The Jaynes-Gibbs principle of maximal entropy and the non-equilibrium propagators of the $O(N)$ $\phi^4$ theory at large $N$

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(March 28, 2022)

We present a novel procedure for calculating non-equilibrium two-point Green’s functions in the $O(N)$ $\phi^4$ theory at large $N$. The non-equilibrium density matrix $\rho$ is constructed via the Jaynes-Gibbs principle of maximal entropy and it is directly implemented into the Dyson-Schwinger equations (DSE) through initial value conditions. In the large $N$ limit we perform an explicit evaluation of two-point Green’s functions for two illustrative choices of $\rho$.

**I. INTRODUCTION**

In the present work we show a particular approach to the non-equilibrium QFT dynamics based in the Jaynes-Gibbs principle of maximal entropy. In contrast to other methods in use the Jaynes-Gibbs method constructs a density matrix $\rho$ directly from the observed macroscopic quantities (e.g. pressure, density of energy, magnetisation, particle current, local momentum, local angular velocity, ionisation rate (if plasma is in question), etc.). The $\rho$ is then implemented through the generalised Kubo-Martin-Schwinger (KMS) conditions into the dynamical equations for Green’s functions. To keep complexity minimal we illustrate our method on a paradigmatic physical system described by the $\phi^4$ theory with $O(N)$ internal symmetry. The plan of this paper is as follows.

In Sec.II we review the Jaynes-Gibbs principle. The rôle of the Shannon entropy is emphasised. Sec.III is devoted to the construction of the DSE for QFT systems away from equilibrium. We use the canonical formalism which appears to be very natural in this context. In order to reflect the density matrix in the dynamical equations we show how to formulate the relevant initial-time conditions. The DSE for two-point Green functions are worked out in Sec.IV. With this mathematical setting, we take in Sec.V the large $N$ limit. In the latter case the DSE for two-point Green functions are decoupled (virtually by chance). We explicitly solve these for two illustrative choices of the initial-time conditions.

**II. INITIAL CONDITIONS, JAYNES-GIBBS PRINCIPLE OF MAXIMAL ENTROPY**

In this section we would like to briefly review the Jaynes-Gibbs principle of maximal entropy (also maximum calibre principle). The objective of the principle is to construct the ‘most probable’ density matrix which fulfils the constraints imposed by experimental/theoretical data.

The standard rules of statistical physics allows us to define the expectation value via the density matrix $\rho$ as $\langle \cdots \rangle = \text{Tr}(\rho \cdots)$, with the trace running over a complete set of physical states describing the ensemble in question at some initial time $t_i$.

The usual approaches trying to determine $\rho$ start with the Liouville equation and hence with the Schrödinger picture. Rather than following this path, we shall use the Heisenberg picture instead. This will prove useful in Sec.III.

In order to determine $\rho$ explicitly we shall resort to the Jaynes-Gibbs principle of maximal entropy. The basic idea is ‘borrowed’ from the information theory. Let us assume that we have criterion of how to characterise the informative content of $\rho$. The most “probable” $\rho$ is then selected out of those $\rho$ which are consistent with ‘whatever’ we know about the system and which have the last informative content (Laplace’s principle of insufficient reasons).

It remains to characterise the information content (measure) $I[\rho]$ of $\rho$. This was done by C. Shannon with the result: $I[\rho] = \text{Tr}(\rho \ln \rho)$.

The density matrix is then chosen to minimise $I[\rho]$. Note that no assumption about the nature of $\rho$ was made; namely there was no assumption whether $\rho$ describes equilibrium or non-equilibrium situation. To put more flesh on the bones, let us rephrase the former. What we actually need to do is to maximise $S_G$ subject to the constraints imposed by our knowledge of expectation values of certain operators $P_1[\phi, \partial \phi], \ldots, P_n[\phi, \partial \phi]$. In contrast to equilibrium, all $P_k[\cdots]$’s need not to be the constants of the motion. So namely if one knows that

$$\langle P_k[\phi, \partial \phi]\rangle = f_k(x_1, x_2, \ldots) , \quad (1)$$

the entropy maximisation leads to

$$\rho = e^{(- \sum_{n=1}^N \int \prod x_j \lambda(x_1, \ldots P_n[\phi, \partial \phi])} / Z[\lambda_1, \ldots, \lambda_n]$$

* It can be shown that $-I[\rho]$ (also called the informative entropy) equals (in base 2 of logarithm) to the expected number of binary (yes/no) questions whose answer takes us from our current state of knowledge to the one certainty.
with the ‘partition function’
\[ Z[\lambda_1, \ldots, \lambda_n] = \text{Tr} \left( e^{-\sum_{i=1}^{n} \int \prod_{j} dt \lambda_i(x_i, \ldots) P_t[\phi, \partial \phi]} \right) \]

It is possible to show that the stationary solution of \( S_G \) is unique and maximal \[12\]. In the previous cases the time integration is not either present at all (\( f_k \) is specified only in the initial time \( t_i \)), or is taken over the gathering interval \((-\tau, t_i)\).

The Lagrange multipliers \( \lambda_k \) might be eliminated if one solves \( n \) simultaneous equations
\[ f_k(x_1, \ldots) = -\frac{\delta \ln Z}{\delta \lambda_k(x_1, \ldots)}. \]

The explicit solution of (2) may be formally written as
\[ \lambda_k(x_1, \ldots) = \frac{\delta S_G[f_1, \ldots, f_n]|_{\text{max}}}{\delta f_k(x_1, \ldots)}. \]

### III. OFF-EQUILIBRIUM DYNAMICAL EQUATIONS

In this section we derive the off-equilibrium Dyson-Schwinger equations using the canonical formalism. We believe that this is a new and far more natural formulation for systems away from equilibrium. The more intuitive path-integral formulation of Calzetta and Hu \[13\] is not particularly suitable in this case, because the connection between kernels \[12\] and initial-time constraints turns out to be rather non-trivial \[13\].

Let us deal first with a single field \( \phi \). We start with the action \( S \) where \( \phi \) is linearly coupled to an external source \( J(x) \). For the fields in the Heisenberg picture, the operator equation of motion can be written as
\[ \frac{\delta S}{\delta \phi(x)} - \frac{\delta S}{\delta \partial \phi(x)} = J(x) = 0, \]

where the index \( J \) emphasises that \( \phi \) is implicitly \( J \)-dependent. It will prove useful in the following to re-express \( \phi \) in such a way that the \( J \)-dependence will become explicit. The latter can be done via an unitary transformation connecting \( \phi \) (governed by \( H - J \phi \)) with \( \phi \) (governed by \( H \)). If \( J(x) \) is switched on at time \( t = t_i \) we have
\[ T C \left( \frac{\delta S[\phi]}{\delta \phi} - J \right) \exp[i \int_C d^4 y J(y) \phi(y)] = 0, \]

with \( T^* \) being the \( T^* \)-ordering. The close-time path \( C \) is the standard Keldysh-Schwinger path. Associating with the upper branch of \( C \) index ‘+’ and with the lower one the index ‘−’ one may introducing the metric \( (\sigma_3)_{\alpha\beta} \) (\( \sigma_3 \) is the usual Pauli matrix and \( \alpha, \beta = \{+, -\} \)) and write \( J_+ \phi_+ - J_- \phi_- = J_\alpha (\sigma_3)^{\alpha\beta} \phi_\beta = J^\alpha (\sigma_3)_{\alpha\beta} \phi_\beta \). For the raised and lowered indices we simply read: \( \phi_+ = \phi^+ \) and \( \phi_- = -\phi^- \) (similarly for \( J_\alpha \)). Taking \( \text{Tr}(\rho \ldots) \) with \( \rho = \rho[\phi, \partial \phi, \ldots] \), we get
\[ \frac{1}{Z[J]} \frac{\delta S}{\delta \phi(x)} \left[ \phi^\alpha(x) = -i \frac{\delta}{\delta J_\alpha(x)} \right] Z[J] = -J^\alpha(x), \]

with \( Z[J] \) being the generating functional for Green’s functions. Because of the \( T^* \)-ordering the time derivatives could be pulled out of \(. . . \). Eq.\(4\) may equivalently be written as
\[ -J^\alpha(x) = \frac{\delta S}{\delta \phi(x)} \left[ \phi^\alpha(x) + i \frac{\delta}{\delta J_\alpha(x)} \right] \mathbb{I}. \]

The \( \mathbb{I} \) indicates the unit. Analogously as for equilibrium systems, we have defined the mean field \( \phi_c \) as
\[ \phi_c(x) = \langle \phi_\alpha(x) \rangle_J = (\sigma_3)_{\alpha\beta} \frac{\delta W[J]}{\delta J_\beta(x)} Z[J] = \exp(iW[J]). \]

Summation over contracted indices is understood. The effective action \( \Gamma[\phi_c] \) is connected with \( W[J] \) via the Legendre transform: \( \Gamma[\phi_c] = W[J] - \int_C d^4 y J(y) \phi_c(y) \).

With this mathematical setting we obtain the usual equilibrium-like identities \[13\]
\[ \frac{\delta \Gamma[\phi_c]}{\delta \phi_c}(x) = -J^\alpha(x), \]
\[ \int d^4 y G_{\alpha\beta}(x, y) (\sigma_3)^{\beta\gamma} \Gamma^{(2)}_{\gamma\gamma}(y, z) = (\sigma_3)_{\alpha\gamma} \delta^4(x - z), \]

with
\[ -G_{\alpha\beta}(x, y) = i(T_C \{ \phi_\alpha(x) \phi_\beta(y) \}) - i \langle \phi_\alpha(x) \langle \phi_\beta(y) \rangle, \]

\[ \frac{\delta^2 \Gamma}{\delta \phi_c(x) \delta \phi^\gamma_c(y)} = \Gamma^{(2)}_{\alpha\gamma}(x, y). \]

For the physical process (i.e. \( J = 0 \)) we have from \((5)\)
\[ \frac{\delta \Gamma[\phi_c]}{\delta \phi^\gamma_c(x)} = \frac{\delta S}{\delta \phi(x)} \left[ \phi_c(x) \right] \]
\[ + i \int d^4 y G_{\alpha\beta}(x, y) (\sigma_3)^{\beta\gamma} \frac{\delta}{\delta \phi^\gamma_c(y)} \mathbb{I} = 0. \]

It is worthy of noticing that the LHS of \((8)\) offers a direct prescription for a calculation of \( \delta \Gamma[\phi_c]/\delta \phi^\gamma_c(x) \).

So far we have not taken into account the constraints. This can be done quite simply. One just sets \( \lambda_i \) in \( \rho \) to be the solution of Eq.\((3)\). Using the identity
\[ e^{A} B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} C_n, \quad C_0 = B, C_n = [A, C_{n-1}], \]

we get then the generalised KMS condition
Here $A = \ln \rho$, $B = \phi(y)$ and $y_0 = t_i$. Similarly we could derive the generalised KMS conditions for the higher point Green’s functions Eq. (8) and its successive $J$ variation provide us with the coupled integro-differential equations. As a result, we get an infinite hierarchy of coupled equations which, if furnished with the corresponding KMS conditions, constitute, in principle, a complete description of the behaviour of a non-equilibrium system.

IV. THE $O(N)$ $\phi^4$ THEORY

Let us illustrate the aforementioned formalism on the $O(N)$ $\phi^4$ theory.

The $O(N)$ $\phi^4$ theory is described by the bare Lagrange function

$$\mathcal{L} = \frac{1}{2} \sum_{a=1}^{N} ((\partial \phi^{a})^2 - m_0^2 (\phi^{a})^2) - \frac{\lambda_0}{8N} \left( \sum_{a=1}^{N} (\phi^{a})^2 \right)^2.$$  \hspace{1cm} (9)

Using the explicit form (9), Eq. (8) reads

$$\frac{\delta \Gamma}{\delta \phi^{a}(x)} = -(\Box + m_0^2) \phi^{a}(x)$$

$$- \frac{\lambda_0}{2N} \left( \sum_{b=1}^{N} \phi^{b}(x)(\phi^{b}(x))^2 + i \phi^{a}(x) \sum_{b=1}^{N} G^{ab}_{\alpha\alpha}(x,x) \right)$$

$$+ 2 \sum_{b=1}^{N} \phi^{b}(x) G^{ab}_{\alpha\alpha}(x,x)$$

$$+ \int d^{4}y \, d^{4}w \, d^{4}z \, \sum_{b=1}^{N} G^{(3)ab\alpha}(y,w,z) \right) = 0.$$  \hspace{1cm} (10)

A successive variation with respect to $J(y)$ generates the DSE for the two-point Green’s functions.

The dynamical equations can be significantly simplified provided that both the density matrix and the Hamiltonian are invariant against rotation in the $N$-dimensional vector space of fields. This fact leads straightforwardly to the following Ward’s identities $\delta \mathcal{W}[J] / \delta J^{a}(z)|_{J=0} = \delta^{a}(z) = 0$, $\forall a$,

$$\frac{\delta^2 \mathcal{W}[J]}{\delta J^{a}(x) \delta J^{b}(y)}|_{J=0} = G_{\alpha\beta}^{ab}(x,y) = \delta^{ab} G_{\alpha\beta}(x,y),$$

$$\Gamma_{\alpha\beta}^{abc}(y_1,y_2,y_3) = 0, \quad \forall a,b,c,$$

$$\Gamma_{\alpha\beta\gamma\delta}^{abcd}(y_1,y_2,y_3,y_4) \propto \delta_{ab} \delta_{cd} + \delta_{ac} \delta_{bd} + \delta_{ad} \delta_{bc}.$$  \hspace{1cm} (11)

With these results we may write the evolution equation for the two-point Green’s function as follows

$$\left( \Box + m_0^2 + \frac{\lambda_0}{2} i \frac{N + 2}{N} G_{\alpha\alpha}(x,x) \right) G_{\alpha\beta}(x,y)$$

$$+ \frac{\lambda_0}{2} \frac{N + 2}{N} \left( G_{\alpha\alpha\beta}(x,x,x,y) \right) = -\delta(y-x)(\sigma_{3})_{\alpha\beta}.$$  \hspace{1cm} (12)

In the following we shall confine ourselves only to such situations where both $\rho$ and $H$ are $O(N)$ invariant.

V. $G_{\alpha\beta}(X, Y)$: $O(N)$ $\phi^4$ THEORY IN THE LARGE $N$ LIMIT

One can show $\Box \Box \Box$ by a detailed study of the large-$N$ approximation (virtually using only the Ward’s identities and properties of $\Gamma_m W$) that the vertex functions $\Gamma^{(2n)}$ must be of order $N!^{-n}$. The latter suggests that in the dynamical equation (10) we can neglect $\Gamma^{(4)}$ terms.

Let us mention one more point. If we perform the expectation value of the Lagrange function (9) we find that this does not depend on $G^{(4)}$ in the $N \rightarrow \infty$ limit, indeed

$$\text{Tr}(\rho \mathcal{L}(x)) = \frac{1}{2} i N \{ \partial_{x} \partial_{y} G^{(4)}(x,y) \}_{x=y} - m_{0}^{2} G^{(4)}(x,x)$$

$$- \frac{\lambda_{0}}{4} \left( \frac{N + 1}{4} \{ G^{(4)}(x,x,x,x) + (G(x,x))^{2} \} \right).$$  \hspace{1cm} (13)

Here we have used the fact that $G^{(4)aa} = 3G^{(4)ab} = 3G^{(4)}$. So we may equally start with the Lagrange function

$$\hat{\mathcal{L}} = \frac{1}{2} \sum_{a=1}^{N} ((\partial \phi^{a}(x))^2 - m_{0}^{2} (\phi^{a}(x))^2)$$

$$- \frac{\lambda_{0}}{4} \sum_{a=1}^{N} (\phi^{a}(x))^{2} G(x,x).$$  \hspace{1cm} (14)

The former fulfills the identity $\langle \hat{\mathcal{L}} \rangle = \langle \mathcal{L} \rangle |_{N \rightarrow \infty}$. It is also simple to see that the DSE derived from $\hat{\mathcal{L}}$ reads

$$\left( \Box_{x} + m_{0}^{2} + \frac{\lambda_{0}}{2} G_{\alpha\alpha}(x,x) \right) G_{\alpha\beta}(y,x)$$

$$= -\delta(x-y)(\sigma_{3})_{\alpha\beta}.$$  \hspace{1cm} (15)

This is precisely the same which one would obtain if the large $N$ limit would be performed in the original DSE (10).

Let us now show how to compute $G_{\alpha\beta}(x,y)$ for some familiar choices of the initial-time constraints.

(i) Equilibrium

In this case the constraints are usually chosen to be the integrals of motion. The only available integral of the
motion is the full Hamiltonian $H$, and the corresponding constraint reads [14]

$$\langle P_k[\phi, \partial \phi] \rangle_{t_i} = \langle H \rangle = \int_0^T dT' C_V(T') = F(T),$$  \hspace{1cm} (13)$$

where $C_V$ is the heat capacity at constant volume $V$. The density matrix $\rho$ maximising $S_G$ is the density matrix of the canonical ensemble: $\rho = \frac{\exp(-\beta H)}{Z[\beta]}$. The Lagrange multiplier $\beta$ is determined from Eq.(3):

$$\beta = \frac{\partial S_G}{\partial F(T)} = \left( \frac{\partial S}{\partial T} \right)_V \left( \frac{\partial F(T)}{\partial T} \right)_V^{-1} = \frac{1}{T}.$$  \hspace{1cm} (14)$$

In this case the KMS condition is the well known relation

$$G_{+-}(x, t; y, 0) = G_{-+}(x, t - i \beta; y, 0).$$  \hspace{1cm} (15)$$

The DSE are those in [13] with $G(x, y) = G(x - y)$. The solutions are the equilibrium propagators in the Keldysh-Schwinger formalism, i.e.

$$iG_{\pm\pm}(k) = \frac{\pm i}{k^2 - m^2_0 + i\varepsilon} + \frac{2\pi f(|k_0|) \delta(k^2 - m^2)}{2\varepsilon}$$

$$iG_{\pm\mp}(p) = 2\pi \{ \theta(\mp k_0) + f(|k_0|) \} \delta(k^2 - m^2),$$  \hspace{1cm} (16)$$

where $f(x) = (\exp(\beta x) - 1)^{-1}$ is the Bose distribution, and $m^2_0 = m^2_0 + \frac{1}{2} \delta G(0)$ is the renormalised mass.

(ii) Non-equilibrium: translationally invariant $G_{\alpha\beta}$

The DSE in the former example were immensely simplified due to the translational invariance of Green’s functions. If we retain the translational invariance this simplicity will be preserved also to non-equilibrium. As an example, let us choose the following initial-time constraint:

$$\langle P_k[\phi, \partial \phi] \rangle_{t_i} = \langle H(k) \rangle = \langle \tilde{H}(k) \rangle = g(k),$$  \hspace{1cm} (17)$$

where $\tilde{H}$ means the effective Hamiltonian density derived from $\tilde{L}$. The density matrix reads

$$\rho = \frac{\exp(-\int d^3k \beta(k) \tilde{H}(k))}{Z[\beta]} = \frac{\exp(-\int d^3k \tilde{\beta}(k) a_k^\dagger a_k)}{Z[\beta]},$$

with $\beta(k) = \tilde{\beta}(k) 2\sqrt{k^2 + m^2_0}$ and $\beta(k) = \frac{gS}{5g(k)}$. The former indicates that the different modes have different ‘temperatures’. The DSE agree with those in the equilibrium case. The generalised KMS conditions are

$$G_{+-}(k) = e^{-\tilde{\beta}(k) k_0/2} G_{-+}(k)$$  \hspace{1cm} (18)$$

The solution of (12) furnished with (18) formally coincides with the solution (16). The only proviso is that $f(|k_0|) \to \frac{1}{e^{\sigma/2} - 1}$.

VI. CONCLUSIONS AND OUTLOOK

We considered the Jaynes-Gibbs principle of maximal entropy. This allowed us to construct the non-equilibrium DSE. For the $O(N) \phi^4$ theory in the $N \to \infty$ limit we have explicitly evaluated propagators for two choices of translationally invariant density matrices. A notable advantage of this approach is that one can get the DSE without going through the Cornwall-Jackiw-Tomboulis formalism, which would be formidably difficult particularly for more than one constraint.

The $O(N) \phi^4$ theory in the large $N$ limit is a nice toy model allowing in many cases to approach the dynamical equations analytically. For suitable choices of the translationally non-invariant initial-time constraints the simplicity of the equations is such that one may solve them exactly. A more detailed report will appear elsewhere [13].

VII. ACKNOWLEDGEMENTS

This work is supported by Fitzwilliam College and CONACYT.

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