2.3.3 Martin–Schwinger hierarchy

So far we have dealt with time-ordered operator correlators, namely

$$\hat{G}_n \equiv \frac{1}{i^n} \mathcal{T}\{\hat{\psi}_H(1)\ldots\hat{\psi}_H(n)\,\hat{\psi}_H^+(n')\ldots\hat{\psi}_H^+(1')\},$$

and found a hierarchy of integro-differential equations connecting

$$\hat{G}_{n-1} \longleftrightarrow \hat{G}_n \Longleftrightarrow \hat{G}_{n+1}.$$

To make further progress, we now need to **define** expectation values and thus Green's functions

$$G_n(1,\ldots,n;1',\ldots,n') \equiv \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\hat{G}_n(1,\ldots,n;1',\ldots,n')\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\right]}$$

$$= \frac{1}{i^n}\,\frac{\mathrm{Tr}\left[\mathcal{T}\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\,\hat{\psi}(1)\ldots\hat{\psi}(n)\,\hat{\psi}^+(n')\ldots\hat{\psi}^+(1')\}\right]}{\mathrm{Tr}\left[\mathcal{T}\{e^{-i\int_\gamma \hat{H}(\bar{z})\,d\bar{z}}\}\right]}.$$

Example: Take G_1 with $z_1 < z_1'$:

$$e^{-\beta\hat{H}^M}\mathcal{T}\{\hat{\psi}_H(1)\hat{\psi}_H^+(1')\} = \pm\,\hat{U}(z_f,z_i)\,\hat{U}(z_i,z_1')\,\hat{\psi}^+(1')\,\hat{U}(z_1',z_1)\,\hat{\psi}(1)\,\hat{U}(z_1,z_i)$$

$$= \underset{\text{fermions}}{\overset{\text{bosons}}{\pm}}\,\mathcal{T}\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\,\hat{\psi}^+(1')\,\hat{\psi}(1)\} = \mathcal{T}\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\,\hat{\psi}(1)\,\hat{\psi}^+(1')\},$$

where we used $e^{-\beta\hat{H}^M} = \hat{U}(z_f,z_i)$ and that field operators (anti-)commute under the $\mathcal{T}$ operator.

Why are the Green's functions G_n (n-body Green's functions) useful?
E.g., G_1 at $z_1 = z$ and $z_1' = z^+ > z$ is proportional to the time-dependent ensemble average of $\hat{\psi}_H^+(x_1')\,\hat{\psi}_H(x_1)$, from which the time-dependent ensemble average of <u>any</u> one-body operator (density, current, ...) can be computed! The same holds true for n-body operators and G_n.

For $z = t_0$: 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 $\hat{\rho}$ and taking the trace:

$$\boxed{\begin{aligned}\left[i\frac{d}{dz_k}-h(k)\right]G_n(1,\dots,n;1',\dots,n') &= \pm i\int d\bar{1}\, v(k;\bar{1})\, G_{n+1}(1,\dots,n,\bar{1};1',\dots,n',\bar{1}^+)\\ &\quad+\sum_{j=1}^{n}(\pm)^{k+j}\delta(k;j')\,G_{n-1}(1,\dots\overline{k}\dots n;1'\dots\overline{j'}\dots n'),\\ G_n(1,\dots,n;1',\dots,n')\left[-i\frac{\overleftarrow{d}}{dz'_k}-h(k')\right] &= \pm i\int d\bar{1}\, v(k';\bar{1})\, G_{n+1}(1,\dots,n,\bar{1}^-;1',\dots,n',\bar{1})\\ &\quad+\sum_{j=1}^{n}(\pm)^{k+j}\delta(j;k')\,G_{n-1}(1,\dots\overline{j}\dots n;1'\dots\overline{k'}\dots n').\end{aligned}}$$

<u>Martin-Schwinger hierarchy</u>.

<u>Important observation:</u> The derivation of these equations only depended on the behavior of operators under $\mathcal{T}$ (contour time-ordering) and on Heisenberg equations of motion on a contour. The exact shape/type of contour was not used. The Martin-Schwinger hierarchy is therefore valid on different contours flexibly!

<u>Another important property:</u> The boundary condition that follows from the definition:

$$\boxed{\begin{aligned}G_n(1,\dots,(x_k,z_i),\dots,n;1',\dots,n') &= \pm\, G_n(1,\dots,(x_k,z_f),\dots,n;1',\dots,n')\\ G_n(1,\dots,n;1',\dots,(x'_k,z_i),\dots,n') &= \pm\, G_n(1,\dots,n;1',\dots,(x'_k,z_f),\dots,n').\end{aligned}}$$

<u>Kubo-Martin-Schwinger relations</u> (Kubo 1957; MAS 1959).

Examples: 1-particle Green's function

$$G_1(x,z_i;x',z') = \pm\, G_1(x,z_f;x',z')$$
$$G_1(x,z;x',z_i) = \pm\, G_1(x,z;x',z_f).$$

Proof of KMS boundary conditions:

The numerator in the definition of G_n is

$$\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar z\,\hat H(\bar z)}\hat\psi(1)\ldots\hat\psi(k-1)\boxed{\hat\psi(x_k,z_f)}\hat\psi(k+1)\ldots\hat\psi(n)\hat\psi^+(n')\ldots\hat\psi^+(1')\right\}\right]=\ldots$$

move this operator outside $\mathcal{T}$
since z_f is the latest
possible time on γ
$\Rightarrow$ $(k-1)$ (anti-) commutations required

$$\ldots=(\pm)^{k-1}\,\mathrm{Tr}\left[\hat\psi(x_k)\,\mathcal{T}\left\{e^{-i\int_\gamma d\bar z\,\hat H(\bar z)}\hat\psi(1)\ldots\hat\psi(k-1)\hat\psi(k+1)\ldots\hat\psi^+(1')\right\}\right]=\ldots$$

no z_f label needed — remember that it was only meant to remind us of the order of operators.

Now cyclically permute under the trace ($\hat\psi(x_k)$ from left to right):

$$\ldots=(\pm)^{k-1}\,\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar z\,\hat H(\bar z)}\hat\psi(1)\ldots\hat\psi(k-1)\hat\psi(k+1)\ldots\hat\psi^+(1')\hat\psi(x_k,z_i)\right\}\right]=\ldots$$

inserted as "earliest" possible under Tr

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

$$\ldots=\underbrace{(\pm)^{k-1}(\pm)^{2n-k}}_{\equiv\,\pm}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar z\,\hat H(\bar z)}\hat\psi(1)\ldots\hat\psi(k-1)\hat\psi(x_k,z_i)\hat\psi(k+1)\ldots\hat\psi^+(1')\right\}\right]$$

$\equiv \pm$ 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 Σ 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 $G(1;2)\equiv G_1(1;2)$:

$$\boxed{\begin{aligned}\left[i\frac{d}{dz_1} - h(1)\right] G(1;1') &= \delta(1;1') \pm i\int d2\, v(1;2)\, G_2(1,2;1',2^+)\\ G(1;1')\left[-i\frac{\overleftarrow{d}}{dz_1'} - h(1')\right] &= \delta(1;1') \pm i\int d2\, v(1';2)\, G_2(1,2^-;1',2)\end{aligned}}$$

EOMs for G.

For G_2 we have the EOMs

$$\left[i\frac{d}{dz_1} - h(1)\right] G_2(1,2;1',2') = \delta(1;1')G(2;2') \pm \delta(1;2')G(2;1') \pm i\int d3\, v(1;3)\, G_3(1,2,3;1',2',3^+)$$

$$\left[i\frac{d}{dz_2} - h(2)\right] G_2(1,2;1',2') = \pm\delta(2;1')G(1;2') + \delta(2;2')G(1;1') \pm i\int d3\, v(2;3)\, G_3(1,2,3;1',2',3^+).$$

$$G_2(1,2;1',2')\left[-i\frac{\overleftarrow{d}}{dz_1'} - h(1')\right] = \delta(1;1')G(2;2') \pm \delta(2;1')G(1;2') \pm i\int d3\, v(1';3)\, G_3(1,2,3^-;1',2',3)$$

$$G_2(1,2;1',2')\left[-i\frac{\overleftarrow{d}}{dz_2'} - h(2')\right] = \pm\delta(1;2')G(2;1') + \delta(2;2')G(1;1') \pm i\int d3\, v(2';3)\, G_3(1,2,3^-;1',2',3).$$

$\Rightarrow$ this suggests to decompose

$$\boxed{G_2(1,2;1',2') = G(1;1')\,G(2;2') \pm G(1;2')\,G(2;1') + \Upsilon(1,2;1',2')}$$

Correlation function, defined via this equation

Check: for $v=0$ this G_2 with $\Upsilon = 0$ satisfies the EOMs.

For example:

$$\left[i\frac{d}{dz_1} - h(1)\right]\left(G(1;1')\,G(2;2') \pm G(1;2')\,G(2;1')\right) = \delta(1;1')\,\delta(2;2') \pm \delta(1;2')\,\delta(2;1')$$

is fulfilled by G for $v=0$ (cf. $v=0$ EOMs for G).

Also: G_2 automatically fulfills KMS boundary conditions when G does.

The <u>approximation</u> $\boxed{G(1,2;1',2') \cong G(1;1')\,G(2;2') \pm G(1;2')\,G(2;1')}$

is called <u>Hartree-Fock approximation</u> for G_2.

Inserting the HF approximation into the EOMs for G gives:

$$\boxed{\begin{aligned}\left[i\frac{d}{dz_1}-h(1)\right]G(1;1') &= \delta(1;1') \pm i\int d2\, v(1;2)\left[G(1;1')G(2;2^+) \pm G(1;2^+)G(2;1')\right]\\ &\equiv \delta(1;1') + \int d2\, \Sigma(1;2)\, G(2;1')\\ G(1;1')\left[-i\frac{\overleftarrow{d}}{dz_1'}-h(1')\right] &= \delta(1;1') \pm i\int d2\, v(1';2)\left[G(1;1')\, G(2^-;2') \pm G(1;2)G(2^-;1')\right]\\ (*)\qquad &\equiv \delta(1;1') + \int d2\, G(1;2)\,\Sigma(2;1')\end{aligned}}$$

Here we have defined the <u>Hartree-Fock self-energy</u>

$$(**)\quad \boxed{\begin{aligned}&\Sigma(1;2) \equiv \delta(1;2)\, V_H(1) + i\, v(1;2)\, G(1;2^+)\\ \text{with}\quad &V_H(1) \equiv \pm i\int d3\, v(1;3)G(3;3^+) = \int dx_3\, V(x_1,x_3,z_1)\, n(x_3,x_1).\end{aligned}}$$

We have used $v(1;3) = \delta(z_1,z_3)\, V(x_1,x_3,z_1)$

$$\pm i\, G(x_3,z_1;x_3,z_1^+) = n(x_3,z_1)$$

V_H is called Hartree potential $\hat{=}$ classical electrostatic potential.

e.g., $V_H(x_1,x_3,z_1) = \dfrac{1}{|\vec{r}_1-\vec{r}_3|}$ for Coulomb interactions.

Second term in Σ: "Fock" or "exchange potential" – local in time, but nonlocal in space $\Longrightarrow$ no classical interpretation!

The equations $(*)$ and $(**)$ must be solved <u>selfconsistently</u>!
(cf. mean-field theory of Hubbard antiferromagnet.)

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 condition to write the solution in integral form.

<u>Definition:</u> The <u>noninteracting</u> Green's function G_0 fulfills the EOMs for $v=0$:

$$\left[i\frac{d}{dz_1}-h(1)\right]G_0(1;1') = \delta(1;1')$$

$$G_0(1;1')\left[-i\frac{\overleftarrow{d}}{dz_1'}-h(1')\right] = \delta(1;1').$$

Using KMS boundary conditions we write

$$\int d1\; G_0(2;1)\left[i\frac{d}{dz_1}-h(1)\right]G(1;1') \overset{\text{partial integration in } \gamma\text{-time}}{=}$$

$$= \int d1\; G_0(2;1)\left[-i\frac{\overleftarrow{d}}{dz_1}-h(1)\right]G(1;1') + \underbrace{i\int dx_1\; G_0(2;x_1,z_1)G(x_1,z_1;1')\Big|_{z_1=z_i}^{z_1=z_f}}_{\text{vanishes because } G \text{ and } G_0 \text{ satisfy KMS}}$$

$$= \int d1\; \delta(2;1)\,G(1;1') = G(2;1').$$

Analogously: $\int d1'\; G(1;1')\left[-i\frac{\overleftarrow{d}}{dz_1'}-h(1')\right]G_0(1';2) = G(1;2).$

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

$$\boxed{\begin{aligned} G(1;2) &= G_0(1;2) + \int d3\,d4\; G_0(1;3)\,\Sigma(3;4)\,G(4;2),\\ G(1;2) &= G_0(1;2) + \int d3\,d4\; G(1;3)\,\Sigma(3;4)\,G_0(4;2).\end{aligned}}$$

<u>Dyson equations</u>

Here the KMS boundary conditions are <u>automatically incorporated</u> via G_0.

<u>Later:</u> The exact G fulfills the same form of equations but with a more complicated self-energy Σ (beyond Hartree-Fock).

Dyson equation = <u>formal</u> solution of the Martin-Schwinger hierarchy.

$\Downarrow$

suggests that we can introduce Σ as a "truncator of the hierarchy".

2.3.5 Exact solution of the hierarchy via Wick's theorem

For $v=0$ the hierarchy couples G_n only to G_{n-1}:

$$\left[i\frac{d}{dz_k}-h(k)\right]G_{0,n}=\sum_{j=1}^{n}(\pm)^{k+j}\delta(k;j')\,G_{0,n-1}(1,..\overline{k}..n;1',..\overline{j'}..n'),$$

$$G_{0,n}\left[-i\frac{\overleftarrow{d}}{dz_k'}-h(k')\right]=\sum_{j=1}^{n}(\pm)^{k+j}\delta(j;k')\,G_{0,n-1}(1..\overline{j}..n;1'..\overline{k'}..n'),$$

which can be solved exactly. Below we will prove that

$$\boxed{G_{0,n}(1,\dots,n;1',\dots,n')=\begin{vmatrix}G_0(1;1') & \dots & G_0(1;n')\\ \vdots & & \vdots\\ G_0(n;1') & \dots & G_0(n;n')\end{vmatrix}_\pm}\quad (*)$$

"Wick's theorem"

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

Here $|A|_\pm \equiv \sum_P(\pm)^P A_{1P(1)}\cdots A_{nP(n)} = \begin{cases}\text{permanent } (+) \text{ for bosons}\\ \text{determinant } (-) \text{ for fermions}\end{cases}$

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 $(*)$: Expand the permanent/determinant along row k:

$$G_{0,n}=\sum_{j=1}^{n}(\pm)^{k+j}G_0(k;j')\,G_{0,n-1}(1,\dots,\overline{k},\dots,n;1,\dots,\overline{j'},\dots n').$$

← direct calculation of what $(*)$ really means.

Apply $\left[i\frac{d}{dz_k}-h(k)\right]$ from left: This fulfills the EOM for $G_{0,n}$.

Expanding along column k gives the second EOM.

⇒ The expansion $(*)$ of $G_{0,n}$ into a permanent/determinant of 1-body noninteracting G_0's is a solution of the noninteracting 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 ± 1-prefactor also multiplies the entire per/det with the same prefactor.)

$\Rightarrow$ it is sufficient to solve the EOMs for G_0 to obtain all $G_{0,n}$'s !

<u>Remark:</u> This derivation of Wick's theorem is completely general. The expansion appears as a natural solution to a boundary value problem for the MS hierarchy.