect disappears in stationary state.

D Gauge invariance

In classical electromagnetism, governed by Maxwell equations, we can define the fields from an scalar and a vector potential

$$\mathbf{E} = -\nabla\phi - \partial_t \mathbf{A} \tag{322}$$
$$\mathbf{B} = \nabla \times \mathbf{A}. \tag{323}$$

Since the rotational of a vector field defined with a gradient is null we can transform $\mathbf{A} \to \mathbf{A} + \nabla\Lambda$ without change the magnetic field but it will change the electric field in the following way: $\mathbf{E} = -\nabla(\phi + \partial_t\Lambda) - \partial_t\mathbf{A}$. To fix this we need to full fill these two transformations

$$\mathbf{A} \to \mathbf{A} + \nabla\Lambda \tag{324a}$$
$$\phi \to \phi - \partial_t\Lambda \tag{324b}$$

so-called gauge transformations. Since this transformations do not change the electromagnetic field every theory constructed over classical electromagnetism must be gauge invariant.

To choose an appropriate potentials one needs to add a restriction. In quantum physics the Coulomb gauge is chosen

$$\nabla \cdot \mathbf{A} = 0. \tag{325}$$

This gauge imposes the transversability of the vector potential.

The Schrödinger equation for a particle in an electromagnetic field is

$$\left[-\imath\partial_t + \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}\right)^2 + q\phi\right]\psi(\mathbf{x}, t) = 0 \tag{326}$$

so if we apply gauge transformations

$$\left[-\imath\partial_t + \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A} - q\nabla\Lambda\right)^2 + q\phi - q\partial_t\Lambda\right]\psi'(\mathbf{x}, t) = 0 \tag{327}$$

Look that if the gauge transform of wave function is the addition of a phase $\psi \to \psi' = \mathrm{e}^{\imath\alpha(\mathbf{x},t)}\psi$ the time derivative is $\partial_t\psi' = \mathrm{e}^{\imath\alpha}\partial_t\psi + \imath\mathrm{e}^{\imath\alpha}\psi\partial_t\alpha$ and similarly with the gradient (recall $\mathbf{p} = -\imath\nabla$) $\nabla\psi' = \mathrm{e}^{\imath\alpha}\nabla\psi + \imath\mathrm{e}^{\imath\alpha}\psi\nabla\alpha$ so introducing it into Schrödinger equation

$$\mathrm{e}^{\imath\alpha}\left[-\imath\partial_t + \partial_t\alpha + \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A} - q\nabla\Lambda + \nabla\alpha\right)^2 + q\phi - q\partial_t\Lambda\right]\psi(\mathbf{x}, t) = 0 \tag{328}$$

and finally in order to recover the original equation $\alpha = q\Lambda$ so $\psi \to \mathrm{e}^{\imath q\Lambda}\psi$. Also, for any operator

$$\langle\psi|\mathcal{O}|\psi\rangle = \langle\psi'|\mathcal{O}'|\psi'\rangle = \left\langle\psi|\mathrm{e}^{-\imath q\Lambda}\mathcal{O}'\mathrm{e}^{\imath q\Lambda}|\psi\right\rangle \tag{329}$$

so $\mathcal{O} \to \mathrm{e}^{\imath q\Lambda}\mathcal{O}\mathrm{e}^{-\imath q\Lambda}$.

When a gauge transformation is applied into a second order electromagnetic hopping new terms appear:

$$\begin{aligned}\bar{\alpha}^{i\mu}_{j\nu}(t) = \sum_{k,w}\big[&\left(\mathbf{t}^{\mu}_{w}(\mathbf{r}_{ik})\cdot\mathbf{A}(t)\right)\left(\mathbf{t}^{w}_{\nu}(\mathbf{r}_{kj})\cdot\mathbf{A}(t)\right) + \left(\mathbf{t}^{\mu}_{w}(\mathbf{r}_{ik})\cdot\mathbf{A}(t)\right)\left(\mathbf{t}^{w}_{\nu}(\mathbf{r}_{kj})\cdot\nabla\Lambda(t)\right)\\ &+ \left(\mathbf{t}^{\mu}_{w}(\mathbf{r}_{ik})\cdot\nabla\Lambda(t)\right)\left(\mathbf{t}^{w}_{\nu}(\mathbf{r}_{kj})\cdot\mathbf{A}(t)\right) + \left(\mathbf{t}^{\mu}_{w}(\mathbf{r}_{ik})\cdot\nabla\Lambda(t)\right)\left(\mathbf{t}^{w}_{\nu}(\mathbf{r}_{kj})\cdot\nabla\Lambda(t)\right)\big]\end{aligned} \tag{330}$$