New Initial Conditions for Quantum Field Simulations after a Quench

M. Sallé, J. Smit and J.C. Vink*
Institute for Theoretical Physics, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

We investigate a new way of using the quantum fluctuations in the vacuum as initial conditions for subsequent classical field dynamics. We show that with this method the field properly thermalizes at later times, whereas the method used previously leads to unphysical results.

1. Initial conditions for a quench

Investigation of initial value problems for quantum fields using numerical simulation are difficult. The dynamics cannot be computed exactly and one has to use e.g. the classical approximation, the large N or Hartree approximation. It is then not obvious how to specify initial conditions properly. Here we focus on this problem and investigate a new way to supply initial conditions for classical dynamics. We shall apply the same strategy to a simulation with the recently proposed Hartree ensemble approximation as well.

As a test case, we consider a quench in a simple 1+1 dimensional $\varphi^4$ model discretized on a lattice, with hamiltonian,

$$ H = \sum_x \left( \frac{1}{2} \pi_x^2 - \frac{1}{2} \varphi_x \Delta \varphi_x + \frac{1}{2} \mu^2 \varphi_x^2 + \frac{1}{4} \lambda \varphi_x^4 \right). $$ (1)

We model a sudden quench by assuming that at $t = 0$ the sign of $\mu^2$ in the potential flips from positive to negative. At $t = 0$ the system is in the vacuum state corresponding to the single-well potential ($\mu^2 > 0$). Classically this would imply that the field is at rest, but triggered by (vacuum) quantum fluctuations, the field modes with momentum $|p| < |\mu|$ will grow exponentially in a “spinodal decomposition” of the field. It is not obvious how one should supply quantum fluctuations as initial conditions for the classical fields. Until now one has followed the prescription that the classical field at $t = 0$ should reproduce the one- and two-point functions evaluated in the quantum theory.

This implies that initial values for the (complex) Fourier amplitudes $\varphi_p$ and $\pi_p$ of the classical field and its velocity $\pi = \dot{\varphi}$, must be drawn from a gaussian ensemble with probability distribution (using $\omega_{0p} = (p^2 + |\mu|^2)^{1/2}$),

$$ P(\varphi, \pi) \propto \exp\left(- \sum_p (|\pi_p|^2 + \omega_{0p}^2 |\varphi_p|^2) / 2 \omega_{0p} \right). $$ (2)

An apparent problem with this prescription is that the initial vacuum fluctuations contribute to the energy density and the equilibrium temperature that would correspond to the amount of energy put into the field diverges when the cut-off is removed, $T \propto 1/a$. One can only hope that in the early stages of the field evolution, this reservoir of spurious energy in the short wavelength modes does not significantly affect the low-energy dynamics.

These problems are absent in the new approach we shall describe next. During the spinodal decomposition, there may be a time window $t_- < t < t_+$ in which $\langle |\varphi_p|^2 \rangle \gg \frac{1}{\lambda}$ while the backreaction can still be ignored, $\lambda \omega_{0p}^2 \ll \lambda |\varphi|^2$. If this is so, one can solve the quantum initial value problem analytically in the approximation $\lambda = 0$ for $t \leq t_0$ with $t_- < t_0 < t_+$. At time $t_0$ we switch to a classical simulation since occupation numbers (of the low momentum modes) have grown sufficiently large. As matching conditions we impose that the one- and two-point functions with subtracted vacuum fluctuations, are reproduced in the ensemble of classical initial conditions.

Using the $\lambda = 0$ solution, we can compute the one- and two-point functions, $\langle \varphi_p \rangle = \langle \pi_p \rangle = 0$, $\langle |\varphi_p|^2 \rangle$ and $\langle |\pi_p|^2 \rangle$. The two-point functions contain contributions from vacuum fluctuations which we would like to subtract. Even though
the quench model at early times is clearly far out of equilibrium, we nonetheless use the following equilibrium relations to define the (time dependent) particle energy $\omega_p$ and number density $n_p$,
\[
\langle |\varphi_p|^2 \rangle = (n_p + \frac{1}{2})/\omega_p, \quad \langle |\pi_p|^2 \rangle = (n_p + \frac{1}{2})\omega_p.
\]

In this way we identify the contribution from vacuum fluctuations by the $\frac{1}{2}$ in these relations. To switch to classical dynamics, we specify a gaussian ensemble of classical fields at $t = t_0$ with
\[
\langle |\varphi_p|^2 \rangle = n_p/\omega_p \quad \text{and} \quad \langle |\pi_p|^2 \rangle = n_p\omega_p.
\]
Even though the analytical calculation gives a tail $n_p \propto 1/p^4$ for large momenta, shall make the further simplification that $n_p = 0$ for the $|p| > \mu$.

For comparison we shall also show results, still using classical dynamics, but using the customary initial ensemble that includes vacuum fluctuations, $n_p \rightarrow n_p + \frac{1}{2}$. In this case one might argue that the coupling constants need to be renormalized, and that somehow the effect of the vacuum fluctuations should be subtracted. As this is a classical theory which is far from equilibrium, it is not clear how to implement such a renormalization in a consistent way.

Finally we use the Hartree ensemble approximation to compute the dynamics. Now we must specify initial conditions for the mean fields and for the mode functions. In order to be as close to classical dynamics as possible, we choose an ensemble of initial conditions, in which the mean fields have the same distribution as the classical fields above at time $t_0$. Vacuum fluctuations are represented by the mode functions, which we choose as plane waves. We refer to ref. [1] for further details of the Hartree ensemble method.

2. Thermalization

In order to study the effect of the different initial conditions, we monitor the thermalization process. Hence we plot the time dependence of the particle number density which, for classical fields, is defined as in [2] but without subtracting the $\frac{1}{2}$, $n_p = (\langle |\varphi_p|^2 \rangle / \langle |\pi_p|^2 \rangle)^{1/2}$. In Figs. 1–3 we show log(1 + 1/n), which is linear in $\omega$ for a Bose-Einstein distribution. We switch from the analytical solution to the numerical method at $t_0m = 0.6$; the results do not change when this time is chosen differently, provided it stays in the range $0.2 \leq t_0m \leq 2$.

In Fig. 1 we use classical dynamics with the customary initial conditions including high momentum vacuum fluctuations, as in ref. [2]. At very early time $tm = 5 - 10$, one recognizes the unstable modes from the large values of $n$ at $\omega < 0.5$. Also the vacuum fluctuations are clearly visible, since they imply that $n \approx \frac{1}{2}$ or log(1 + 1/n) $\approx 1.1$.

At later times modes with larger momenta thermalize with a classical distribution, indicated by the curved line $n_p = T/\omega_p$. Eventually, at $tm > 3000$ all modes have thermalized and the corresponding temperature has become unphysically large. The temperature we obtain from fitting the (low $\omega$) part of the spectrum, is plotted in Fig. 1. After an initial decrease one clearly sees the unphysical rising of the temperature for $tm > 75$.

Next we use the new initial conditions, which do not include vacuum fluctuations. As can be seen in Fig. 2, the low-momentum modes at early times behave similarly to the previous case. But now the number density is exponentially suppressed for large momenta. At larger times we see that the distribution gradually moves towards a classical shape, but this happens much more slowly than in Fig. 1.

The lack of spurious vacuum energy in the simulation of Fig. 2 also has a pronounced effect on
the temperature we obtain by fitting \( n \) against \( T/\omega \) for low \( \omega \). Now the initial temperature drop continues, as energy continues to dissipate from the low momentum modes towards higher momenta.

Finally we use the Hartree ensemble method to compute the field dynamics. For increasing time, more and more modes thermalize and align towards a Bose-Einstein distribution. At the largest time that we simulated, \( t_m = 3000 \) the particle numbers follow a BE distribution over a significant range of energies.

The temperature, obtained from fitting the low-momentum part of the spectrum with a BE-distribution, is shown in Fig. 4. At very early times, \( t < 50 \), the behavior appears to be the same as in the previous classical simulations. At later times the temperature decreases very slowly, much more slowly than with the classical dynamics. This is understandable because the particle number densities at high momenta remain exponentially suppressed.

3. Conclusion

Using vacuum fluctuations as seeds for subsequent classical dynamics has to be done with care. The straightforward way, choosing an initial classical ensemble that reproduces the quantum two-point functions, leads to misleading results at late times: the temperature of low-energy particles that equilibrate keeps rising and will eventually reach an unphysical value \( T \propto 1/a \). We have further demonstrated that the new prescription for initial conditions gives quite reasonable results, both when used with classical and with Hartree ensemble dynamics.

REFERENCES

1. M. Sallé, J. Smit and J.C. Vink, Phys.Rev. D64 (2001) 025016, hep-ph/0012346 and hep-ph/0012362.

2. S. Yu. Khlebnikov and I.I. Tkachev, Phys.Rev.Lett. 77 (1996) 219; Phys.Lett. B390 (1997) 80; Phys.Rev.Lett. 79 (1997) 1607; G. Felder and L. Kofman, Phys.Rev. D63 (2001) 103503; G. Felder, L. Kofman and A. Linde, hep-th/0106179; G. Felder, J. Garcia-Bellido, P.B. Green, L. Kofman; A. Linde and I. Tkachev, Phys.Rev.Lett. 87 (2001) 011601; A. Rajantii and E.J. Copeland, Phys.Rev.Lett. 85 (2000) 916;