Initial conditions for simulated ‘tachyonic preheating’ and the Hartree ensemble approximation

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In numerical simulations studying preheating in the classical approximation there is the problem how to derive the classical initial conditions from the quantum vacuum fluctuations. In past treatments, the initial conditions often put an energy density into the classical field of order of the cutoff, leading to a divergent temperature after thermalization. We suggest a solution to the problem which follows naturally from a Hartree ensemble approximation, introduced recently as an improvement over the standard Hartree approximation. We study the effects on particle numbers of the various treatments, within the context of ‘tachyonic preheating’ in 1+1 dimensional $\varphi^4$ theory.

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1 Introduction

Numerical simulations of quantum field dynamics in real time are currently carried out by first making approximations. For systems out of equilibrium the classical approximation can be quite useful, for example in studying reheating after inflation \cite{1\textsuperscript{-}8}. In addition there are Hartree (gaussian), Dyson-Schwinger and 2PI-functional approximations, possibly supported by large $N$ considerations. These have the advantage of being formulated in the quantum theory where potential divergencies are taken care of by renormalization.

Even if the system is homogeneous it may be important to allow for inhomogeneous realizations in order to capture non-perturbative effects. Recently we have formulated a Hartree ensemble approximation \cite{9,10}, in which an overall homogeneous density matrix is represented as an ensemble of typically inhomogeneous initial configurations, which are then evolved in time using the Hartree approximation. With this method we found that the poor thermalization properties of the homogeneous Hartree approximation are much improved.

Here we shall describe an application of this method to the problem of spinodal or tachyonic instability. This process has been put forward as an efficient mechanism for preheating. In ref. \cite{4,5} it was studied numerically, using the classical approximation with initial values based on quantum fluctuations. However, these initial conditions (of the type also used in the other studies in \cite{1\textsuperscript{-}8}) lead to problems: the final temperature is of order of the cutoff. Below we propose improved initial conditions for the classical approximation which do not have this problem and we compare with results obtained using the previously employed initial conditions, in classical and Hartree dynamics.

We also draw the attention to a fruitful definition of particle numbers and energies for systems out of equilibrium, which was introduced in \cite{9}, and for the fermionic case in \cite{13}.

2 Hartree ensemble approximation

Our tests are carried out in in 1+1 dimensional $\varphi^4$ theory. The quantum hamiltonian is given by

$$\hat{H} = \int dx \left( \frac{1}{2} \hat{\pi}^2 + \frac{1}{2} (\nabla \hat{\varphi})^2 + \frac{1}{2} \mu^2 \hat{\varphi}^2 + \frac{1}{4} \lambda \hat{\varphi}^4 \right),$$

from which follow the Heisenberg operator equations

$$\dot{\hat{\varphi}} = \hat{\pi}, \quad \dot{\hat{\pi}} = (\nabla^2 - \mu^2) \hat{\varphi} - \lambda \hat{\varphi}^3.$$ (2)

We discretize the field on a space-time lattice, with lattice spacings $a$ and $a_t$, such that $\nabla \varphi \to (\varphi_{x+a} - \varphi_x)/a$, $\varphi \to [\varphi_x(t+a_t) - \varphi_x(t)]/a_t$. The number of spatial lattice sites is $N$, the volume $L = Na$ and we use periodic boundary conditions. The Hartree approximation
implies that the fields can be expanded in terms of mode functions
\[ \tilde{\varphi}_x = \varphi_x + \sum_\alpha (f_\alpha^* \hat{b}_\alpha + f_\alpha \hat{b}_\alpha^*), \quad \tilde{\pi}_x = \pi_x + \sum_\alpha (\tilde{f}_\alpha^* \hat{b}_\alpha + \tilde{f}_\alpha \hat{b}_\alpha^*), \tag{3} \]
in which \( \varphi_x \) and \( \pi_x = \tilde{\varphi}_x \) are the mean fields. The creation and annihilation operators \( \hat{b}_\alpha^*, \hat{b}_\alpha \) are time-independent, with \([\hat{b}_\alpha, \hat{b}_\beta^*] = \delta_{\alpha\beta}\), while the mode functions \( f_\alpha^* \) are time-dependent. Furthermore, the density operator (which is time-independent in the Heisenberg picture) is gaussian, such that it is completely specified by giving the initial values of the one and two-point functions, \( \langle \hat{\varphi}_x \hat{\varphi}_y \rangle = \varphi_x \varphi_y, \langle \hat{\varphi}_x \hat{\pi}_y + \hat{\pi}_y \hat{\varphi}_x \rangle = \pi_x, \langle \hat{\pi}_x \hat{\pi}_y \rangle \). With a suitable choice of initial mode functions these can be rephrased as \( \langle \hat{b}_\alpha^* \hat{b}_\beta \rangle = n_\alpha^0 \delta_{\alpha\beta} \), with \( \langle \hat{b}_\alpha \rangle = \langle \hat{b}_\alpha^* \rangle = \langle \hat{b}_\alpha \hat{b}_\alpha \rangle = \langle \hat{b}_\alpha^* \hat{b}_\alpha^* \rangle = 0 \). In case the gaussian state is pure, the \( n_\alpha^0 = 0 \), and the Hartree equations for the mean field and mode functions take the form of a set of coupled non-linear partial differential equations,
\[ \begin{align*}
\ddot{\varphi}_x &= \nabla^2 \varphi_x - \left( \mu^2 + \lambda \varphi_x^2 + 3\lambda \sum_\alpha f_\alpha^* f_\alpha \right) \varphi_x, \\
\ddot{f}_x^\beta &= \nabla^2 f_x^\beta - \left( \mu^2 + 3\lambda \varphi_x^2 + 3\lambda \sum_\alpha f_\alpha^* f_\alpha \right) f_x^\beta. \tag{4} \end{align*} \]

In 1+1 dimensions the mode sum is only logarithmically divergent as the lattice spacing \( a \rightarrow 0 \), which is taken care of by mass renormalization. In the following we assume the divergence to be subtracted from the mode sum, such that \( \mu^2 \) is a renormalized mass parameter, with particle mass \( m^2 = \mu^2 \) (symmetric phase) and \( m^2 = -2\mu^2 \) (broken phase).

In the Hartree ensemble approximation the density operator \( \hat{\rho} \) is written as a superposition in terms of gaussian coherent pure states \( |i\rangle \),
\[ \hat{\rho} = \sum_i p_i |i\rangle \langle i|, \tag{5} \]
and the Hartree approximation is applied to each state \( |i\rangle \) individually. Note that \( \hat{\rho} \) does not have to be gaussian or pure-state. Given \( \hat{\rho} \) and a choice of the set of coherent states \( |i\rangle \), the probabilities \( p_i \) are uniquely defined in simple cases, e.g. a free thermal ensemble \( \mathbb{F} \). However, we shall use \( \mathbb{F} \) to formulate approximations to the true \( \hat{\rho} \), such that the initial values of the one and two-point functions are reproduced. We see this as a sort of coarse graining: not all details of the true \( \hat{\rho} \) are kept, only those referring to the important low momentum modes of the one and two point functions \( \langle \hat{\varphi}_x \rangle, \ldots, \langle \hat{\pi}_x \hat{\pi}_y \rangle \).

Even if \( \varphi_x = \langle \hat{\varphi}_x \rangle = \sum_i p_i |i\rangle \langle i| \hat{\varphi}_x |i\rangle \) is homogeneous (independent of \( x \)), the individual \( \varphi_x^{(i)} = \langle i | \hat{\varphi}_x | i \rangle \) are typically inhomogeneous. This is important for thermalization, because the modes interact non-linearly with the inhomogeneous \( \varphi_x^{(i)} \): the particles can scatter.
3 Particle number

One needs a definition of particle number $n_k$ and frequency $\omega_k$ which is reasonably intuitive and robust, such that it can be applied to systems out of equilibrium. Some coarse graining will have to be involved and the following definition takes this to the extreme of using an average over the whole volume: we define $n_k$ and $\omega_k$ at each time by the equations

$$
\langle \hat{\psi}_k \hat{\psi}^\dagger_k \rangle_{\text{conn}} = \left( n_k + \frac{1}{2} \right) \frac{1}{\omega_k}, \quad \langle \hat{n}_k \hat{n}^\dagger_k \rangle_{\text{conn}} = \left( n_k + \frac{1}{2} \right) \omega_k,
$$

(6)

where $\hat{\psi}_k = \sum_x e^{-ikx} \hat{\varphi}_x / \sqrt{L}$ and $\langle \hat{\psi}_k \hat{\psi}^\dagger_k \rangle_{\text{conn}} = \langle \hat{\varphi}_k \hat{\varphi}^\dagger_k \rangle - \langle \hat{\varphi}_k \rangle \langle \hat{\varphi}_k^\dagger \rangle$, etc. For a free system these formulas produce the standard distribution functions and frequencies, while for systems out of equilibrium the above definitions have been used successfully in [9, 10]. A corresponding definition for fermions was introduced in [13], which also mentions the relation to Wigner functions. Here we note in particular that the above equations can be easily solved, with positive $\omega_k$, and we always have found $n_k$ to be positive.

The above formulas can also be applied to classical fields, with

$$
\overline{\varphi_k \varphi^\dagger_k}_{\text{conn}} = n_k \frac{1}{\omega_k}, \quad \overline{n_k n^\dagger_k}_{\text{conn}} = n_k \omega_k,
$$

(7)

where $\overline{\cdot}$ denotes a classical average (typically over initial configurations).

4 Initial conditions

Consider a quench, a sudden change of the sign of the renormalized mass parameter $\mu^2$ from positive to negative values at time $t = 0$. This is supposed to mimic the effect of a rapid phase transition (cf. figure 1). Because the potential at $t = 0^+$ is unstable, Fourier modes of the field with wave vector $|k| < |\mu|$ are unstable and grow exponentially. Occupation numbers grow large and non-linearities become important, which fact has been dealt with numerically using the classical approximation.

The question is how to start the simulation, and, can we do better and stay within the quantum theory? Classically, the ground state at $t = 0^-$ implies that the fields and canonical momenta are zero, so nothing would happen subsequently. Quantum fluctuations are invoked to start the process. At $t = 0^-$ the system is in a single well ground state. Neglecting non-linearities the quantum fluctuations are characterized by

$$
n_k = 0, \quad \omega_k = \omega_k^0 = \sqrt{|\mu|^2 + k^2}.
$$

(8)

These expectation values can be reproduced with the classical ensemble distribution

$$
p(\varphi, \pi) \propto \prod_k \exp \left[ -\frac{\pi_k^2 \pi_k + \omega_k^2 \varphi_k \varphi_k^*}{\omega_k(n_k + 1/2)} \right],
$$

(9)
with \( n_k = 0 \) and \( \omega_k = \omega_k^0 \). The type of initial conditions used in [1]-[8] correspond to generating configurations from this distribution and using these as initial values for the subsequent classical evolution. A problem with this is that the total energy density \( \sum_k \omega_k^0/2L \) diverges \( \propto a^{-2} \) for lattice spacing \( a \to 0 \), and after equilibration the classical temperature \( T \) also diverges \( \propto a^{-1} \). Renormalization of this divergence is not possible out of equilibrium (in equilibrium one can attempt to do this with temperature dependent counterterms [11, 12]).

The Hartree approximation does not have this problem as it is formulated in the quantum theory. However, with homogeneous initial conditions it has insufficient scattering to obtain thermalization.

To improve this situation we proceed as follows. We solve the Heisenberg equations analytically for small times, when the modes grow exponentially \( \propto \exp(t\sqrt{|\mu|^2 - |k|^2}) \). Non-linearities become important roughly when \( |\mu|^2 \varphi^2/2 = \lambda \varphi^2/4 \), at the spinodal time \( t_{sp} \equiv \frac{1}{2}|\mu| \ln(2|\mu|^2/\lambda) \). At some resampling time \( 0 < t_{rs} < t_{sp} \) we provide a gaussian distribution (9), for initial values \( \varphi_k \) and \( \pi_k \) of the unstable modes, based on the analytically calculated two-point functions \( \langle \hat{\varphi}_k^{\dagger} \hat{\varphi}_k \rangle \) and \( \langle \hat{\pi}_k^{\dagger} \hat{\pi}_k \rangle \) (in the analytic solution \( \langle \hat{\varphi}_k \rangle = \langle \hat{\pi}_k \rangle = \langle \hat{\varphi}_k^{\dagger} \hat{\varphi}_k \rangle = 0 \)):

- In the classical approximation, the distribution is chosen of the form (9) with \( n_k + 1/2 \to n_k \) (so dropping the 1/2), such that the analytically calculated particle distribution \( n_k \) is reproduced by (9). The high momentum modes in (9) are suppressed by \( n_k \) dropping to zero (like \( k^{-4} \) as it turns out). We actually keep only the unstable modes in the initialization as for these typically \( n_k \gg 1 \). The resulting energy density is finite.

- In the Hartree ensemble approximation we also use the form (9) to generate initial values for the mean fields in each Hartree realization, again with \( n_k + 1/2 \to n_k \). The mode functions are initialized as vacuum plane waves \( \alpha \to k \),

\[
 f_k^x = \frac{e^{ikx - i\omega_k t}}{\sqrt{2L\omega_k^{\text{vac}}}} \quad \omega_k^{\text{vac}} = \sqrt{m^2 + k^2}, \quad m^2 = -2\mu^2, \quad (10)
\]

where \( m \) is the mass of the particles and the gaussian coherent states are specified by \( b_k|i\rangle = 0 \). (It would perhaps have been logically more consistent to use \( \omega_k \) in
\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Particle distributions at various times using ‘old’ initial conditions. The straight line is a fit to the data at small \(\omega_k\). The classical distribution \(n_k = T/\omega_k\) with the same temperature is also indicated (curved line).}
\end{figure}

\section{Numerical tests}

We used relatively weak coupling, \(v^2 = m^2/2\lambda = 6\), a lattice spacing \(am = 0.2\) and volume \(Lm = 102.4\). Figure 2 shows the particle distribution for several times, obtained by classical evolution using the ‘old’ initial conditions at \(t = 0^+\), i.e. (9) with \(n_k + 1/2 \to 1/2\) (so keeping the 1/2) and \(\omega_k = \omega_k^0\). Plotted is \(\ln(1 + 1/n_k)\) versus \(\omega_k\), which would give a straight line with slope \(1/T\) for a Bose-Einstein distribution \(n_k^{-1} = \exp(\omega_k/T) - 1\). One clearly sees at time \(tm = 10\) that the high momentum modes, which have not been affected yet by the evolution, are populated according to the vacuum fluctuations: their effective classical particle number (from (6) and (7)) is \(1/2\) and \(\ln(1 + 1/0.5) \approx 1.1\). At later times the distribution approaches the classical \(T/\omega_k\).

Next we show results using the proposed ‘new’ initial conditions for the classical evolution. With the parameters used here there are then 23 unstable modes (12 with \(k \geq 0\)). The spinodal time \(t_{sp}m \approx 1.8\) and the resampling time was chosen to be \(t_{rs}m \approx 1\). Figure 3 shows the results for this case. We see that initially \(n_k\) drops very fast as a function of \(k\) (cf. \(tm = 10\)). At intermediate times the distribution resembles a Bose-Einstein form. The approach to the classical distribution is much slower than in the previous case, the flow of energy to the higher momentum modes is evidently slow.

Results using the Hartree ensemble approximation are shown in figure 4-left. In this case we see a slow approach to a Bose-Einstein distribution, within the same time span as in the previous cases. However, we expect the distribution to approach a classical
form on a much larger time scale, typically by a factor of 100 \[10\].

Finally, figure 4-right shows how the temperature (as determined by the slope in figs. 2-4 at low momenta) evolves in time for the three cases. In the first case we see the temperature gradually rising, eventually \(T\) will get of order \(1/a\). In the second case \(T\) drops slowly as the energy is being equipartitioned from the low momentum modes to all modes. For the Hartree ensemble case the temperature remains reasonably constant after the initial transient. We checked that the same temperature is obtained using a smaller resampling time.

6 Conclusion

The divergences in the energy density and the classical temperature are cured by our proposal for obtaining initial conditions for classical simulations. It makes a big difference at
later times. The Hartree ensemble approximation appears to be a significant improvement over the classical treatments. However, this method is numerically expensive and further tests are needed in 3+1 dimensions.

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