Time evolution of correlation functions for classical and quantum anharmonic oscillators

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The time evolution of the correlation functions of an ensemble of anharmonic N-component oscillators with O(N) symmetry is described by a flow equation, exact up to corrections of order 1/N\(^2\). We find effective irreversibility. Nevertheless, analytical and numerical investigation reveals that the system does not reach thermal equilibrium for large times, even when N → ∞. Depending on the initial distribution, the dynamics is asymptotically stable or it exhibits growing modes which break the conditions for the validity of the 1/N expansion for large time. We investigate both classical and quantum systems, the latter being the limit of an O(N) symmetric scalar quantum field theory in zero spatial dimensions.

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Recently much progress was made in understanding the evolution of quantum field theories away from thermal equilibrium in the leading 1/N approximation. However this approach has its shortcomings. The omission of scattering leads to infinitely many conserved quantities which prevent thermalization.

In we have taken the first step in an investigation of the evolution of an O(N) symmetric scalar field theory in next to leading order 1/N. The resulting system describes the evolution of the 2-point functions of the fields and their conjugate momenta. At this level we can hope to answer the fundamental question of whether the inclusion of scattering leads to thermalization.

A full treatment of the non-linear behavior for the field theory requires much greater computational resources than at the leading order. One should therefore gain as much insight as possible in simple realizations of the problem. In this letter we study the limit of zero spatial dimensions of an O(N) symmetric \(\varphi^4\)-theory, or, equivalently the evolution of an ensemble of quantum anharmonic oscillators. Our approach is based on the effective action which generates the equal time one particle irreducible (1PI) correlation functions.

The time evolution of the effective action \(\Gamma\) obeys

\[
\partial_t \Gamma[\phi, \pi; t] = - \left( \mathcal{L}_c + \mathcal{L}_q \right) \Gamma[\phi, \pi; t],
\]

where the first operator, \(\mathcal{L}_c\), generates the classical evolution, whereas \(\mathcal{L}_q\) determines the dynamics of the quantum effects. We will deal with the specific example of an O(N) symmetric ensemble of anharmonic oscillators \(Q_a, a = 1, \ldots, N\), obeying the microscopic equations of motion \(\partial_t^2 Q_a = -m^2 Q_a - \frac{1}{2} Q_b Q_b Q_a\). The arguments of \(\Gamma\) are the mean values of the coordinates \(\phi_a = \langle Q_a \rangle\) and their conjugate momenta \(\pi_a = \langle \dot{Q}_a \rangle\) (in the presence of sources). From \(\mathcal{L}_c\), one infers

\[
\mathcal{L}_{cl} = \frac{\delta}{\delta \phi_a} - m^2 \phi_a \frac{\delta}{\delta \pi_a} \frac{\lambda}{2} \left[ \phi_b \phi_b \phi_a + \phi_a G_{ab} \phi^b \right].
\]

On the level of 1PI 2 and 4 point functions the most general form of \(\Gamma\) consistent with O(N) symmetry is

\[
\Gamma = \frac{1}{2} \left\{ A \phi_a^* \phi_a + B \pi_a^2 + 2C \pi_a \phi_a \right\} + \frac{1}{8} \left\{ u \phi_a \phi_a \phi_a \phi_b + v \pi_a \phi_a \phi_a \phi_b + w \pi_a \phi_a \phi_a \phi_b \phi_a + s \left[ \pi_a \pi_b \phi_a \phi_a - \pi_a \pi_b \phi_a \phi_b \right] \right\}
\]

The time dependence of \(A(t), \ldots, z(t)\) gives directly the time dependence of the propagator and the 4-point vertices. Higher vertices only induce corrections \(\sim 1/N^2\). We emphasize that the truncation still retains connected n-point functions of arbitrary order to the extent that they are constructed from 4-vertices and propagators \((G_{ab} = G_{ab} = (Q_a(t)Q_b(t) - (Q_a(t))\langle Q_b(t) \rangle)\), etc.

The exact equations for the inverse two point functions, with \(G = B/(AB - C^2)\) and \(c = C/B\), read

\[
\partial_t G = -2c G, \quad \partial_t B = -2(c + \gamma) B,
\]

\[
\partial_t c = \omega^2 - \frac{1}{BG} + \gamma c + c^2.
\]

Here, the time dependent frequency, \(\omega\), and \(\gamma\) are:

\[
\omega^2 = m^2 + \frac{N + 2}{2} \lambda G \left[ 1 - \frac{G^2}{4} \left[ 4u - 3v + 2wc^2 - ye^3 \right] \right],
\]

\[
\gamma = \frac{N + 2}{8} \lambda G^3 \left[ v - wc + 3ye^2 - 2z e^3 \right].
\]

For large \(N\), with \(\lambda, u, v, w, s, y, z\) scaling like 1/N, one may expand in small 1/N. We see that \(\gamma \sim 1/N\) and \(\omega\) becomes independent of \(u, v, \ldots, z\), in leading order. In the limit \(N \to \infty\) the system of evolution equations for the
inverse 2-point functions is closed. In this approximation $B/G$ becomes an additional conserved quantity [3].

For a solution of (4-6) at finite $N$, however, one needs the time dependent 4-point functions. Their evolution involves, in turn the 6-point functions. The exact system is not closed and for any practical purpose we have to proceed to some approximation. Below we simply omit all contributions from 1PI 6-point vertices. Then the evolution equations for the quartic couplings are

$$\begin{align*}
\partial_t u &= \omega^2 v + 4\lambda B c - \lambda^2 B^2 c^3 - \lambda B G^2 \left\{ 2(N+8) u \right\}, \\
\partial_t v &= 2\omega^2 w - 4u - \gamma v + 4\lambda B - 3\lambda^2 B^3 c^2 - \lambda B G^2 \left\{ 2(N+8) u + [(N-10)w - 3(N-1)s]c^2 + (N+8)yc^3 \right\}, \\
\partial_t w &= 3\omega^2 y - 3v - 2\gamma w - 3\lambda h B^3 c - \lambda B G^2 \left\{ (N+8) v + [(N-10)w - 3(N-1)s]c^2 + 2(N+8)zc^3 \right\}, \\
\partial_t s &= 2\omega^2 y - 2v - 2\gamma s - 2\lambda h B^3 c - \lambda B G^2 \left\{ (N+6) v - 2[4w + (N-1)s]c + (N+2)yc^2 + 8zc^3 \right\}, \\
\partial_t y &= 4\omega^2 z - 2w - 3\gamma y - \lambda h B^3 c - \lambda B G^2 \left\{ (N+2) w - (N-1)s - (N+8)y c^2 \right\}, \\
\partial_t z &= -y - 4\gamma z.
\end{align*}$$

Here we have omitted some terms $\sim 1/N^2$. The neglected 6-point functions can also be treated consistently as being $\sim 1/N^2$. Thus, our set of evolution Eqs. (4-6) contains all contributions in the next to leading order $1/N$. The average energy $\epsilon = \epsilon_1 + \epsilon_2 = \langle H \rangle$,

$$\begin{align*}
\epsilon_1 &= \frac{N}{2} \left\{ B^{-1} + \left[ m^2 + c^2 + \frac{N+2}{4} \lambda G \right] G \right\}, \\
\epsilon_2 &= -\frac{N(N+2)}{8} \lambda G^4 \left[ u - vc + wc^2 - yc^3 + zc^4 \right],
\end{align*}$$

is conserved by the exact evolution equations, as well as by our truncation. Our system meets at least some basic conditions for thermalization: The number of interacting degrees of freedom $N$ can be arbitrarily large and scattering effects are included.

A first hint that the approach to equilibrium for large times is not obvious, however, comes from the study of possible time invariant solutions. The fixed points of the system Eqs. (4-6) correspond to stationary probability distributions. They obey, for $\omega^2 > 0$,

$$\begin{align*}
G_s^{-1} &= \omega^2 B_s, \quad c_s = 0, \quad v_s = 0, \quad y_s = 0, \\
u_s &= \frac{\lambda B_s + (\omega^2/2) w_s}{1 + \frac{N+8}{2} \lambda / (\omega^2 B_s)}, \\
w_s &= \frac{2\omega^2 z_s + \frac{N-1}{2} \lambda (\omega^3 B_s)^{-1} s_s - \frac{3\lambda h^2 B^3_s}{1 + \frac{N+2}{2} \lambda / (\omega^2 B_s)}}{\langle H \rangle - \langle B \rangle}.
\end{align*}$$

We observe a large manifold of fixed points since Eqs. (8) have solutions for arbitrary $B_s$, $s_s$ and $z_s$. This property seems not to be an artifact of the truncation. The fixed point manifold becomes even larger if one includes the six point functions and seems to characterize any higher (finite) polynomial truncation. Classical thermodynamic equilibrium, at temperature $T$ (for $h = 0$) corresponds to the particular point in this manifold:

$$\begin{align*}
B_{eq} &= \beta = 1/T, \quad c_{eq} = 0, \quad G_{eq} = \frac{T}{\omega_{eq}^2}, \\
v_{eq} &= w_{eq} = s_{eq} = y_{eq} = z_{eq} = 0, \\
u_{eq} &= \frac{\lambda}{T} \left( 1 + \frac{N+8}{2} \frac{\lambda T}{\omega_{eq}^4} \right)^{-1},
\end{align*}$$

where $\omega_{eq}$ obeys

$$\left( \omega_{eq}^4 - m^2 \omega_{eq}^2 - \frac{N+2}{2} \lambda T \right) \left( 1 + \frac{2}{N+8} \frac{\omega_{eq}^4}{\lambda T} \right) = -\frac{N+2}{N+8} \lambda T,$$

with $\lim_{N \to \infty} \omega_{eq}^2 = \frac{1}{2} (m^2 + \sqrt{m^4 + 4N \lambda T})$.

The thermal fixed point in the quantum system occurs for non-zero $w_s, z_s$. In particular, we find in the quantum system a fixed point which differs from the classical equilibrium fixed point only by $z_s = \lambda h^2 B^2_s / (4\omega^2)$, instead of $z_{eq} = 0$. For this fixed point, all correlation functions involving only $\phi$ are the same as for classical equilibrium. Inversely, for every fixed point of the quantum system there is one for the classical system, differing only by a shift in $z_s$. Up to this shift, the quantum equilibrium could be reached by the classical system!

An obstruction to thermalization arises from the existence of an infinite set of conserved quantities. Besides $\langle H \rangle$, also arbitrary powers $\langle H^p (L^2)^q \rangle$ (with $L^2$ the squared generalized angular momentum) are conserved. For thermal equilibrium $\langle L^2 \rangle$ or $\langle H^2 \rangle - \langle H \rangle^2$ are computable as functions of $T$, e.g. $\langle L^2 \rangle_{eq} = N(N-1)T^2 / \omega_{eq}^2$. Initial values of conserved quantities away from equilibrium prevent thermalization.

For classical statistics ($h = 0$), we have shown [3] that the dynamical system describing the linearized motion orthogonal to the fixed point manifold is characterized by three doubly degenerate eigenvalues which are strictly imaginary. Consequently the motion is purely oscillatory. To probe the behavior in the non-linear regime, away from the fixed point manifold, we have solved the system of differential Eqs. (4-6) numerically for various initial conditions. Unless otherwise stated, we consider below the the parameters $N = 10$, $m^2 = 1$, $\lambda = 1/N$ and $h = 0$.

We first show, in Fig. 1, the result of Gaussian initial conditions with $G(0) = 0.18069$, $B(0) = 5$ and all other initial couplings zero. After a rapid initial increase of $u$ the typical behavior becomes purely oscillatory. This confirms the results of our small fluctuation analysis and
depends, however, on the initial condition as specified by a stable mean value independent of \( \tau \). We see that for \( \Delta \) not too large the system thermalizes. In a strict sense. Nevertheless, the time averages of the correlation functions can never be approached to different initial \( (L^2) \). For \( \Delta > 0 \) we find a clear signal that the '2-point function' \( (Q^2) \) never thermalizes. This constitutes the most important result of this letter.

The situation for the quantum system is not very different, as seen by comparing Figs. B and C. For negative \( m^2 = -1 \) we show in Figs. B and D the results of the classical \( (h = 0) \) and quantum \( (h = 1) \) evolution for \( T = 1 \) and with \( G_{\text{eq}}(T), u_{\text{eq}}(T) \) adapted appropriately.

\[ G(0) = G_{\text{eq}}(T)(1 + \Delta), \quad u(0) = u_{\text{eq}}(T), \]
\[ c(0) = v(0) = y(0) = w(0) = s(0) = z(0) = 0, \quad (11) \]
\[ B(0)^{-1} = T - \Delta G_{\text{eq}}(T) \left[ m^2 + \frac{N + 2}{4} \lambda G_{\text{eq}}(T)(2 + \Delta) \right. \]
\[ \left. - \frac{N + 2}{4} \lambda G_{\text{eq}}^3(T) u_{\text{eq}}(T) \right] \left( 4 + 6 \Delta + 4 \Delta^2 + \Delta^3 \right) \]
\[ + \frac{N + 2}{4} \lambda G_{\text{eq}}^4(0) \left( u(0) - u_{\text{eq}}(T) \right). \]

Here \( T \) is the equilibrium temperature and \( G_{\text{eq}}(T), u_{\text{eq}}(T) \) the corresponding values in Eqs. (3). The initial condition for \( B(0) \) is chosen such that the energy of the system \( \epsilon = \Delta (3T + G_{\text{eq}}(T)m^2) \), is independent of \( \Delta \). Thus, the initial conditions correspond all to the same effective temperature and the large time behavior should become independent of \( \Delta \) if the system thermalizes. In Fig. 2B we plot \( \langle G(t) \rangle_{100} \) for the initial conditions of (11). We see that for \( \Delta \) not too large \( \langle G \rangle_{100} \) for has for large \( t \) a stable mean value independent of \( \tau \). The mean value depends, however, on the initial condition as specified by \( \Delta \). The curves correspond to the same effective \( T \), but to different initial \( (L^2) \). For \( \Delta > 0 \) we find a clear signal that the '2-point function' \( (Q^2) \) never thermalizes. This constitutes the most important result of this letter.

We repeated the analysis of Fig. 2 for different \( N \) with similar results, even for very large \( N \). The dependence of \( \langle G \rangle \) on \( \Delta \) becomes independent of \( N \) as \( N \to \infty \).

The odd number of degrees of freedom and the absence of more conservation laws hints to the fact that the real nonlinear system of flow equations should not be Hamiltonian, albeit being energy conserving. The spectrum of a Hamiltonian system is semi-positive definite and the system is stable in the sense that it has no growing modes. Otherwise this property is lost. Of course the existence of one growing mode implies others since the energy must be preserved by the evolution. This is precisely what happens to the full nonlinear system in the strong anharmonic regime. As already visible in Fig. 2B the system becomes unstable if the initial conditions are far from the fixed point manifold. More precisely this means that the couplings grow large and the validity of the \( 1/N \) expansion breaks down for large \( t \). A useful criterion for the validity of the \( 1/N \) expansion requires that the contribution to \( \epsilon \) proportional to \( u \), \( |\epsilon_{\text{u}}| = \frac{N(N+2)}{8} |G^4 u| \), remains smaller then \( \frac{1}{T} \). We denote by \( t_e \) the time when this condition is violated and plot \( t_e \) as a function of \( \Delta \) in Fig. 3A for \( T = 1 \) and \( T = 5 \). The initial conditions are chosen here without the \( \Delta \) terms in \( B(0) \), i.e. \( B(0) = 1/T \). For \( \Delta \leq \Delta_c \) the \( 1/N \) expansion remains valid at least for \( t \leq 10^4 \). (The critical values are \( \Delta_c = 0.655(1.012) \).
for \( T = 1(5) \) and \( \hbar = 0 \) and \( \Delta_\epsilon = 0.346(\Delta_\epsilon \leq 10^{-6}) \) for \( T = 1(5) \) and \( \hbar = 1 \). For \( \Delta > \Delta_\epsilon \) one observes a very peculiar behavior of \( t_c(\Delta) \) with discontinuities at certain values of \( \Delta \). It suggests a chaotic dependence of the correlation functions on the initial conditions! (This type of behavior has been observed at leading \( 1/N \) [6].) This should not be confused with the much more common chaotic behavior for individual solutions of the equations of motion. The latter, once averaged in an ensemble, often leads to regular behavior of the correlation functions. Note that there are restrictions on the initial values of the correlation functions as they must be consistent with a positive probability distribution. We have not systematically investigated these conditions so far.

Below we address the behavior for \( \Delta > \Delta_\epsilon \) in more detail in order to shed some light on the origin of the instability. Fig. 3 shows a typical evolution for initial conditions generating instabilities. Notice that \( u(t) \) grows unbounded for large times while \( \omega^2(t) \) becomes negative. The power spectrum shows how the system goes stiff, particularly for the 4-point functions. In order to ensure the accuracy of our numerical integration we have used two independent methods, one based on an adaptive step algorithm and another especially tailored to handle stiff problems. Although the latter is intrinsically less precise we observed that instabilities occurred for coincident \( t_c \). We conclude they are inherent to the dynamical system and robust to the choice of numerical integrator.

From Fig. 3 it is apparent that many frequencies are shared among the 2 and 4-point functions. This may lead to secular instabilities since products of the 2-point functions act as sources for the dynamical equations of the 4-point functions. Secular instabilities result from an oscillator being driven at its own natural frequency and result initially in linear growth of its amplitude. For a given frequency \( \omega \) shared by all degrees of freedom odd products of the 2-point functions can generate secular growth of the 4-point functions. In the quantum case these terms are more common, which may explain why the quantum motion generally becomes unstable sooner.

FIG. 3. \( t_c \) vs. \( \Delta \), for \( T = 1, 5 \) and \( B(0) = 1, 0.2 \). The discontinuities seem to arise at arbitrary small steps in \( \Delta \). For \( \Delta \) such that no point is plotted \( t_c > 10^4 \).

Below we address the behavior for \( \Delta > \Delta_\epsilon \) in more detail in order to shed some light on the origin of the instability. Fig. 4 shows a typical evolution for initial conditions generating instabilities. Notice that \( u(t) \) grows unbounded for large times while \( \omega^2(t) \) becomes negative. The power spectrum shows how the system goes stiff, particularly for the 4-point functions. In order to ensure the accuracy of our numerical integration we have used two independent methods, one based on an adaptive step algorithm and another especially tailored to handle stiff problems. Although the latter is intrinsically less precise we observed that instabilities occurred for coincident \( t_c \). We conclude they are inherent to the dynamical system and robust to the choice of numerical integrator.

In conclusion, we have presented a detailed study of the time evolution of correlation functions for ensembles of \( N \)-component quantum and classical anharmonic oscillators. Our truncation method converges for large \( N \) and is well suited to describe an approach to thermal equilibrium. Nevertheless, we find that the isolated systems do not thermalize! It will be very interesting to see if similar features persist in field theory or if effective thermalization occurs in the presence of many frequencies for the linear problem, due to dephasing [1,2].

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