Nonequilibrium time evolution in quantum field theory

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The time development of equal-time correlation functions in quantum mechanics and quantum field theory is described by an exact evolution equation for generating functionals. This permits a comparison between classical and quantum evolution in nonequilibrium systems. [S1063-651X(97)05909-6]

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In a statistical description of nature only expectation values or correlations are observable. The dynamical laws describe how a given (complete) set of correlation functions at some initial time t_0 has evolved at some later time t. In a very general context this constitutes a differential evolution equation for the correlation functions or their generating functionals. Different dynamical laws, i.e., the difference between a classical and a quantum description, manifest themselves only in different evolution equations. For quantum mechanics of a few degrees of freedom we are accustomed to using the Schrödinger equation for pure states and to evaluate time-dependent expectation values in an ensemble specified by a density matrix. The classical counterpart is Newton's equations with the ensemble described by a probability distribution for initial values. For many degrees of freedom a more direct formulation of the dynamics in terms of an evolution equation for generating functionals of correlation functions may be advantageous. Then one only deals with the relevant observable information and may avoid additional complication in intermediate steps of their computation. For classical equations of motion such an evolution equation has been established recently [1]. It is the purpose of this work to develop the counterpart for quantum mechanics and quantum field theory.

The resulting evolution equation in quantum field theory is a functional differential equation. Its practical use depends on the ability to find realistic truncations for the time-dependent effective action—the generating functional for the 1PI Green's functions. Nevertheless, already at the present formal stage a comparison between classical and quantum evolution equations sheds some light on current dynamical simulations of nonequilibrium quantum field theory problems within a classical approximation for the field equations. It also provides a systematic framework to compute quantum corrections to a classical evolution, as relevant, for example, for inflationary periods in early cosmology.

Consider a system with an arbitrary number of degrees of freedom described by conjugate operators $Q_i, P_i, i=1,\ldots,n$, $[Q_i,P_i]=i\delta_{ij}$, $[Q_i,Q_j]=[P_i,P_j]=0(\hbar\equiv 1)$. The Hamiltonian is given by

$$H=\frac{1}{2m}P^2+V[Q], \tag{1}$$

where $P^2=P_iP_i$ is a scalar product (summation of repeated indices is always implied) and $V[Q]=V(Q_1\cdots Q_n)$. (Systems with different masses m_i can be brought to this form by simultaneous rescaling of Q_i and P_i—in fact, we could also use a scaling with $m=1$. Our formalism can be generalized for arbitrary $H[P,Q]$ but we restrict the discussion here to the most common form of quadratic in the momenta.) In the Heisenberg picture the operators Q and P depend on time according to

$$\dot{Q}_i=\frac{1}{m}P_i, \quad \dot{P}_i=-V_i[Q]. \tag{2}$$

(We use a notation $V_i=\partial V/\partial Q_i, V_{ij}=\partial^2 V/\partial Q_i\partial Q_j$, etc.) Let us now define the generating functional

$$Z[j,h,t]=\mathrm{Tr}(e^{jQ(t)+hP(t)}\rho) \tag{3}$$

where ρ is the density matrix which is time independent in the Heisenberg picture. It is a function (or functional for $n\to\infty$) of the time-independent sources j_i and h_i. The coefficients of its Taylor expansion

$$Z[j,h,t]=\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\frac{1}{k!\,l!}z^{(k,l)}_{q_1\cdots q_k,r_1\cdots r_l}(t)\times j_{q_1}\cdots j_{q_k}h_{r_1}\cdots h_{r_l} \tag{4}$$

are time-dependent symmetrized expectation values of correlation functions. For a one-component example ($n=1$),

$$z^{(k,l)}(t)=\langle (Q^kP^l)_s(t)\rangle=\mathrm{Tr}\{(Q^k(t)P^l(t))_s\rho\}, \tag{5}$$

the symmetrized ordering $(\,)_s$ stands for an equally weighted sum over all $(k+l)!/k!\,l!$ possibilities to form different chains of k operators Q and l operators P, i.e.,

$$(Q^2P^2)_s=\frac{1}{6}(Q^2P^2+QP^2Q+P^2Q^2+PQ^2P+QPQP+PQPQ). \tag{6}$$

The generalization to arbitrary n is obvious. Knowledge of $Z[j,h,t]$ contains complete information about the system. Macroscopic quantities and thermodynamic functions can be expressed in terms of correlation functions [2].

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The time dependence of Z obeys the evolution equation ($\partial_t Z$ is the time derivative at fixed j and h)

$$\partial_t Z = i\,\mathrm{Tr}([H, e^{jQ+hP}]\rho). \tag{7}$$

Our aim is to express the right-hand side in terms of Z and its derivatives with respect to j and h. In order to deal with the problem of ordering the noncommuting operators we use

$$i[H, e^{jQ+hP}] = \frac{1}{m} j_i \frac{\partial}{\partial h_i} e^{jQ+hP} + iV\left[\frac{\partial}{\partial \beta}\right][e^{\beta Q}, e^{jQ+hP}]\big|_{\beta=0} \tag{8}$$

and evaluate the commutator with the Campbell-Baker-Hausdorff formula

$$[e^{\beta Q}, e^{jQ+hP}] = (e^{(i/2)\beta h} - e^{-(i/2)\beta h}) e^{(\beta+j)Q+hP}. \tag{9}$$

For each of the two contributions on the right-hand side, one can express $\partial/\partial\beta$ by an appropriate combination of $\partial/\partial j$ and h. This leads to

$$i[V[Q], e^{jQ+hP}] = i\left(V\left[\frac{\partial}{\partial j} + \frac{i}{2}h\right] - V\left[\frac{\partial}{\partial j} - \frac{i}{2}h\right]\right) e^{jQ+hP} \tag{10}$$

and Eqs. (8) and (10) can now be inserted in the trace (7). Our final result is a linear partial differential equation for the evolution of Z with a simple structure:

$$\partial_t Z = \mathcal{L}^{(Z)} Z,$$

$$\mathcal{L}^{(Z)} = \frac{1}{m} j_i \frac{\partial}{\partial h_i} + i\left(V\left[\frac{\partial}{\partial j} + \frac{i}{2}h\right] - V\left[\frac{\partial}{\partial j} - \frac{i}{2}h\right]\right). \tag{11}$$

For a comparison with the time evolution of Z in classical statistics [1] we expand V in powers of h

$$iV\left[\frac{\partial}{\partial j} + \frac{i}{2}h\right] - iV\left[\frac{\partial}{\partial j} - \frac{i}{2}h\right]$$
$$= -V_i\left[\frac{\partial}{\partial j}\right]h_i + \frac{1}{24}V_{ijk}\left[\frac{\partial}{\partial j}\right]h_i h_j h_k - \frac{1}{1920}V_{ijklm}\left[\frac{\partial}{\partial j}\right]h_i h_j h_k h_l h_m + \cdots. \tag{12}$$

The first term in this expansion reproduces the classical evolution equation. This leads to the important observation that for linear equations of motion (H quadratic in Q and P) there is no difference in the time evolution of correlation functions between quantum statistics and classical statistics. The higher order terms appearing for nonlinear equations of motion can be viewed as quantum corrections to the classical evolution. Restoring $\hbar$, they involve powers $\hbar^2$, $\hbar^4$, etc. For V containing only up to quartic terms the quantum correction $\Delta\mathcal{L}^{(Z)}_{\mathrm{QM}}$ reads explicitly ($V_{ijk} \equiv V_{ijk}[0]$)

$$\mathcal{L}^{(Z)} = \mathcal{L}^{(Z)}_{\mathrm{cl}} + \Delta\mathcal{L}^{(Z)}_{\mathrm{QM}}, \quad \mathcal{L}^{(Z)}_{\mathrm{cl}} = \frac{1}{m} j_i \frac{\partial}{\partial h_i} - h_i V_i\left[\frac{\partial}{\partial j}\right],$$
$$\Delta\mathcal{L}^{(Z)}_{\mathrm{QM}} = \frac{1}{24}V_{ijk}h_i h_j h_k + \frac{1}{24}V_{ijkl}h_i h_j h_k \frac{\partial}{\partial j_l}. \tag{13}$$

It may be instructive to consider two examples. We first take a single anharmonic oscillator with

$$V(Q) = \frac{1}{2}m\omega^2\left(Q^2 + \frac{4}{3}\sqrt{2m\omega}\,\gamma Q^3 + 2m\omega\,\delta Q^4\right). \tag{14}$$

In terms of a complex source

$$J = \frac{1}{\sqrt{2m\omega}}(j + im\omega h), \tag{15}$$

which is conjugate to the creation operator $a^\dagger$ of the harmonic oscillator, the evolution equation reads

$$\partial_t Z = -i\omega\left\{ J^*\frac{\partial}{\partial J^*} - J\frac{\partial}{\partial J} + (J^*-J)\left[\gamma\left(\frac{\partial}{\partial J^*} + \frac{\partial}{\partial J}\right)^2 + \delta\left(\frac{\partial}{\partial J^*} + \frac{\partial}{\partial J}\right)^3\right] + \frac{\gamma}{12}(J^*-J)^3 + \frac{\delta}{4}(J^*-J)^3\left(\frac{\partial}{\partial J^*} + \frac{\partial}{\partial J}\right)\right\} Z. \tag{16}$$

In our picture the state of the system at a given time t is described by $Z[J,t]$. For the harmonic oscillator ($\gamma = \delta = 0$) the stationary states or fixed points of Z ($\partial_t Z = 0$) are exactly those for which all terms in Z involve an equal number of powers of J and J^*. They correspond to incoherent mixtures of eigenstates of the number operator $a^\dagger a$ or energy eigenstates. It is intriguing that due to the equivalence of the quantum and classical evolution for linear equations of motion the quantum mechanical energy eigenstates can also be viewed as classically stationary probability distributions for commuting coordinate and momentum variables. For $\gamma, \delta \neq 0$ these particular states are not stationary any more. We know, nevertheless, that Eq. (16) must admit an infinite number of fixed point solutions which correspond exactly to incoherent mixtures of energy eigenstates of the anharmonic oscillator. This follows from the general observation that Eq. (7) is equivalent to

$$\partial_t Z = -i\,\mathrm{Tr}(e^{jQ+hP}[H, \rho]) \tag{17}$$

and $H(t) = H(t_0)$. Every ρ which commutes with H defines a stationary state. An important qualitative difference between the quantum and classical evolution equation can be easily seen if we neglect δ. The quantum mechanical evolution equation for $\ln Z$ contains a ''correction'' term $(\gamma/12)(J^*-J)^3$ which acts as an additional constant ''force'' on the connected correlation function for P^3, i.e., $\Delta\partial_t\langle P^3\rangle_c = \frac{1}{12}\omega\gamma(2m\omega)^{3/2}$. A cubic potential is not bounded from below. The local minimum at the origin is separated from the unstable part by a barrier. A classically stable initial ensemble with all energies below the barrier becomes un-

stable in quantum mechanics due to tunneling, as reflected by the additional ''force.'' The essential features of this effect are not changed if we restore stability by a small positive nonzero δ. Once reexpressed in terms of real sources j and h, Eq. (16) is a real partial linear differential equation for a function of three variables $Z(j,h,t)$. A linear combination of two solutions is again a solution. A numerical solution of this equation contains at once the information about the time evolution of all expectation values of arbitrary powers of Q and P. In particular, it seems interesting to investigate the outcome for classically chaotic systems.

Our second example is a linear chain of oscillators (with mass m scaled to one and $d=1$)

$$H=\sum_i \left\{\frac{1}{2}P_i^2+\frac{1}{2}\mu^2 Q_i^2+\frac{1}{3}\nu a^{-d/2}Q_i^3+\frac{1}{8}\lambda a^{-d}Q_i^4 + \frac{1}{2a^2}(Q_{i+1}-Q_i)^2\right\}. \tag{18}$$

Here a is the distance between two oscillators on the chain and we take periodic boundary conditions with a fixed length $\Omega=\Sigma_{i=1}^n a$. The evolution equation reads

$$\partial_t Z=\sum_i \left\{ j_i\frac{\partial}{\partial h_i}+\frac{1}{a^2}h_i\left(\frac{\partial}{\partial j_{i+1}}-2\frac{\partial}{\partial j_i}+\frac{\partial}{\partial j_{i-1}}\right) -h_i\left[\mu^2\frac{\partial}{\partial j_i}+\nu a^{-d/2}\left(\frac{\partial}{\partial j_i}\right)^2+\frac{1}{2}\lambda a^{-d}\left(\frac{\partial}{\partial j_i}\right)^3\right] +\frac{1}{12}\nu a^{-d/2}h_i^3+\frac{1}{8}\lambda a^{-d}h_i^3\frac{\partial}{\partial j_i}\right\}Z. \tag{19}$$

Again, the last two terms are the quantum corrections.

The transition to a field theory can be made by taking the limit $a\to 0$ while keeping a nonzero ''volume'' Ω. With the replacements $a^{-d/2}Q_i\to\tilde{\varphi}(x)$, $a^{-d/2}P_i\to\tilde{\pi}(x), a^d\Sigma_i \to\int d^dx$, $a^{-(d/2+1)}(Q_{i+1}-Q_i)\to\partial\tilde{\varphi}/\partial x_i$—we generalize here to an arbitrary dimension d—the Hamiltonian (18) becomes

$$H=\int d^dx\left\{\frac{1}{2}\tilde{\pi}^2(x)+\frac{1}{2}\partial_i\tilde{\varphi}(x)\partial_i\tilde{\varphi}(x)+U(\tilde{\varphi}(x))\right\},$$
$$U(\tilde{\varphi}(x))=\frac{1}{2}\mu^2\tilde{\varphi}^2(x)+\frac{1}{3}\nu\tilde{\varphi}^3(x)+\frac{1}{8}\lambda\tilde{\varphi}^4(x). \tag{20}$$

This is the Hamiltonian of a relativistic scalar field theory with field equations $\dot{\tilde{\varphi}}(x)=\tilde{\pi}(x)$, $\dot{\tilde{\pi}}=\ddot{\tilde{\varphi}}=\Delta\tilde{\varphi}-\partial U/\partial\tilde{\varphi}$. Since also the commutation relation $[a^{-d}\delta_{ij}\to\delta(x-x')]$,

$$[\tilde{\varphi}(x),\tilde{\pi}(x')]=i\delta(x-x'), \tag{21}$$

is covariant under Lorentz transformations, our system describes a Lorentz-invariant quantum field theory. Here Z becomes a functional of the sources $j_\varphi(x), j_\pi(x)$ which are related to the sources in the discrete version by $a^{-d/2}j_i\to j_\varphi(x)$, $a^{-d/2}h_i\to j_\pi(x)$, $a^{-d/2}(\partial/\partial j_i)\to\delta/\delta j_\varphi(x)$ and $a^{-d/2}(\partial/\partial h_i)\to\delta/\delta j_\pi(x)$, i.e., $Z=\mathrm{Tr}\{\exp(\int d^dx[j_\varphi(x)\tilde{\varphi}(x)+j_\pi(x)\tilde{\pi}(x)])\rho\}$. We finally arrive at the time evolution equation for a scalar quantum field theory

$$\partial_t Z[j_\varphi,j_\pi,t]=\int d^dx\left\{ j_\varphi(x)\frac{\delta}{\delta j_\pi(x)}+j_\pi(x)\Delta\frac{\delta}{\delta j_\varphi(x)} +iU\left(\frac{\delta}{\delta j_\varphi(x)}+\frac{i}{2}j_\pi(x)\right) -iU\left(\frac{\delta}{\delta j_\varphi(x)}-\frac{i}{2}j_\pi(x)\right)\right\}Z[j_\varphi,j_\pi,t]. \tag{22}$$

Its generalization to several scalar fields $\tilde{\varphi}_a(x)$ is straightforward—with $\tilde{\pi}^2\to\tilde{\pi}_a\tilde{\pi}_a$, $\partial_i\tilde{\varphi}\partial_i\tilde{\varphi}\to\partial_i\tilde{\varphi}_a\partial_i\tilde{\varphi}_a$ in H (12) and the commutation relation $[\tilde{\varphi}_a(x),\tilde{\pi}_b(x')] =i\delta(x-x')\delta_{ab}$ we only have to replace $j_\varphi(\delta/\delta j_\pi)\to j_{\varphi_a}(\delta/\delta j_{\pi_a})$, $j_\pi\Delta(\delta/\delta j_\varphi)\to j_{\pi_a}\Delta(\delta/\delta j_{\phi_a})$ in Eq. (22). All symmetries of $U(\tilde{\varphi})$ are preserved by the evolution equation in the sense that an initially symmetric state remains so at a later time. This does not preclude spontaneous symmetry breaking in the course of the evolution—it may be detected by adding a small symmetry breaking linear term in U or by starting with a slightly asymmetric initial state.

Equation (22) is a functional differential equation and its approximate solution has to proceed by some truncation. For this purpose it seems an advantage to switch to the generating functional for the 1PI Green's functions, $\Gamma[\varphi,\pi,t]=-\ln Z[j,t]+\int d^dx[j_\varphi(x)\varphi(x)+j_\pi(x)\pi(x)]$, where $\varphi(x)=\partial\ln Z/\delta j_\varphi(x)$, $\pi(x)=\delta\ln Z/\delta j_\pi(x)$. The derivation of the evolution equation for the effective action Γ proceeds as in Ref. [1] and here we only give the result for the Hamiltonian (20) with $\partial_t\Gamma$ a time derivative at fixed φ and π:

$$\partial_t\Gamma=-(\mathcal{L}_{\mathrm{cl}}^{(\Gamma)}+\Delta\mathcal{L}_{\mathrm{QM}}^{(\Gamma)})\Gamma,$$
$$\mathcal{L}_{\mathrm{cl}}^{(\Gamma)}=\int d^dx\left\{\pi(x)\frac{\delta}{\delta\varphi(x)}+\varphi(x)(\Delta-\mu^2)\frac{\delta}{\delta\pi(x)}-\left[\nu[\varphi^2(x)+G_{\varphi\varphi}(x,x)]+\frac{\lambda}{2}\left(\varphi^3(x)+3\varphi(x)G_{\varphi\varphi}(x,x) -\int dx_1dx_2dx_3G_{\varphi\gamma_1}(x,x_1)G_{\varphi\gamma_2}(x,x_2)G_{\varphi\gamma_3}(x,x_3)\frac{\delta^3\Gamma}{\delta\hat{\varphi}_{\gamma_1}(x_1)\delta\hat{\varphi}_{\gamma_2}(x_2)\delta\hat{\varphi}_{\gamma_3}(x_3)}\right)\right]\frac{\delta}{\delta\pi(x)}\right\},$$
$$\Delta\mathcal{L}_{\mathrm{QM}}^{(\Gamma)}\Gamma=\int d^dx\left\{\frac{\nu}{12}\left(\frac{\delta\Gamma}{\delta\pi(x)}\right)^3+\frac{\lambda}{8}\varphi(x)\left(\frac{\delta\Gamma}{\delta\pi(x)}\right)^3\right\}. \tag{23}$$

Here $G_{\gamma\gamma'}(x,x')=\langle\hat{\tilde{\varphi}}_\gamma(x)\hat{\tilde{\varphi}}_{\gamma'}(x')\rangle_j-\hat{\tilde{\varphi}}_\gamma(x)\hat{\tilde{\varphi}}_{\gamma'}(x')$ is the propagator in the presence of sources where $\hat{\varphi}_\gamma$, $\gamma=\varphi,\pi$ is shorthand for (φ,π). The propagator can in turn be expressed by the inverse of the matrix of second functional derivatives of Γ, i.e., $G_{\gamma\gamma'}(x,x')=(\Gamma^{(2)})^{-1}_{\gamma\gamma'}(x,x')$. Note that $\Gamma^{(2)}$ has indices (x,γ) and (x',γ') with $\gamma=(\varphi,\pi)$. We observe that $\mathcal{L}_{\rm cl}^{(\Gamma)}$ plays the role of the classical Liouville operator, with φ^n replaced by $\langle\tilde{\varphi}^n\rangle$. The difference $\langle\tilde{\varphi}^n\rangle-\varphi^n$ is accounted for by the terms involving G. They induce a dependence of $\mathcal{L}$ on Γ and turn the evolution equation nonlinear. The quantum corrections are all proportional to $(\delta\Gamma/\delta\pi)^3$.

The evolution equation (23) has a fixed point $\Gamma_*(\beta)$ corresponding to thermal equilibrium where $\rho=Z_0^{-1}e^{-\beta H}$, $Z_0=\mathrm{Tr}e^{-\beta H}$ in Eq. (3). This can be computed by functional integral methods [3]. It is far from obvious, however, if and in what sense the solutions of Eq. (23) with nonequilibrium initial conditions approach this fixed point. A uniform approach is not possible due to the existence of infinitely many other fixed points which correspond to incoherent mixtures of eigenstates of H. At best, the equilibrium fixed point can be approached if we restrict the discussion to correlation functions of suitably averaged fields (coarse graining) or to other subsystems. Thermalization can also be achieved by a coupling to an environment, thus introducing a stochastic element in the equations of motion. A truncation of $\Gamma[\varphi,\pi,t]$ may destroy the existence of the infinitely many fixed points. Information about higher 1PI correlations or their precise momentum dependence is omitted in this way. It is conceivable that truncated equations have a more uniform approach to the fixed point than the exact ones. Good truncations should at least retain those terms that play an important role in the computation of $\Gamma_*(\beta)$ by the solution of renormalization group equations in dependence on a coarse graining scale [4]. A better understanding of the impact of truncations will be crucial for the practical use of the present formalism.

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[1] C. Wetterich, e-print hep-th/9612206; e-print hep-th/9702125.
[2] R. Balescu, *Equilibrium and Non-Equilibrium Statistical Mechanics* (Wiley, New York, 1975).
[3] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Oxford University Press, New York, 1989).
[4] C. Wetterich, Nucl. Phys. **B352**, 529 (1991); Phys. Lett. B **301**, 90 (1993); Z. Phys. C **60**, 461 (1993).