THE GENERATING FUNCTIONAL OF THERMAL CORRELATORS
FOR FERMIONS

NOTES BY LUCA G. MOLINARI

Abstract. Time-ordered thermal correlators and thermal Green functions may be obtained from generating functionals, which depend on external fields linearly coupled to the operators that enter the correlators. For Green functions the generator depends on Grassmann fields.
Here the operator approach is used. In another note, a representation of the generator as a functional integral with coherent states will be given. It has the great advantage of treating fields and source-fields on an equal footing.

1. Introduction

Consider a many-particle system with Hamiltonian $\hat{H}$, in thermal equilibrium at inverse temperature β and chemical potential μ. The thermal average of an operator is

$$\langle \hat{O} \rangle_K = \frac{1}{Z_K} \mathrm{tr}(\, e^{-\beta \hat{K}} \hat{O}\,) \tag{1}$$

where $\hat{K} = \hat{H} - \mu \hat{N}$ and $Z_K = \mathrm{tr}(e^{-\beta \hat{K}})$ is the partition function and $\Omega = -(1/\beta)\log Z_K$ is the thermodynamic potential. The evolution in imaginary time of an operator is:

$$\hat{O}_K(\tau) = e^{\frac{1}{\hbar}\tau \hat{K}} \hat{O}\, e^{-\frac{1}{\hbar}\tau \hat{K}}, \quad 0 \le \tau \le \hbar\beta. \tag{2}$$

Suppose that we are interested in thermal time-ordered correlators of the density, $\langle \mathcal{T} \hat{n}_K(x_1) \dots \hat{n}_K(x_n) \rangle_K$, where x_j stands for τ_j and position $\mathbf{x}_j$. Such correlators may be obtained from a generating functional. To this end, the Hamiltonian is modified by a term that couples the density operators $\hat{n}(\mathbf{x})$ to a fictitious external field $\varphi(\mathbf{x}, \tau)$ that depends on τ:

$$\hat{V}(\tau) = \int d\mathbf{x}\, \hat{n}(\mathbf{x}) \varphi(\mathbf{x}, \tau) \tag{3}$$

In presence of time-dependent sources, the time-evolution is given by a two-parameter propagator $\hat{\mathscr{U}}(\tau, \tau')$, that solves the Schrödinger equation $[\hat{K} + \hat{V}(\tau)]\hat{\mathscr{U}}(\tau, \tau') = -\hbar \partial_\tau \hat{\mathscr{U}}(\tau, \tau')$. In the interaction picture it factors into a source-free and a residual propagator:

$$\hat{\mathscr{U}}(\tau, 0) = e^{-\frac{1}{\hbar}\tau \hat{K}} \hat{\mathscr{U}}_I(\tau, 0) \tag{4}$$

Date: 2014, revised 2019.

The latter solves the equation $\hat{V}_K(\tau)\hat{\mathscr{U}}_I(\tau,0) = -\hbar\partial_\tau \hat{\mathscr{U}}_I(\tau,0)$, and can be represented as a Dyson time-ordered expansion:

$$\mathscr{U}_I(\tau,0) = \mathcal{T}\exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' V_K(\tau')\right] = \mathcal{T}\exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' \int d\mathbf{x}'\, \hat{n}_K(\mathbf{x}',\tau')\varphi(\mathbf{x}',\tau')\right]$$

The system with sources is not in thermal equilibrium. However, it is useful to introduce a source-dependent partition function that generalizes Gibbs' static expression. Setting $\tau = \hbar\beta$ in (4) and taking the trace:

$$Z[\varphi] = \operatorname{tr} \hat{\mathscr{U}}(\hbar\beta, 0) = \operatorname{tr}[e^{-\beta\hat{K}}\hat{\mathscr{U}}_I(\hbar\beta,0)] = Z_K\langle \hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K$$

This is the generating functional of the density correlators:

$$Z[\varphi] = Z_K\Big\langle \mathcal{T}\exp\Big\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\, \hat{n}_K(\mathbf{x},\tau)\varphi(\mathbf{x},\tau)\Big\}\Big\rangle_K \tag{5}$$

The expansion in the source-field gives the thermal correlators *i.e. in absence of the sources* (here $x = (\mathbf{x},\tau)$):

$$\frac{Z[\varphi]}{Z_K} = 1 + \sum_{r=1}^\infty \frac{(-1)^r}{r!\hbar^r}\int dx_1\dots dx_r \langle \mathcal{T}\hat{n}_K(x_1)\dots\hat{n}_K(x_r)\rangle_K\, \varphi(x_r)\dots\varphi(x_1)$$

Alternatively, functional derivatives of $Z[\varphi]$ in the source-field give correlators *in presence of sources* (which may be put to zero in the end). For example,

$$\hbar^2 \frac{\delta^2 Z[\varphi]}{\delta\varphi(x)\delta\varphi(x')} = Z_K\langle \mathcal{T}\mathscr{U}(\hbar\beta,0)\hat{n}(x)\hat{n}(x')\rangle_K = Z[\varphi]\langle \mathcal{T}\hat{n}(x)\hat{n}(x')\rangle_\varphi$$

where we define the average in presence of the sources as:

$$\begin{aligned}\langle \mathcal{T}\hat{n}(x_1)...\hat{n}(x_n)\rangle_\varphi =& \frac{\langle \mathcal{T}\mathscr{U}(\hbar\beta,0)\hat{n}(x_1)...\hat{n}(x_n)\rangle_K}{\langle \mathscr{U}(\hbar\beta,0)\rangle_K} \\ =& (-\hbar)^n \frac{1}{Z[\varphi]}\frac{\delta^n Z[\varphi]}{\delta\varphi(x_1)...\delta\varphi(x_n)}\end{aligned} \tag{6}$$

The thermal correlator is:

$$\langle \mathcal{T}\hat{n}(x_1)...\hat{n}(x_n)\rangle_K = (-\hbar)^n \frac{1}{Z[\varphi]}\frac{\delta^n Z[\varphi]}{\delta\varphi(x_1)...\delta\varphi(x_n)}\Big|_{\varphi=0} \tag{7}$$

2. Green functions

Since field operators are a basis for operators, the generating functional of their thermal correlators is of special interest. Such correlators are named Green functions. In absence of sources (thermal average):

$$(-1)^r \mathscr{G}(x_1\dots x_r; y_1\dots y_s) = \langle \mathcal{T}\hat{\psi}_K(x_1)\dots\hat{\psi}_K(x_r)\hat{\psi}_K^\dagger(y_s)\dots\hat{\psi}_K^\dagger(y_1)\rangle_K$$

Note the ordering of space-spin and time arguments. They are obtained from a generating functional with two independent Grassmann sources:

$$Z[\overline{\eta},\eta] = Z_K\Big\langle \mathcal{T}\exp\Big\{-\int dx\,[\overline{\eta}(x)\hat{\psi}_K(x) + \hat{\psi}_K^\dagger(x)\eta(x)]\Big\}\Big\rangle_K \tag{8}$$

In evaluating derivatives within a $\mathcal{T}$-ordering, the Grassmann derivatives and the field operators exactly anticommute:

$$\frac{\delta}{\delta\overline{\eta}(x_1)}\cdots\frac{\delta}{\delta\overline{\eta}(x_r)}\frac{\delta}{\delta\eta(y_s)}\cdots\frac{\delta}{\delta\eta(y_1)}\Big\langle\mathcal{T}e^{-\int dx\,[\overline{\eta}(x)\hat\psi(x)+\hat\psi^\dagger(x)\eta(x)]}\Big\rangle_K$$
$$=\Big\langle\mathcal{T}\frac{\delta}{\delta\overline{\eta}(x_1)}\cdots\frac{\delta}{\delta\overline{\eta}(x_r)}e^{-\int dx\,\overline{\eta}(x)\hat\psi(x)}\frac{\delta}{\delta\eta(y_s)}\cdots\frac{\delta}{\delta\eta(y_1)}e^{-\int dx\,\hat\psi^\dagger(x)\eta(x)}\Big\rangle_K$$

Now, the leftmost derivative $\delta/\delta\overline{\eta}(x_1)$ is anticommuted with the next $r-1$ derivatives. Its action on the source replaces it with the operator $-\hat\psi(x_1)$ which is anticommuted back to the left with the same number of sign changes. This is done for all derivatives in $\bar\eta(x_j)$. The derivatives $\delta/\delta\eta(x_j)\exp[-\int dx\hat\psi^\dagger(x)\eta(x)]$ give factors $+\hat\psi^\dagger(x_j)$. The result is:

$$=(-1)^r\Big\langle\mathcal{T}\hat\psi(x_1)\ldots\hat\psi(x_r)e^{-\int dx\,\overline{\eta}(x)\hat\psi(x)}\hat\psi^\dagger(y_s)\ldots\hat\psi^\dagger(y_1)e^{-\int dx\,\hat\psi^\dagger(x)\eta(x)}\Big\rangle_K$$
$$=(-1)^r\Big\langle\mathcal{T}\mathscr{U}_I(\hbar\beta,0)\hat\psi(x_1)\ldots\hat\psi(x_r)\hat\psi^\dagger(y_s)\ldots\hat\psi^\dagger(y_1)\Big\rangle_K$$

If sources are not put to zero, a correlator with sources is obtained:

$$\frac{(-1)^r}{Z[\overline{\eta},\eta]}\frac{\delta}{\delta\overline{\eta}(x_1)}\cdots\frac{\delta}{\delta\overline{\eta}(x_r)}\frac{\delta}{\delta\eta(y_s)}\cdots\frac{\delta}{\delta\eta(y_1)}Z[\overline{\eta},\eta]$$
$$=\frac{\langle\mathcal{T}\hat{\mathscr{U}}_I(\hbar\beta,0)\hat\psi_K(x_1)\ldots\hat\psi_K(x_r)\hat\psi^\dagger{}_K(y_s)\ldots\hat\psi^\dagger{}_K(y_1)\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K}$$
$$=\langle\mathcal{T}\hat\psi(x_1)\ldots\hat\psi(x_r)\hat\psi^\dagger(y_s)\ldots\hat\psi^\dagger(y_1)\rangle_{\overline{\eta},\eta}\tag{9}$$

The factor $Z[\bar\eta,\eta]^{-1}$ normalizes the measure in presence of the sources. Now sources may be turned off and:

$$\mathscr{G}(x_1\ldots x_r,y_1\ldots y_s)=\frac{1}{Z_K}\frac{\delta^{r+s}Z[\overline{\eta},\eta]}{\delta\overline{\eta}(x_1)\ldots\delta\overline{\eta}(x_r)\delta\eta(y_s)\ldots\delta\eta(y_1)}\Big|_{\eta,\overline{\eta}=0}\tag{10}$$

Double derivatives give two-point time-ordered correlators:

$$\mathscr{G}(x,y)=-\langle\mathcal{T}\hat\psi_K(x)\hat\psi^\dagger{}_K(y)\rangle_K=\frac{1}{Z[\overline{\eta},\eta]}\frac{\delta^2Z[\overline{\eta},\eta]}{\delta\overline{\eta}(x)\delta\eta(y)}\Big|_0\tag{11}$$

$$\mathscr{F}(x,y)=-\langle\mathcal{T}\psi_K(x)\psi_K(y)\rangle_K=-\frac{1}{Z[\overline{\eta},\eta]}\frac{\delta^2Z[\overline{\eta},\eta]}{\delta\overline{\eta}(x)\delta\overline{\eta}(y)}\Big|_0\tag{12}$$

$$\mathscr{F}^\dagger(x,y)=-\langle\mathcal{T}\psi^\dagger{}_K(x)\psi^\dagger{}_K(y)\rangle_K=--\frac{1}{Z[\overline{\eta},\eta]}\frac{\delta^2Z[\overline{\eta},\eta]}{\delta\eta(x)\delta\eta(y)}\Big|_0\tag{13}$$

The anomalous Green functions $\mathscr{F}(x,y)$ and $\mathscr{F}^\dagger(x,y)$ are non-zero in systems which do not conserve the number of particles, as the B.C.S. model of superconductivity or Bogoliubov's model for superfluidity.

2.1. **The classical field.** A single functional derivative gives the average of the Fermi field in presence of the sources, named *classical field* (a Grassmann field):

$$\boxed{\psi_{c\ell}(x)=:\langle\hat\psi(x)\rangle_{\bar\eta\eta}=\frac{\langle\mathcal{T}\hat{\mathscr{U}}_I(\hbar\beta,0)\hat\psi_K(x)\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K}=-\frac{1}{Z[\overline{\eta},\eta]}\frac{\delta Z[\overline{\eta},\eta]}{\delta\overline{\eta}(x)}}\tag{14}$$

Similarly one obtains

$$\overline{\psi}_{c\ell}(x) = \frac{\delta}{\delta\eta(x)} \log Z[\overline{\eta},\eta].$$

If the sources are turned off, the thermal averages of the Fermi fields are time independent. They may be nonzero in theories where the total number of particles is not an exact symmetry, as in superfluidity.
Another derivative and anticommutations give:

$$\begin{aligned}\frac{\delta\psi_{c\ell}(x)}{\delta\eta(y)} &= -\frac{1}{Z[\overline{\eta},\eta]}\frac{\delta^2 Z[\overline{\eta},\eta]}{\delta\eta(y)\delta\overline{\eta}(x)} + \frac{1}{Z^2[\overline{\eta},\eta]}\frac{\delta Z[\overline{\eta},\eta]}{\delta\eta(y)}\frac{\delta Z[\overline{\eta},\eta]}{\delta\overline{\eta}(x)}\\ &= -\langle\mathcal{T}\hat\psi(x)\hat\psi^\dagger(y)\rangle_{\eta\overline{\eta}} + \psi_{c\ell}(x)\bar\psi_{c\ell}(y)\end{aligned}$$

Let's specify the $\mathcal{T}$-ordering in the numerator of (14):

$$\psi_{c\ell}(x) = \frac{\langle\hat{\mathscr{U}}_I(\hbar\beta,\tau)e^{\frac{1}{\hbar}\tau\hat K}\hat\psi(\mathbf{x})e^{-\frac{1}{\hbar}\tau\hat K}\hat{\mathscr{U}}_I(\tau,0)\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K} = \frac{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\hat{\mathscr{U}}(\tau,0)^{-1}\hat\psi(\mathbf{x})\hat{\mathscr{U}}(\tau,0)\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K}$$

The equation of motion of the classical field is governed by $\hat K + \hbar\int dx\,[\overline{\eta}(\mathbf{x},\tau)\hat\psi(\mathbf{x}) + \hat\psi^\dagger(\mathbf{x})\eta(\mathbf{x},\tau)]$. Then:

$$\begin{aligned}-\hbar\frac{\partial\psi_{c\ell}(x)}{\partial\tau} &= \frac{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\hat{\mathscr{U}}(\tau,0)^{-1}[\hat\psi(\mathbf{x}),\hat K]\hat{\mathscr{U}}(\tau,0)\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K} + \hbar\eta(x)\\ &= \frac{\langle\hat{\mathscr{U}}_I(\hbar\beta,\tau)[\hat\psi_K(\mathbf{x},\tau),\hat K]\hat{\mathscr{U}}_I(\tau,0)\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K} + \hbar\eta(x)\\ &= \frac{\langle\mathcal{T}\hat{\mathscr{U}}_I(\hbar\beta,0)[\hat\psi_K(x),\hat K]\rangle_K}{\langle\hat{\mathscr{U}}_I(\hbar\beta,0)\rangle_K} + \hbar\eta(x)\end{aligned} \tag{15}$$

3. Independent fermions and Wick's theorem

The equation of motion (15) can be analytically solved for a quadratic Hamiltonian. The result can be used to evaluate the generator of Green functions. Let $\hat K_0 = \int d\mathbf{x}\,\hat\psi^\dagger(\mathbf{x})[h(\mathbf{x})-\mu]\hat\psi(\mathbf{x})$. The equation for the classical field is:

$$\left[\hbar\frac{\partial}{\partial\tau} + h(\mathbf{x}) - \mu\right]\psi_{c\ell}(\mathbf{x},\tau) = -\hbar\eta(\mathbf{x},\tau)$$

A functional derivative in $\eta(x')$ followed by turn-off of the sources, gives the equation for the thermal propagator of non-interacting particles:

$$\left[\hbar\frac{\partial}{\partial\tau} + h(\mathbf{x}) - \mu\right]\mathscr{G}_0(\mathbf{x},\tau;\mathbf{x}',\tau') = -\hbar\,\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau') \tag{16}$$

This Green function is used to solve the equation for the classical field:

$$\psi_{c\ell}(x) = -\frac{\delta}{\delta\overline{\eta}(x)}\log Z[\overline{\eta},\eta] = \int dy\,\mathscr{G}_0(x,y)\eta(y)$$

A functional integration gives the partition function with sources:

$$\boxed{Z_0[\overline{\eta},\eta] = Z_0\exp\left\{-\int dxdy\,\overline{\eta}(x)\mathscr{G}_0(x,y)\eta(y)\right\}} \tag{17}$$

Proposition 3.1 (Wick expansion). *For independent fermions, the thermal Green functions of a k creation and k destruction operators factor in two-point Green functions:*

$$\boxed{\mathscr{G}_0(x_1 \dots x_n; y_1 \dots y_n) = \det\{\mathscr{G}_0(x_i, y_j)\}_{ij=1\dots n}} \tag{18}$$

Proof. The expansion in the source fields of both sides of (17) is $(i = x_i, i' = y_i)$:

$$\sum_r \sum_{r'} \frac{(-1)^{r+r'}}{r!\, r'!} \int d1 \dots dr \int d1' \dots dr' \, \langle \overline{\eta}_1 \hat{\psi}_1 \dots \overline{\eta}_r \hat{\psi}_r \hat{\psi}^\dagger_{1'} \eta_{1'} \dots \hat{\psi}^\dagger_{r'} \eta_{r'} \rangle_0$$
$$= \sum_k \frac{(-1)^k}{k!} \int d1d1' \dots dkdk' \, \overline{\eta}_1 \mathscr{G}_0(1, 1') \eta_{1'} \dots \overline{\eta}_k \mathscr{G}_0(k, k') \eta_{k'}$$

Terms with unequal numbers of $\hat{\psi}$ and $\hat{\psi}^\dagger$ operators have null expectation. Comparison order by order in the sources gives the equality:

$$\frac{1}{(k!)^2} \int d1 \dots dk \int d1' \dots dk' \, \langle \overline{\eta}_1 \hat{\psi}_1 \dots \overline{\eta}_k \hat{\psi}_k \hat{\psi}^\dagger_{1'} \eta_{1'} \dots \hat{\psi}^\dagger_{k'} \eta_{k'} \rangle_0$$
$$= \frac{(-1)^k}{k!} \int d1d1' \dots dkdk' \overline{\eta}_1 \mathscr{G}_0(1, 1') \eta_{1'} \dots \overline{\eta}_k \mathscr{G}_0(k, k') \eta_{k'}$$

The sources exit the thermal average as $\overline{\eta}_1 \eta_{1'} \dots \overline{\eta}_k \eta_{k'} \, \langle \hat{\psi}_1 \dots \hat{\psi}_k \hat{\psi}^\dagger_{1'} \dots \hat{\psi}^\dagger_{k'} \rangle_0$. Equality follows after total antisymmetrization (sum on weighted permutations) of the right hand side. $\square$