Finite Temperature Simulations from Quantum Field Dynamics?

Mischa Sallé, Jan Smit and Jeroen C. Vink

Institute for Theoretical Physics, University of Amsterdam
Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

We describe a Hartree ensemble method to approximately solve the Heisenberg equations for the $\varphi^4$ model in $1+1$ dimensions. We compute the energies and number densities of the quantum particles described by the $\varphi$ field and find that the particles initially thermalize with a Bose-Einstein distribution for the particle density. Gradually, however, the distribution changes towards classical equipartition. Using suitable initial conditions quantum thermalization is achieved much faster than the onset of this undesirable equipartition. We also show how the numerical efficiency of our method can be significantly improved.

1. Hartree ensemble approximation

Non-perturbative equilibrium properties of quantum field theories are studied with great success using numerical lattice techniques. Similarly one would like to investigate quantum field dynamics non-perturbatively. This has obvious applications to e.g. heavy ion collisions and early universe physics. Furthermore, it could be used to study equilibrium properties in cases where Monte Carlo methods do not work, such as in QCD at finite density or chiral gauge theories.

Using Monte Carlo techniques to compute the Minkowski time path integral is, of course, not possible. Neither can one directly solve the Heisenberg equations for the quantum field operators. Hence one has to resort to approximations, such as classical dynamics \cite{2} (for recent work see \cite{3}), large $n$ or Hartree (see e.g. \cite{4}). Here we discuss a different type of Hartree or gaussian approximation than used previously, in which we use an ensemble of gaussian wavefunctions to compute Green functions. Ref. \cite{1} also contains a discussion of this method and a detailed presentation will appear elsewhere.

We use the lattice $\varphi^4$ model in $1+1$ dimensions as a test model, which has the following Heisenberg operator equations,

$$\dot{\varphi}_x = \pi, \quad \dot{\pi}_x = (\Delta - \mu^2)\varphi - \lambda\varphi^3,$$

where $\Delta$ the lattice laplacian, $\mu$ the bare mass parameter and $\lambda$ the coupling constant (we use lattice units $a = 1$). The Hartree approximation assumes that the wavefunction used to compute the Green functions is of gaussian form, such that the field operator can be written as

$$\hat{\varphi}_x = \varphi_x + \sum_\alpha [f^\alpha_x \hat{a}_\alpha + f^{*\alpha}_x \hat{a}^\dagger_\alpha],$$

with $\hat{a}_\alpha$ and $\hat{a}^\dagger_\alpha$ time-independent creation and annihilation operators and time-dependent mean field $\varphi$ and mode functions $f^\alpha$. All information is contained in the one- and two-point functions, which can be expressed (for gaussian pure states) as

$$\langle \hat{\varphi}_x \rangle = \varphi_x, \quad \langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}} = \sum_\alpha f^\alpha_x f^{*\alpha}_y.$$

The mode functions represent the width of the wave function, allowing for quantum fluctuations around the mean field. With Hartree dynamics we therefore expect to improve the classical dynamics. Of course we cannot expect to capture all quantum effects, e.g. tunneling is beyond the scope of the gaussian approximation.

The Heisenberg equations \cite{4} provide self-consistent equations for the mean field $\varphi$ and the mode functions $f^\alpha$,

$$\dot{\varphi}_x = \Delta \varphi_x - [\mu^2 + \lambda(\varphi^2_x + 3 \sum_\alpha f^\alpha_x f^{*\alpha}_x)]\varphi_x,$$

$$\dot{f}^\alpha_x = \Delta f^\alpha_x - [\mu^2 + \lambda(3\varphi^2_x + 3 \sum_\alpha f^\alpha_x f^{*\alpha}_x)]f^\alpha_x$$

with $\Delta$ the lattice laplacian, $\mu$ the bare mass parameter and $\lambda$ the coupling constant (we use lattice units $a = 1$). The Hartree approximation assumes that the wavefunction used to compute the Green functions is of gaussian form, such that the field operator can be written as

$$\hat{\varphi}_x = \varphi_x + \sum_\alpha [f^\alpha_x \hat{a}_\alpha + f^{*\alpha}_x \hat{a}^\dagger_\alpha],$$

with $\hat{a}_\alpha$ and $\hat{a}^\dagger_\alpha$ time-independent creation and annihilation operators and time-dependent mean field $\varphi$ and mode functions $f^\alpha$. All information is contained in the one- and two-point functions, which can be expressed (for gaussian pure states) as

$$\langle \hat{\varphi}_x \rangle = \varphi_x, \quad \langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}} = \sum_\alpha f^\alpha_x f^{*\alpha}_y.$$

The mode functions represent the width of the wave function, allowing for quantum fluctuations around the mean field. With Hartree dynamics we therefore expect to improve the classical dynamics. Of course we cannot expect to capture all quantum effects, e.g. tunneling is beyond the scope of the gaussian approximation.
In order to simulate a more general density matrix instead of the pure gaussian state assumed in eq. (3), we average over a suitable ensemble of Hartree realizations by specifying different initial conditions and/or coarsening in time. In this way we compute Green functions with a non-gaussian density matrix \( \hat{\rho} \), as

\[
\langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}} = \sum_i p_i [\langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}} + \varphi_x^{(i)} \varphi_y^{(i)}] - (\sum_i p_i \varphi_x^{(i)})(\sum_j p_j \varphi_y^{(j)}).
\]

It should be stressed that for typical Hartree realizations the mean field \( \varphi_x \) is inhomogeneous in space. This is different from the ensemble average of \( \hat{\varphi} \) which may, of course, be homogeneous. We also note that the equations (4) can in fact be derived from a hamiltonian. Since the equations are also strongly non-linear, this suggests that the system will evolve to an equilibrium distribution with equipartition of energy, as in classical statistical physics.

2. Observables

To assess the viability of our Hartree ensemble approximation, we solve the equations (4) starting from a number of initial conditions. We compute the particle number densities and energies from the connected two-point functions of \( \varphi \) and \( \pi \), after coarse-graining in space and time and averaging over initial conditions,

\[
\frac{1}{N} \sum_{x,z} e^{-ikz} \langle \varphi_{x+z} \varphi_x \rangle_{\text{conn}} = \frac{n_k + \frac{1}{2}}{\omega_k},
\]

(6)

\[
\frac{1}{N} \sum_{x,z} e^{-ikz} \langle \pi_{x+z} \pi_x \rangle_{\text{conn}} = (n_k + \frac{1}{2})\omega_k.
\]

(7)

The over-bar indicates averaging over some time-interval and initial conditions as in eq. (3), \( \omega_k \) is the energy, \( n_k \) the (number) density of particles with momentum \( k \) and \( N \) the number of lattice sites.

For weak couplings, such as we will use in our numerical work, the particle densities should have a Bose-Einstein (BE) distribution,

\[
n_k = 1/(e^{\omega_k/T} - 1), \quad \omega_k^2 = m^2(T) + 2 - 2 \cos(k),
\]

(8)

Figure 1. Particle number densities as a function of \( \omega \) at various times. The straight line gives a BE distribution with temperature \( T/m = 1.7 \). (The lattice volume \( Lm = 32 \), coupling \( \lambda/m^2 = 0.083 \) and inverse lattice spacing \( 1/am = 8 \); \( m \equiv m(T = 0) \).)

with \( T \) the temperature and \( m(T) \) an effective finite temperature mass. We have verified that this is indeed the case using Monte Carlo simulations of the euclidian time version of the model.

3. Numerical results

First we use initial conditions which correspond to fields far out of equilibrium: gaussians with mean fields that have just a few low momenta modes,

\[
\varphi_x = v, \quad \pi_x = A \sum_j \cos(k_j x + \alpha_j).
\]

(9)

The \( \alpha_j \) are random phases and the \( A \) is a suitable amplitude. Initially the mode functions are plane waves, \( e^{ikx}/\sqrt{2\omega L} \), such that all energy resides in the mean field.

The results in Fig. 1 show that fast, well before \( tm \approx 200 \), a BE distribution is established for particles with low momenta. Slowly this thermalization progresses to particles with higher momenta, while the temperature \( T \approx 1.7m \) remains roughly constant. Such a thermalization does not happen when using a single Hartree realization with a homogeneous mean field \( \varphi \). The difference may be understood, because particles in our method can scatter via the inhomogeneities in the mean field.
Next we want to speed-up the thermalization of the high momentum modes. Therefore we use different initial conditions in which the energy is distributed more realistically over the Fourier modes of the mean field. The modes are the same as before but mean fields are drawn from an ensemble with a BE-like probability distribution,

\[ p(\varphi_k, \pi_k) \propto \exp\left[-(e^{\omega_k/T_0} - 1)(\pi_k^2 + \omega_k^2 \varphi_k^2)/2\omega_k\right]. \]  

(10)

We also want to probe large time scales, which were not yet reached in the weak coupling simulation of fig. 1.

Fig. 2a shows the particle density computed without the mean field part in eq. (6). Already at \( tm = 20 \) a credible BE distribution has established, with a temperature that increases until it saturates at \( T \approx 1.0 m \) at \( tm = 100 \) (\( T = 0 \) at \( t = 0 \)). Fig. 2b shows the densities at \( tm = 100 \), now with the mean field contribution included. The straight line is a BE distribution at \( T \approx 1.01 m \).

At very large times, Fig. 2c, the BE distribution persists in the large \( \omega \) region, albeit with a slightly higher temperature \( T \approx 1.14 m \), but for small \( \omega \) one clearly sees deviations. The particle densities here can be fitted rather well with the classical form \( n = T cl/\omega \) (dashed curve). The corresponding classical temperature slowly decreases, as energy disperses more and more to the large momentum modes. It is remarkable that the “decay time” of this temperature is some two orders of magnitude larger than the warming-up time shown in Fig. 2a.

Finally, in Fig. 3 we show data for a large time \( tm \approx 25000 \) and at a higher (initial) temperature, \( T_0 = 5 m \). Here equipartition has extended to all modes with \( \omega < \sim 12 m \), as is evident from the accuracy of the fitted curve \( n = 1.9 m/\omega \) (dashed line).

Even though the timescales of relaxation to a BE distribution and relaxation to classical equipartition appear to be widely separated, the simulations of Fig. 2 could not easily be used to study finite temperature equilibrium physics: only around \( tm = 100 - 200 \) there may be a window in which the fields have thermalized to a BE distribution, without significant deviations due to the up coming classical equipartition. To increase such a window we did a simulation at weaker coupling and higher temperature. Now we find density distributions as shown in Fig. 4. Already af-
Figure 4. Particle number densities as a function of $\omega$, starting from BE type initial conditions. The straight line through the origin is a BE distribution with temperature $T/m = 6.7$. ($Lm = 23$, $\lambda/m^2 = 0.083$ and $1/am = 22$).

After a relatively short time, before $tm \approx 100$, the particles have acquired a BE distribution up to large momenta $\omega/m \approx 12$. Note that even with the BE-type initial conditions, the fields initially are out of equilibrium: energy is initially carried by the mean field only but within a time span of $tm \approx 200$ it is redistributed over the modes.

Finally we try to improve the efficiency of our method. Since we have to solve for $N$ mode functions, on a lattice with $N$ sites, the CPU time for one time-step grows $\propto N^2$. However, mode functions corresponding to particles with momenta much larger than $T$ should be irrelevant, since these particle densities are exponentially suppressed. This suggests that we can discard such modes. This is tested in Fig. 5, where we compare simulation results using all mode functions with results obtained using only a quarter of the mode functions. This corresponds with mode functions with initial plane wave energy $\omega \lesssim 17m$. Clearly the results for particles with significant densities $n$ are indistinguishable. For particles with energy larger than $\approx 17m$, there are no longer mode functions that can provide the vacuum fluctuations and consequently the particle density defined by (7) drops to $-1/2$.

4. Conclusion

Using a Hartree ensemble method, we have demonstrated that we can simulate approximate quantum thermalization in a weakly coupled scalar field model in real time. Only after times much longer than typical equilibration times, the approximate nature of the dynamics shows up in deviations from the BE distribution towards classical equipartition. We have furthermore found that these simulations can be done efficiently using a limited number of mode functions.

REFERENCES

1. M. Sallé, J. Smit and J.C. Vink, in proceedings of SEWM2000, hep-ph/0009120.
2. D. Grigoriev and V. Rubakov, Nucl. Phys. B299 (1988) 67.
3. G. Aarts, G.F. Bonini and C. Wetterich, hep-ph/0003262, hep-ph/0007357.
4. B. Mihaila, T. Athan, F. Cooper, J. Dawson and S. Habib, hep-ph/0003103.