Time Evolution of Non-Equilibrium Effective Action

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Abstract

The time evolution of correlation functions in statistical systems is described by an exact functional differential equation for the corresponding generating functionals. This allows for a systematic discussion of non-equilibrium physics and the approach to equilibrium without the need of solving the non-linear microscopic equations of motion or computing the time dependence of the probability distribution explicitly.

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A description of the time evolution of statistical systems is needed in very diverse areas of science, ranging from the growth of density fluctuations in the early universe to the evolution of a population of bacteria. As a typical problem we may consider a given distribution of density fluctuations in the early universe at the time when the photons decouple - say a Gaussian distribution around central values given by a flat Harrison-Zeldovich spectrum - and ask how it looks like when the galaxies form. For small fluctuations the underlying gravitational equations of motion (or field equations) can be linearized and approximate solutions found [1]. For large density contrasts, however, the nonlinearities in the field equations become important and the analytical discussion becomes more involved. Most approaches to this problem therefore use numerical simulations. The observed galaxy correlation function shows a power-like decay and similar for clusters. This raises the challenge to understand the exponents analytically - perhaps by the attraction of the nonlinear system to a suitable partial fixed point, similar to the renormalization flow of couplings in the theory of critical phenomena.

Examples from particle physics include the rate of baryon number-violating processes at high temperature and the discussion of a possible formation of a disordered chiral condensate [2] in heavy ion collisions. After such a collision the distribution of pion fields is not given by the equilibrium distribution corresponding to the ground state. The time evolution of the non-equilibrium distribution could produce spectacular coherent effects. In statistical physics one may ask how a system evolves to equilibrium after a quench or starting in a metastable state. We propose here a method how such questions can be addressed directly on the level of correlation functions without solving the (nonlinear) equations of motions or computing the time evolution of the probability distribution. It is based on an exact functional differential equation for the time evolution of generating functionals for the correlations functions. The microscopic laws or equations of motion reflect themselves in the precise form of this evolution equation. Many general aspects, as the approach to possible fixed points for $t \to \infty$, are, however, independent of this precise form.

Consider a system of degrees of freedom $\chi_m(t)$ whose time evolution is determined by a differential equation of motion

$$\frac{d}{dt}\chi_m = \dot{\chi}_m = F_m[\chi] = \sum_{k=0}^{\infty} f^{(k)}_{mn_1\ldots n_k}\chi_{n_1}\cdots\chi_{n_k} \tag{1}$$

(We always sum over repeated indices and use $\chi_{-n} = \chi_n^*$ with a summation over positive and negative values of n if χ_n is a complex variable. In case of continuous field equations for $\chi(x,t)$ the index summation corresponds to an integration over x or a corresponding momentum summation for Fourier modes. The equation of motion is nonlinear unless $f^{(k)}$ vanishes for $k > 1$ and F_m can also depend on t.) We assume that with given initial values $\chi_m^0 = \chi_m(t_0)$ eq. (1) has a solution $\chi_m(t;\chi^0)$, but we will not need its explicit form. The initial probability distribution $\sim \exp -S_0[\chi^0]$ at time t_0 describes an ensemble of initial conditions. The correlation functions for the variables χ_m at some time $t > t_0$ are then given by

$$< \chi_{n_1}(t)...\chi_{n_i}(t) >= Z^{-1} \int D\chi^0 \ \chi_{n_1}(t;\chi^0)...\chi_{n_i}(t;\chi^0) \exp -S_0[\chi^0] \qquad (2)$$

with $Z = \int D\chi^0 \exp -S_0[\chi^0]$ and $\int D\chi^0 \equiv \int \prod_m d\chi^0_m$. Inserting the equation of motion we see that the evolution of the mean value of χ_m involves the higher correlation functions

$$\frac{d}{dt} < \chi_m(t) >= \sum_{k=0}^{\infty} f^{(k)}_{mn_1...n_k} < \chi_{n_1}(t)...\chi_{n_k}(t) > \qquad (3)$$

Writing down similar equations for the correlation functions one arrives at an infinite system of differential equations for the time dependence of the n-point functions.

Insight in the behaviour of this system can be gained from the generating functional for time-dependent n-point functions

$$Z[j,t] = \int D\chi^0 \exp\{-S_0[\chi^0] + j^*_m \chi_m(t;\chi^0)\} \qquad (4)$$

or the related functionals for the connected correlation functions $W[j,t] = \ln Z[j,t]$ or the 1PI irreducible correlation functions

$$\begin{aligned} \Gamma[\varphi,t] &= -\ln Z[j,t] + j^*_m \varphi_m, \\ \varphi_m &= \frac{\partial \ln Z[j]}{\partial j^*_m} \end{aligned} \qquad (5)$$

We will concentrate here on the time evolution of the non-equilibrium effective action $\Gamma[\varphi,t]$. Knowledge of $\Gamma[\varphi,t]$ contains all information on the time evolution of correlation functions. In particular, the mean value $< \chi_m(t) >$ corresponds to the (time-dependent) value of φ_m for which Γ has its minimum. We should emphasize that in contrast to the equilibrium effective action the non-equilibrium effective action $\Gamma[\varphi,t]$ depends on the specific probability distribution for the initial values χ^0 at $t = t_0$, as specified by $S_0[\chi^0]$ or, equivalently, by $\Gamma[\varphi,t_0]$. Nevertheless, some features, as the approach to a possible equilibrium state for $t \to \infty$, can become independent of the initial conditions.

The time dependence of $\Gamma[\varphi,t]$ is specified by an exact evolution equation (∂_t is the time derivative at fixed φ)

$$\partial_t \Gamma[\varphi] = -\frac{\partial \Gamma[\varphi]}{\partial \varphi_m} \hat{F}_m[\varphi] \qquad (6)$$

$$\begin{aligned} &\hat{F}_m[\varphi] = f^{(0)}_m + f^{(1)}_{mn}\varphi_n + f^{(2)}_{mn_1,-n_2}\{\varphi_{n_1}\varphi^*_{n_2} + (\Gamma^{(2)})^{-1}_{n_1n_2}\} \\ &+ f^{(3)}_{mn_1n_2,-n_3}\{\varphi_{n_1}\varphi_{n_2}\varphi^*_{n_3} + \varphi_{n_1}(\Gamma^{(2)})^{-1}_{n_2n_3} + \varphi_{n_2}(\Gamma^{(2)})^{-1}_{n_1n_3} + \varphi_{n^*_3}(\Gamma^{(2)})^{-1}_{n_1,-n_2} \\ &-(\Gamma^{(2)})^{-1}_{n_1p_1}(\Gamma^{(2)})^{-1}_{n_2p_2}(\Gamma^{(2)})^{-1}_{p_3n_3} \frac{\partial^3 \Gamma}{\partial \varphi^*_{p_1}\partial \varphi^*_{p_2}\partial \varphi_{p_3}}\} \end{aligned}$$

$$+\sum_{k=4}^{\infty} f^{(k)}_{mn_1\dots n_{k-1},-n_k}(\varphi_{n_1}+(\Gamma^{(2)})^{-1}_{n_1p_1}\frac{\partial}{\partial\varphi^*_{p_1}})$$
$$\dots(\varphi_{n_{k-2}}+(\Gamma^{(2)})^{-1}_{n_{k-2}p_{k-2}}\frac{\partial}{\partial\varphi^*_{p_{k-2}}})(\varphi_{n_{k-1}}\varphi^*_{n_k}+(\Gamma^{(2)})^{-1}_{n_{k-1}n_k}) \tag{7}$$

Here the matrix $\Gamma^{(2)}[\varphi]$ is given by the second derivatives

$$(\Gamma^{(2)})_{mn}=\frac{\partial^2\Gamma[\varphi]}{\partial\varphi^*_m\partial\varphi_n} \tag{8}$$

and its inverse $(\Gamma^{(2)})^{-1}$ denotes the effective (φ-dependent) propagator. Eq. (6) is the central equation of this letter and we observe that it simplifies considerably if the equation of motion contains only up to quadratic ($k=2$) or cubic ($k=3$) terms. In the limit of infinitely many degrees of freedom $\chi_m(t)\equiv\chi(x,t)$, it is a functional differential equation and $\partial/\partial\varphi_m$ may be replaced by $\delta/\delta\varphi(x)$. Eq. (6) follows from the evolution equation for $Z[j,t]$ (with ∂_t at fixed j here)

$$\partial_t Z[j]=j^*_m F_m[\frac{\partial}{\partial j^*}]Z[j] \tag{9}$$

and the identity $\partial_t\Gamma_{|\varphi}=-\partial_t\ln Z_{|j}$. In turn, eq. (9) can be proven by taking a time derivative of eq. (4), inserting the equation of motion (1) under the (functional) integral and expressing the powers of $\chi_{n_i}(t)$ by derivatives with respect to $j^*_{n_i}$.

The evolution equation for the mean value $\bar\varphi_m(t)=<\chi_m(t)>$ obtains from the minimum condition $(\partial\Gamma/\partial\varphi_m)(\bar\varphi(t))=0$ which is valid for all t

$$\frac{d}{dt}\bar\varphi_m(t)=\hat F_m(\bar\varphi(t)) \tag{10}$$

Comparing the "macroscopic" equation of motion (10) which includes the fluctuations with the microscopic one (1) for a particular configuration, we see that the influence of the fluctuations appears through the terms in $\hat F_m$ (7) which involve the propagator $(\Gamma^{(2)})^{-1}$ and those involving higher φ-derivatives of Γ. The mean values of the connected two-point correlation function $<\chi_m(t)\chi^*_n(t)>-<\chi_m(t)><\chi^*_n(t)>$ $=(\Gamma^{(2)})^{-1}_{mn}(\bar\varphi(t))$ evolves according to

$$\frac{d}{dt}P_{mn}\equiv\frac{d}{dt}\Gamma^{(2)}_{mn}(\bar\varphi(t))=A^*_{pm}P_{pn}+P_{mp}A_{pn}$$
$$A_{mn}=-\frac{\partial\hat F_m}{\partial\varphi_n}(\bar\varphi(t)) \tag{11}$$

In the limit where $\partial\hat F_m[\varphi]/\partial\varphi_n$ is independent of φ (in particular for a linear equation of motion where $A_{mn}=-f^{(1)}_{mn}$) one can solve eq. (6) explicitly. The time evolution of all 1PI n-point functions is given by appropriate contractions with A similar to eq. (11) and therefore determined by the eigenvalues of A. For small nonlinearities one can perturbatively expand around this solution. Of course, the magnitude of the nonlinear effects is not only determined by the values of the coefficients $f^{(k)}$ but also by the size of the fluctuations.

Let us next come to the interesting question if the evolution equation (6) has fixed points $\Gamma_*[\varphi]$ which are approached for $t \to \infty$. Such fixed points could correspond to possible equilibrium distributions to which the system is attracted. The existence of fixed points (solutions of $\partial_t \Gamma[\varphi] = 0$) obviously depends on the precise form of the equation of motion (1). We concentrate in the following on conservative equations of motion

$$\dot{\chi}_{1s} = B_{st} \frac{\partial U}{\partial \chi^*_{2t}}, \quad \dot{\chi}_{2s} = -B^\dagger_{st} \frac{\partial U}{\partial \chi^*_{1t}} \tag{12}$$

which can be derived from some generalized potential $U[\chi]$ which is conserved if U does not depend explicitly on time ($dU/dt = \partial_t U_{|\chi}$). For conserved U one can show that

$$Z_*[j, \beta] = \int D\chi \exp(-\beta U[\chi] + j^*_m \chi_m) \tag{13}$$

is a fixed point of eq. (9). (Here $m = (1, s), (2, s)$ is a collective index.) The Legendre transform (5) $\Gamma_*[\varphi, \beta]$ is then a fixed point for the evolution equation (6) for arbitrary values of β. The proof relies on the invariance of the measure $D\chi$ under variable shifts $\chi'_m = \chi_m + \epsilon_m$ wich constant (infinitestimal) ϵ_m. Expanding

$$U[\chi] = \sum_{k=0}^{\infty} \frac{1}{k!} u^{(k)}_{n_1 \dots n_k} \chi_{n_1} \chi_{n_2} \cdots \chi_{n_k} \tag{14}$$

the shift invariance implies the Schwinger-Dyson equation [3]

$$\beta \sum_{k=0}^{\infty} \frac{1}{k!} u^{(k+1)}_{n_1 \dots n_k, -m} Z^{-1}_*[j] \frac{\partial}{\partial j^*_{n_1}} \cdots \frac{\partial}{\partial j^*_{n_k}} Z_*[j] = j_m \tag{15}$$

The coefficients $f^{(k)}$ in the equation of motion (1) are directly related to $u^{(k+1)}$ and the right-hand side of eq. (9) vanishes due to the relative minus sign in (12).

The symplectic structure of eq. (12) is typical for second-order equations of motions

$$\ddot{\chi}_m = -\frac{\partial V[\chi]}{\partial \chi^*_m} \tag{16}$$

Identifying χ_1 with χ and χ_2 with $\pi \equiv \dot{\chi}$ the equation of motion takes the form (12) with $B_{st} = \delta_{st}$ and

$$U = V[\chi] + \frac{1}{2} \pi^*_m \pi_m \tag{17}$$

We interpret U as the total energy of the system and β as the inverse temperature. The "kinetic part" of Z_* which involves the sources for π_m factorizes as a trivial Gaussian. The remaining part of Z_* is the partition function for a system χ_m with (potential) energy $V[\chi]$ in thermodynamic equilibrium at temperature $1/\beta$. We note that the concept of temperature arises here without any notion of interaction with some external heat bath! Since U is conserved and $< U >= -\partial \ln Z_*[j=0]/\partial\beta$ the temperature is uniquely fixed by the initial value $< U > [t_0]$ if $Z_*[0,\beta]$ is monotonic in the appropriate range.

If the thermodynamic equilibrium partition function Z_* were the only fixed point of the system and attractive for $t \to \infty$, we could be sure that initial conditions not too far from equilibrium would "thermalize", i.e. $\Gamma[\varphi, t \to \infty] = \Gamma_*[\varphi]$. The approach to the equilibrium fixed point may, however, be obstructed by the existence of conserved quantities A_i besides U. The fixed point can be reached only if the initial values of all A_i coincide with the equilibrium values. The generic situation may be similar to quantum mechanics where the trace of arbitrary powers of the density matrix is conserved. In what sense (reduction of effective degrees of freedom, time averaging) an equilibrium state can be reached under such circumstances is an interesting and subtle question.

Let us finally turn to more practical applications of eq. (6) to non-equilibrium situations. Exact solutions are out of reach and one has to ressort to approximations by truncating the most general form of $\Gamma[\varphi, t]$ to an object of manageable size. The truncation has to be adapted to the particular system and the success of the method in the nonlinear non-equilibrium domain will depend on the ability to conceive a realistic truncation. As an example we consider the $O(N)$ symmetric φ^4-theory in d dimensions, with equation of motion ($i = 1..d, a = 1...N, \chi_a(x,t)$ real)

$$\ddot{\chi}_a(x,t) = \partial_i\partial_i\chi_a(x,t) - m^2\chi_a(x,t) - \frac{1}{2}\lambda\chi_b(x,t)\chi_b(x,t)\chi_a(x,t) \tag{18}$$

For $\lambda \to \infty$ with fixed negative m^2/λ this corresponds to Ising or Heisenberg models, and for $d = 3, N = 4$ and $m^2 < 0$ this is the equation used in numerical simulations of pion dynamics related to the investigation of a possible disordered chiral condensate. For the non-equilibrium effective action we use the truncation

$$\begin{aligned}\Gamma[\varphi, t] \; &= \; \frac{1}{2}\beta \int \frac{d^dq}{(2\pi)^d}\{A(q)\varphi_a^*(q)\varphi_a(q) + B(q)\pi_a^*(q)\pi_a(q) + 2C(q)\pi_a^*(q)\varphi_a(q)\} \\ &+ \frac{1}{2}\beta \int d^dx\{u\;\rho^2(x) + v\rho(x)\pi_a(x)\varphi_a(x)\}\end{aligned} \tag{19}$$

with $\rho = \frac{1}{2}\varphi_a\varphi_a, \varphi_a(q) = \int d^dx e^{iq_ix_i}\varphi_a(x) = \varphi_a^*(-q)$. The evolution equation (6) describes the time dependence of the real functions $A(q), B(q), C(q)$ which depend here only on the invariant q_iq_i, and the constants u and v. Inserting (19) in (6) and omitting on the r.h.s. terms $\sim v$, one finds after some algebra

$$\begin{aligned}\partial_tA(q) \; &= \; 2\omega_q^2C(q),\; \partial_tB(q) = -2C(q) \\ \partial_tC(q) \; &= \; \omega_q^2B(q) - A(q) \\ \partial_tu \; &= \; 4\lambda C(0)K \\ \partial_tv \; &= \; -2u + 2\lambda B(0)K\end{aligned} \tag{20}$$

with

$$\begin{aligned}
\omega_q^2 &= q^2+m^2+\frac{N+2}{2}\frac{\lambda}{\beta}\Big(\int\frac{d^dq'}{(2\pi)^d}G(q') \\
&\quad -\frac{u}{\beta}\int\frac{d^dq'}{(2\pi)^d}\frac{d^dq''}{(2\pi)^d}G(q')G(q'')G(q+q'-q'')\Big) \\
K &= 1-\frac{N+8}{2}\frac{u}{\beta}\int\frac{d^dq}{(2\pi)^d}G^2(q) \\
&\quad +\frac{3N+20}{2}\left(\frac{u}{\beta}\right)^2\int\frac{d^dq}{(2\pi)^d}\frac{d^dq'}{(2\pi)^d}G^2(q)G(q')G(q-q') \\
G(q) &= B(q)/(A(q)B(q)-C^2(q))
\end{aligned} \tag{21}$$

We assume here that the system is regularized by a momentum cutoff for q^2. For a given initial distribution specified by A, B, C, u and v for $t=t_0$ the system (20) (or a simplified version with $B(q)=B(0), C(q)=C(0), A(q)=A(0)+Zq^2$) could be solved numerically. (Note that eq. (20) implies that $A(q)B(q)-C^2(q)$ is a conserved quantity for every q.) Results may be compared with direct numerical simulations which solve eq. (18) numerically and average over initial conditions. In particular, the expectation value of a space-independent field obeys ($\bar\rho=\frac{1}{2}\bar\varphi_a\bar\varphi_a$)

$$A(0)+u\bar\rho-\frac{1}{B(0)}(C^2(0)+2vC(0)\bar\rho+\frac{3}{4}v^2\bar\rho^2)=0 \tag{22}$$

or $\bar\varphi_a=0$. It is easy to verify that the system (20) has the equilibrium fixed point (13) with $C_*(q)=0, v_*=0, B_*(q)=1$ and $A_*(q)=\omega_q^2, u_*=\lambda K$. The two last conditions are the (classical!) Schwinger-Dyson equations for the propagator and the quartic scalar coupling in the appropriate truncation. In thermodynamic equilibrium the system exhibits spontaneous symmetry breaking for $A_*(0)<0$. The contributions involving C an v on the r.h.s. of eq. (22) describe the non-equilibrium deviation of $\bar\rho$ from its equilibrium value $\bar\rho_*=-A_*(0)/u_*$. Not too far from equilibrium $B(0)$ is positive and the non-equilibrium effective mass term $A(0)-C^2(0)/B(0)$ is smaller than in equilibrium, thus enhancing the tendency to spontaneous symmetry breaking.

We finally remark that the present formalism can be extended to stochastic equations of motion and the description of correlation functions at unequal time. This will permit to establish the contact to path integral formulations [4] and quantum field theory.

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