2.3.3 Martin–Schwinger hierarchy

So far we have dealt with time-ordered operator correlators, namely
\[ \hat{G}_n = \frac{1}{i^n} \int \{ \hat{\Phi}_H(x_1) \ldots \hat{\Phi}_H(x_n) \hat{\Phi}^+_H(x_n') \ldots \hat{\Phi}^+_H(x_1') \}, \]

and found a hierarchy of integro-differential equations connecting
\[ \hat{G}_{n-1} \leftrightarrow \hat{G}_n \leftrightarrow \hat{G}_{n+1}. \]

To make further progress, we now need to define expectation values
and thus Green's functions
\[ G_n(x_1, \ldots, x_n; y_1, \ldots, y_n) = \frac{\text{Tr} \left[ e^{-\beta \hat{H}_n} \hat{G}_n(x_1, \ldots, x_n) \right]}{\text{Tr} \left[ e^{-\beta \hat{H}_n} \right]} \]
\[ = \frac{1}{i^n} \left( \int \left\{ e^{-i \int d\tau \hat{A}(\tau) \hat{\Phi}(\tau) \ldots \hat{\Phi}(\tau) \hat{\Phi}^+(\tau) \ldots \hat{\Phi}^+(\tau) \} \right\} \right) \]
\[ \text{Tr} \left[ \int \left\{ e^{-i \int d\tau \hat{A}(\tau) \hat{\Phi}(\tau) \ldots \hat{\Phi}(\tau) \hat{\Phi}^+(\tau) \ldots \hat{\Phi}^+(\tau) \} \right\} \right]. \]

Example: Take \( G_n \) with \( z_1 < z_1' \):
\[ e^{-\beta \hat{H}_n} \int \{ \hat{\Phi}_H(x_1) \hat{\Phi}^+_H(x_1') \} = \pm \int \{ e^{-i \int d\tau \hat{A}_B(\tau) \hat{\Phi}^+(\tau) \hat{\Phi}(\tau) \} = \int \{ e^{-i \int d\tau \hat{A}(\tau) \hat{\Phi}(\tau) \hat{\Phi}^+(\tau) \} \]
where we used \( e^{-\beta \hat{A}_B^n} = \hat{U}(z_1, z_1') \) and that field operators \((\hat{\Phi}, \hat{\Phi}^+)\) commute under the \( \int \) operator.

Why are the Green's functions \( G_n \) (n-body Green's functions) useful? E.g., \( G_n \) at \( z, z' \) and \( z_1 = z + z' z \) is proportional to the time-dependent ensemble average of \( \hat{\Phi}_H^+(x_1) \hat{\Phi}_H(x_1') \), from which the time-dependent ensemble average of any one-body operator (density, current, ... ) can be computed! The same holds true for \( n \)-body operators and \( G_n \).

For \( t = t_0 \): generalization to \( n \)-particle density matrices in thermal equilibrium.
The equation hierarchy in 2.3.2 immediately implies, by multiplication with the appropriate density matrix \( \tilde{\rho} \) and taking the trace:

\[
\left[ -i \frac{d}{d\tau_k} - h(k) \right] G_n \left( \tau_1, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right) = \pm i \sum_{i,j} \delta_{ij} \left( \tau_j \right) G_n \left( \tau_1, \ldots, \tau_{i-1}, \tau_{i+1}, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right) \\
+ \sum_{j=1}^{n} \left( \pm \right)^{k+j} \delta \left( \tau_j \right) G_{n-1} \left( \tau_1, \ldots, \tau_{j-1}, \tau_{j+1}, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right)
\]

\[
G_n \left( \tau_1, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right) \left[ -i \frac{d}{d\tau_k} - h(k) \right] = \pm i \sum_{i,j} \delta_{ij} \left( \tau_j \right) G_{n+1} \left( \tau_1, \ldots, \tau_{i-1}, \tau_{i+1}, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right) \\
+ \sum_{j=1}^{n} \left( \pm \right)^{k+j} \delta \left( \tau_j \right) G_{n-1} \left( \tau_1, \ldots, \tau_{j-1}, \tau_{j+1}, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right)
\]

**Marko-Schwinger hierarchy.**

**Important observation:** The derivation of these equations only depended on the behavior of operators under \( J \) (contour line ordering) and on Heisenberg equations of motion on a contour. The exact shape/type of contour was not used. The Marko-Schwinger hierarchy is therefore valid on different contours flexibly!

**Another important property:** The boundary condition that follows from the definition:

\[
G_n \left( \tau_1, \ldots, \tau_{k+1}, \tau_{k+2}, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right) = \pm G_n \left( \tau_1, \ldots, \tau_{k+1}, \tau_{k+2}, \ldots, \tau_n ; \tau'_1, \ldots, \tau'_n \right)
\]

\[
G_n \left( \tau_1, \ldots, \tau_n ; \tau'_1, \ldots, \tau_{k-1}, \tau_{k+1}, \ldots, \tau'_n \right) = \pm G_n \left( \tau_1, \ldots, \tau_n ; \tau'_1, \ldots, \tau_{k-1}, \tau_{k+1}, \ldots, \tau'_n \right)
\]

**Kubo-Marko-Schwinger relations** (Kubo 1957; MDS 1953)

**Examples:** 1-particle Green's function

\[
G_1 \left( x, \tau ; x', \tau' \right) = \pm G_1 \left( x, \tau ; x, \tau' \right)
\]

\[
G_1 \left( x, \tau ; x', \tau' \right) = \pm G_1 \left( x, \tau ; x', \tau' \right)
\]
Proof of KMS boundary conditions:

The numerator in the definition of $G$ is

\[ \text{Tr} \left[ \mathcal{J} e^{-i \int d^3 \vec{x} \hat{A}(\vec{x})} \hat{\psi}(\vec{x}) \ldots \hat{\psi}(k-1) \hat{\psi}(k) \hat{\psi}^\dagger(k+1) \ldots \hat{\psi}^\dagger(n) \hat{\psi}^\dagger(n+1) \ldots \hat{\psi}^\dagger(1) \right] = \ldots \]

Move this operator outside $\mathcal{J}$

since $\mathcal{J}$ is the latest possible time on $\Gamma$

\[ \Rightarrow (k-1) \text{ (and -) commutation required} \]

\[ \ldots = (\pm)^{k-1} \text{Tr} \left[ e^{-i \int d^3 \vec{x} \hat{A}(\vec{x})} \hat{\psi}(\vec{x}) \ldots \hat{\psi}(k-1) \hat{\psi}(k+1) \ldots \hat{\psi}^\dagger(n) \right] \]

No $\mathcal{J}$ label needed — remember that it was only meant to remind us of the order of operators.

Now cyclically permute under the trace (from left to right):

\[ \ldots = (\pm)^{k-1} \text{Tr} \left[ \mathcal{J} e^{-i \int d^3 \vec{x} \hat{A}(\vec{x})} \hat{\psi}(\vec{x}) \ldots \hat{\psi}(k-1) \hat{\psi}^\dagger(k+1) \ldots \hat{\psi}^\dagger(n) \right] \]

Now move back by 2n-k slab to original position:

\[ \ldots = (\pm)^{k-1} (\pm)^{2n-k} \left[ e^{-i \int d^3 \vec{x} \hat{A}(\vec{x})} \hat{\psi}(\vec{x}) \ldots \hat{\psi}(k-1) \hat{\psi}^\dagger(k+1) \ldots \hat{\psi}^\dagger(n) \right] \]

\[ \pm \text{ since k cancels and 2n is always even. Q.e.d.} \]

2.3.4 Truncation of the hierarchy — Hartree-Fock self-energy

Goal: Motivate the self-energy $\Sigma$ as one possible "tool" to truncate the infinite Martin-Schwinger hierarchy.

$\Rightarrow$ basis for many-body perturbation theory and Feynman diagrams.

Focus on 1-body Green's function $G(\vec{x},2) \equiv G(\vec{x},1;2)$;
\[ \left[ i \frac{d}{dt} - h(t) \right] G(\lambda, \lambda') = \delta(\lambda, \lambda') + i \int d^2 r \, \psi(1, 2) \, G_z(1, 2, \lambda, \lambda') \]

\[ G(\lambda, \lambda') \left[ -i \frac{d}{d\lambda} - h(\lambda) \right] = \delta(\lambda, \lambda') + i \int d^2 r \, \psi(1, 2) \, G_z(1, 2, \lambda, \lambda') \]

EOMs for \( G \).

For \( G_z \) we have the EOMs:

\[ \left[ i \frac{d}{dt} - h(1) \right] G_z(1, 2, 1', 2') = \delta(1, 1') G(2, 2') + \delta(1, 2') G(2, 1') + i \int d^3 k \psi(1, 3) G_z(k, 3, 1', 2') \]

\[ \left[ i \frac{d}{dt} - h(2) \right] G_z(1, 2, 1', 2') = \delta(2, 1') G(1, 2') + \delta(2, 2') G(1, 1') + i \int d^3 k \psi(2, 3) G_z(1, 2, 3', 1', 2') \]

\[ G_z(1, 2, 1', 2') \left[ -i \frac{d}{d\lambda} - h(\lambda) \right] = \delta(\lambda, \lambda') G(1, 2') + \delta(\lambda, 2') G(1, 1') + i \int d^3 k \psi(1, 3) G_z(1, 2, 3', 1', 2') \]

\[ G_z(1, 2, 1', 2') \left[ -i \frac{d}{d\lambda} - h(\lambda) \right] = \delta(\lambda, \lambda') G(1, 2') + \delta(\lambda, 2') G(1, 1') + i \int d^3 k \psi(2, 3) G_z(1, 2, 3', 1', 2') \]

This suggests to decompose:

\[ G_z(\lambda, \lambda') = G(\lambda, \lambda') G(2, 2') + G(\lambda, 2') G(2, \lambda') + \sum \]

Correlation function, defined via this equation.

Check: for \( \nu = 0 \) this \( G_z \) with \( \Gamma = 0 \) satisfies the EOMs.

For example:

\[ \left[ i \frac{d}{dt} - h(1) \right] \left( G(\lambda, \lambda') G(2, 2') + G(\lambda, 2') G(2, \lambda') \right) = \delta(\lambda, \lambda') \delta(2, 2') + \delta(\lambda, 2') \delta(2, \lambda') \]

is fulfilled by \( G \) for \( \nu = 0 \) (cf. \( \nu = 0 \) EOMs for \( G \)).

Also: \( G_z \) automatically fulfills KMS boundary conditions when \( G \) does.

The approximation \( G(1, 2, 1', 2') \approx G(\lambda, \lambda') G(2, 2') + G(\lambda, 2') G(2, \lambda') \)

is called Hartree-Fock approximation for \( G_z \).
Inserting the HF approximation into the EOMs for $G$ gives:

\[
\begin{bmatrix}
\frac{d}{dt} - h(1)
\end{bmatrix} G(1,1) = \delta(1,1) + \int d2 \, v(1,2) \left[ G(1,1) G(2,2) \pm G(1,2) G(2,1) \right]
\]

\[\equiv \delta(1,1) + \int d2 \, \Sigma(1,2) G(2,1)\]

\[
G(1,1) \left[ -i \frac{d}{dt} - h(1) \right] = \delta(1,1) + i \int d2 \, v(1,2) \left[ G(1,1) G(2,2) \pm G(1,2) G(2,1) \right]
\]

\[\equiv \delta(1,1) + \int d2 \, G(1,2) \Sigma(2,1)\]

Here we have defined the **Hartree-Fock self-energy**

\[\Sigma(1,2) = \delta(1,2) V_\text{HF}(1) + i \, v(1,2) \, G(1,2^+)\]

with

\[V_\text{HF}(1) \equiv \pm i \int d3 \, v(1,3) G(3,3^+) = \int dx_3 \, v(x_1, x_3, z_3) \eta(x_3, z_3)\]

we have used

\[v(1,3) = \delta(x_1, x_3) \eta(x_1, x_3, z_3) + i \, G(x_1, x_3; z_3, z_3^+) \eta(x_3, z_3)\]

$V_\text{HF}$ is called Hartree potential = classical electrostatic potential.

E.g., $V_\text{HF}(x_1, x_3, z_3) = \frac{1}{|x_1 - x_3|}$ for Coulomb interactions.

Second term in $\Sigma$: "Fock" or "exchange potential" — local in time, but non-local in space \(\Rightarrow\) no classical interpretation!\nn

The equations (3.x) and (4.xx) must be solved self-consistently!

(c.f. mean-field theory of Hubbard and ferromagnet.)

Reason: $\Sigma = \Sigma[G]$, the self-energy is a functional of $G$.

\[\Rightarrow\] nonlinear equations \(\Rightarrow\) nonperturbative in $v$!

We will now use the KMS boundary conditions to write the solution in integral form.
**Definition:** The noninteracting Green's function \( G_0 \) fulfills the EOMs for \( \nu = 0 \):

\[
\left[ i \frac{d}{d\tau} - h(\tau) \right] G_0(\tau; \tau') = \delta(\tau - \tau')
\]

\[
G_0(\tau; \tau') \left[ - i \frac{\delta}{d\tau} - h(\tau) \right] = \delta(\tau - \tau').
\]

Using KMS boundary conditions we write

\[
\int d\tau \; G_0(\tau; \tau') \left[ i \frac{d}{d\tau} - h(\tau) \right] G(\tau; \tau') = \int_{\tau = \tau'}^{\tau = \tau'} d\tau \; G_0(\tau; \tau') \left[ - i \frac{\delta}{d\tau} - h(\tau) \right] G(\tau; \tau') + \int d\tau \; G_0(\tau; \tau') \Sigma(\tau, \tau') G(\tau; \tau')
\]

\[
\int_{\tau = \tau'}^{\tau = \tau'} d\tau \; G_0(\tau; \tau') \left[ - i \frac{\delta}{d\tau} - h(\tau) \right] G(\tau; \tau') \bigg|_{\tau = \tau'}^{\tau = \tau'} = 0
\]

\[
\int d\tau \; G_0(\tau; \tau') \left[ - i \frac{\delta}{d\tau} - h(\tau) \right] G(\tau; \tau') = G(\tau; \tau')
\]

Analogously:

\[
\int d\tau \; G(\tau; \tau') \left[ - i \frac{\delta}{d\tau} - h(\tau) \right] G_0(\tau; \tau') = G(\tau; \tau')
\]

Multiplying \((*)\) from right/left (first/second eq.) with \( G_0 \) and using the above identities we obtain the following two equivalent equations for \( G \):

\[
G(\tau; \tau') = G_0(\tau; \tau') + \int d\tau' d\tau'' G_0(\tau; \tau') \Sigma(\tau'; \tau'') G(\tau'; \tau'')
\]

\[
G(\tau; \tau') = G_0(\tau; \tau') + \int d\tau' d\tau'' G_0(\tau; \tau') \Sigma(\tau'; \tau'') G(\tau'; \tau'')
\]

**Dyson equations**

Here the KMS boundary conditions are automatically incorporated in \( G_0 \).

**Later:** The exact \( G \) fulfills the same form of equations but with a more complicated self-energy \( \Sigma \) (beyond Hartree-Fock).

**Dyson equation:** Formal solution of the Mathieu-Schwinger hierarchy.

\[
\text{suggest that we can introduce } \Sigma \text{ as a "truncated of the hierarchy".}
\]
2.3.5 Exact solution of the hierarchy via Wick's theorem

For \( \nu = 0 \) the hierarchy couples \( G_0 \) only to \( G_{n-1} \):

\[
\begin{align*}
\left[i \frac{d}{dt} - h(k)\right] G_{0n} &= \sum_{j=1}^{n} (\pm)^{k+j} \delta(k,j) G_{0n-1} (1, \ldots, \hat{n}, 1', \ldots, n'), \\
G_{0n} \left[-i \frac{d}{dt} - h(k)\right] &= \sum_{j=1}^{n} (\pm)^{k+j} \delta(j,k) G_{0n-1} (1, \ldots, \hat{n}, 1', \ldots, n'),
\end{align*}
\]

which can be solved exactly. Below we will prove that

\[
G_{0n} (1, \ldots, n; 1', \ldots, n') = \begin{bmatrix} G_0 (1,1') & \cdots & G_0 (1,n') \\
\vdots & \ddots & \vdots \\
G_0 (n,1') & \cdots & G_0 (n,n') \end{bmatrix}^+ \tag{\text{	extit{Wick's theorem}}}
\]

with \( G_0 \equiv G_{0,1} \) (as before).

Here \( |A|^+ \equiv \sum_{P} (\pm)^{p} A_{1P} \cdots A_{nP} \) = \text{permanent} \hspace{1cm} (\text{for bosons}) \text{ determinant} \hspace{1cm} (\text{for fermions})

of the \( n \times n \)-matrix \( A \). Here \( A_{ij} \equiv G_0 (i,j) \).

Note that we have already seen this for the special case \( G_2 \).

**Proof of (\text{	extit{Wick's theorem}}):** Expand the permanent/determinant along row \( k \):

\[
G_{0n} = \sum_{j=1}^{n} (\pm)^{k+j} G_0 (k,j) G_{0n-1} (1, \ldots, \hat{j}, \ldots, n'; 1', \ldots, n').
\]

Apply \( \left[i \frac{d}{dt} - h(k)\right] \) from left. This fulfills the \( n \)-EDM for \( G_{0n} \).

Expanding along column \( k \) gives the second EDM.

\( \Rightarrow \) The expansion (\text{	extit{Wick's theorem}}) \( G_{0n} \) into a permanent/determinant of

1-body noninteracting \( G_0 's \) is a solution of the noninteracting

\( \text{Martin-Schwinger hierarchy} \).

Also: KMS automatically incorporated via KMS for 1-body \( G_0 's \). (multiplication of \( G_0 \) in a row/column with a \( \pm 1 \)-prefactor also multiplies the entire per/det with the same prefactor)
it is sufficient to solve the EOMs for $G_0$ to obtain all $G_n$'s!

Remark: This derivation of Wick's theorem is completely general. The expansion appears as a natural solution to a boundary value problem for the $\Phi^4$ hierarchy.