Real time quantum field theory on a computer: The Hartree ensemble approximation
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In this chapter we will introduce the Hartree approximation, applied to the $\lambda \varphi^4$ model. We will discuss the equilibrium states using the effective potential and calculate the full quantum equilibrium state using a Monte Carlo simulation.

In order to describe the equilibration behaviour, we need to resort to approximations, of which on the one hand the classical and on the other hand the large $n$ and Hartree are the most commonly used. In order to study quantum equilibration, one is forced to use one of the latter two. To prevent subtleties with would-be Goldstone bosons, we only consider the Hartree approximation.

When using homogeneous initial conditions, Hartree (Gaussian) dynamical approximations are known to have problems with thermalization, because of insufficient scattering. We attempt to improve on this by writing an arbitrary density matrix as a superposition of Gaussian pure states and applying the Hartree approximation to each member of such an ensemble. Particles can then scatter via their back-reaction on the typically inhomogeneous mean fields.

We will numerically study this Hartree ensemble approximation, starting from initial states which are far from equilibrium and numerically compute the time evolution of particle distribution functions. We will see that they do indeed display approximate thermalization on intermediate time scales by approaching a Bose-Einstein (BE) form. However, for very large times the distributions drift towards classical-like equipartition. We will study a very small system at strong coupling for a long period of time in order to obtain the final equilibrium distribution.
2.1 GAUSSIAN APPROXIMATION

We will study the $\lambda \varphi^4$ theory, which has the following action\(^1\)

$$\mathcal{L} = -\partial_\mu \varphi \partial^\mu \varphi - \frac{1}{2} \mu^2 \varphi^2 - \frac{1}{4} \lambda \varphi^4, \quad (2.1)$$

resulting in the following Heisenberg field equation for the quantum field at times $x^0 > 0$,

$$(-\partial^2 + \mu^2)\hat{\varphi}(x) + \lambda \hat{\varphi}(x)^3 = 0. \quad (2.2)$$

For exact evaluation we would have to specify the infinite set of matrix elements of $\hat{\varphi}(x,0)$ and $\partial_0 \hat{\varphi}(x,0)$ as initial conditions. In practise, of course, less detail is needed. Taking the expectation value in an initial state at time $x^0 = 0$ leads to

$$\langle \hat{\varphi}(x) \rangle = \varphi(x), \quad (2.3a)$$

$$\langle T\hat{\varphi}(x_1)\hat{\varphi}(x_2) \rangle = \varphi(x_1)\varphi(x_2) - iG(x_1, x_2), \quad (2.3b)$$

$$\langle T\hat{\varphi}(x_1)\hat{\varphi}(x_2)\hat{\varphi}(x_3) \rangle = \varphi(x_1)\varphi(x_2)\varphi(x_3) - i\varphi(x_1)G(x_2, x_3) + 2 \text{ perm.}$$

$$+ (-i)^2 G(x_1, x_2, x_3), \quad (2.3c)$$

$$\langle T\hat{\varphi}(x_1)\cdots\hat{\varphi}(x_4) \rangle = \varphi(x_1)\cdots\varphi(x_4) - i\varphi(x_1)\varphi(x_2)G(x_3, x_4) + 6 \text{ perm.}$$

$$+ \varphi(x_1)(-i)^2 G(x_2, x_3, x_4) + 3 \text{ perm.}$$

$$+ (-i)^2 G(x_1, x_2)G(x_3, x_4) + 2 \text{ perm.}$$

$$+ (-i)^3 G(x_1, \ldots, x_4), \quad (2.3d)$$

etc. Here $T$ denotes time ordering and

$$\langle \hat{\varphi}(x_1)\cdots\hat{\varphi}(x_n) \rangle \equiv \text{Tr} \hat{\varphi}(x_1)\cdots\hat{\varphi}(x_n), \quad (2.4)$$

where $\hat{\rho}$ is the initial density operator; $\varphi$ is the mean field (or classical field) and the $G$’s are correlation functions (connected Green functions). Taking the expectation value of (2.2) and neglecting the three point correlation function $G(x, x, x)$ gives the approximate equation

$$[-\partial^2 + \mu^2 + \lambda \varphi(x)^2 - 3i\lambda G(x, x)]\varphi(x) = 0. \quad (2.5)$$

To use it we need an equation for the two-point function. Such an equation can be found by multiplying (2.2) by $\hat{\varphi}(y)$ and taking again the expectation value in the initial state. This leads to the approximate equation

$$[-\partial^2 + \mu^2 + 3\lambda \varphi(x)^2 - 3i\lambda G(x, x)]G(x, y) = \delta^4(x - y), \quad (2.6)$$

\(^1\)Throughout this thesis I will use the metric $g_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$, in this section we assume 3+1 dimensions.
where we used the canonical commutation relations and dropped the three and four-point correlation functions. We shall comment on their neglect at the end of this section. Since only the two-point function appears, equations (2.5), (2.6) are exact if the Hamiltonian and density matrix are approximated by Gaussian forms. Given the neglect of the higher correlation functions the initial density matrix does not have to be Gaussian \textit{per se}, but its non-Gaussianity does not enter in eqs. (2.5), (2.6). For clarity we shall now assume the \textit{bra-kets} $\langle \cdots \rangle$ to refer to a Gaussian density operator $\hat{\rho}$. Later we will consider non-Gaussian operators by further averaging over initial conditions, as in (1.5), which will be indicated by $\langle \cdots \rangle$.

An intuitive as well as practical way of computing the two-point function, is in terms of mode functions $f_{\alpha}(x)$. We write

\[-iG(x,y) = \theta(x^0 - y^0)C(x,y) + \theta(y^0 - x^0)C(y,x), \quad (2.7)\]

such that

\[C(x,y) = \langle [\hat{\phi}(x) - \varphi(x)][\hat{\phi}(y) - \varphi(y)] \rangle. \quad (2.8)\]

It follows from (2.6) that $C(x,y)$ satisfies the homogeneous equation (i.e. $\delta^4(x - y) \to 0$), in the variable $x$ as well as in $y$, as if $\hat{\phi}(x) - \varphi(x)$ satisfies this equation. We can now introduce mode functions $f_{\alpha}(x)$, satisfying the homogeneous equation

\[-\partial^2 + \mu^2 + 3\lambda \varphi(x)^2 + 3\lambda C(x,x)] f_{\alpha}(x) = 0, \quad (2.9)\]

$(-iG(x,x) = C(x,x))$ and write:

\[\hat{\phi}(x) \overset{\text{g.a.}}{=} \varphi(x) + \sum_{\alpha} [\hat{b}_{\alpha} f_{\alpha}(x) + \hat{b}^\dagger_{\alpha} f^*_{\alpha}(x)]. \quad (2.10)\]

where the $\hat{b}_{\alpha}$ and $\hat{b}^\dagger_{\alpha}$ are spacetime independent and “g.a.” means “Gaussian approximation”. The wave equation (2.9) for the $f_{\alpha}$ is of the Klein-Gordon type and we require the mode functions to be orthogonal and complete in the Klein-Gordon sense (using finite volume notation),

\[
\begin{aligned}
\int d^3x \ [f^*_{\alpha}(x) i\partial_0 f_{\beta}(x) - i\partial_0 f^*_{\alpha}(x)f_{\beta}(x)] &= \delta_{\alpha\beta}, \\
\int d^3x \ [f_{\alpha}(x) i\partial_0 f_{\beta}(x) - i\partial_0 f_{\alpha}(x)f_{\beta}(x)] &= 0, \\
\sum_{\alpha} [-if_{\alpha}(x) \partial_0 f^*_{\alpha}(y) + if^*_{\alpha}(x) \partial_0 f_{\alpha}(y)]_{x^0 = y^0} &= \delta^3(x - y), \\
\sum_{\alpha} [f_{\alpha}(x)f^*_{\alpha}(y) - f^*_{\alpha}(x)f_{\alpha}(y)]_{x^0 = y^0} &= 0, \\
\sum_{\alpha} [\partial_0 f_{\alpha}(x) \partial_0 f^*_{\alpha}(y) - \partial_0 f^*_{\alpha}(x)\partial_0 f_{\alpha}(y)]_{x^0 = y^0} &= 0.
\end{aligned}
\]
The above orthogonality and completeness relations are preserved by the equation of motion (2.9) for the \( f_\alpha \). The canonical commutation relations for \( \hat{\phi} \) and \( \partial_0 \hat{\phi} \) translate into
\[
[\hat{b}_\alpha, \hat{b}^\dagger_\beta] = \delta_{\alpha\beta}, \quad [\hat{b}_\alpha, \hat{b}_\beta] = [\hat{b}^\dagger_\alpha, \hat{b}^\dagger_\beta] = 0. \tag{2.12}
\]
The initial condition implies \( \langle \hat{b}_\alpha \rangle = 0 \) and we have to specify \( E_{\alpha\beta} \equiv \langle \hat{b}_\alpha \hat{b}_\beta \rangle \) and \( N_{\alpha\beta} \equiv \langle \hat{b}^\dagger_\alpha \hat{b}^\dagger_\beta \rangle \). The matrices \( N \) and \( E \) are subject to constraints which follow from their definition as expectation values of operators in Hilbert space. We shall assume that a Bogoliubov transformation \( \hat{b}_\alpha \rightarrow \sum_\beta [A_{\alpha\beta} \hat{b}_\beta + B_{\alpha\beta} \hat{b}^\dagger_\beta] \) can be made such that \( E_{\alpha\beta} \rightarrow 0 \) and \( N_{\alpha\beta} \propto \delta_{\alpha\beta} \). This transformation produces new mode functions which are linear combinations of the \( f \) and \( f^\ast \). In the new basis we only have to specify as initial conditions
\[
\langle \hat{b}^\dagger_\alpha \hat{b}_\beta \rangle \equiv n^0_\alpha \delta_{\alpha\beta}, \quad n^0_\alpha \geq 0, \tag{2.13}
\]
in terms of which
\[
C(x, y) = \sum_\alpha [(1 + n^0_\alpha) f_\alpha(x)f^\ast_\alpha(y) + n^0_\alpha f^\ast_\alpha(x)f_\alpha(y)]. \tag{2.14}
\]
Equation (2.10) expresses the fact that in the Gaussian approximation the field \( \phi'(x) \equiv \phi(x) - \varphi(x) \) is a generalised free field, i.e. its correlation functions are completely determined by the two-point function. Its linear field equation (i.e. (2.9) with \( f_\alpha \rightarrow \phi' \)) is equivalent to the Heisenberg equations of motion of the effective Gaussian Hamiltonian operator
\[
\hat{H}_{g.a.} = \int d^3x \left[ \frac{1}{2} \hat{\phi}'^2 + \frac{1}{2} (\nabla \phi')^2 + \frac{1}{2} m^2_{\text{eff}} \phi'^2 + \epsilon_{\text{eff}} \right], \tag{2.15}
\]
where the spacetime dependent effective mass \( m^2_{\text{eff}} \) is given by
\[
m^2_{\text{eff}}(x) = 3\lambda \varphi(x)^2 + 3\lambda C(x, x). \tag{2.16}
\]
We also introduced an effective c-number energy density \( \epsilon_{\text{eff}} \), which is determined by requiring \( \langle \hat{H}_{g.a.} \rangle = \langle \hat{H} \rangle \):
\[
\epsilon_{\text{eff}}(x) = \frac{1}{2} \pi(x)^2 + \frac{1}{2} [\nabla \varphi(x)]^2 + \frac{1}{2} \mu^2 \varphi(x)^2 + \frac{1}{4} \lambda \varphi(x)^4 - \frac{3}{4} \lambda C(x, x)^2. \tag{2.17}
\]
Summarising, the Gaussian approximation consists of the equations (2.5), (2.9), (2.13) and (2.14), together with the orthogonality and completeness conditions (2.11) for the mode functions and some initial condition for the mean field and mode.
\[-i \frac{\delta \Sigma}{\delta \phi} = \quad \quad + \quad \quad \]

Figure 2.1: Diagrammatic illustration of $\delta \Sigma/\delta \phi$, with $\Sigma$ the self-energy functional defined by $\Gamma = S - \Sigma$. The lines and full dots represent the exact propagators (correlation functions) and vertex functions, the other vertices represent the bare vertex functions as given by the classical action $S$.

\[-i \frac{\delta^2 \Sigma}{\delta \phi \delta \phi} = \quad \quad + \quad \quad + \cdots \]

Figure 2.2: Diagrams for the self-energy part of the inverse correlation function $G^{-1} = -\delta^2S/\delta \phi \delta \phi + \delta^2 \Sigma/\delta \phi \delta \phi$. The $\cdots$ represent the two-loop diagrams obtained by differentiating the diagrams in Fig. 2.1.

functions. For the sake of clarity we write down the equations of motion again, explicitly specifying space and time derivatives:

\[\ddot{\phi} = \Delta \phi - [\mu^2 + \lambda \phi^2 + 3\lambda C] \phi, \quad (2.18a)\]
\[\ddot{f}_\alpha = \Delta f_\alpha - [\mu^2 + 3\lambda \phi^2 + 3\lambda C] f_\alpha, \quad (2.18b)\]

with

\[C = \sum_\alpha (2n^0_\alpha + 1)|f_\alpha|^2, \quad n^0_\alpha = \langle \hat{b}^\dagger_\alpha \hat{b}_\alpha \rangle. \quad (2.18c)\]

The Gaussian approximation can be justified in the limit of large $n$ for the $O(n)$ model. The resulting field equations are very similar: we only need to make the replacement $3 \rightarrow 1$ in eqs. (2.5) and (2.9).

The above derivation in terms of the Heisenberg equations of motion can be put into the systematic framework of the Dyson-Schwinger hierarchy. These equations follow from functionally differentiating an exact equation of motion $\delta \Gamma/\delta \phi = -J$ with respect to $J$ and setting $J = 0$ afterwards. Here $\Gamma$ is the effective action (with time integration along the usual Keldysh-Schwinger contour) and $J$ an external source. We shall not go into details here, instead we just comment on the systematics, using diagrams (for a derivation, see for instance Ref. [46]). Fig. 2.1 illustrates
the exact equation for the mean field. The Gaussian approximation (2.5) is obtained by dropping the two-loop diagram. By differentiating the diagrams in Fig. 2.1 we get the exact equation for the two-point correlation function illustrated in Fig. 2.2. The Gaussian approximation (2.6) can be obtained from this by: a) dropping the two-loop contributions and b) dropping the second one-loop diagram. The neglect of the two-loop terms may be reasonable at weak coupling, and even the second approximation may be justifiable if the product of the three point couplings (one bare, the other dressed) is substantially smaller than the (bare) four point coupling in the first one-loop diagram. However, since the bare three point vertex \( \delta S/\delta \phi \propto \lambda \phi \), we see that this is not likely if \( \phi = O(\lambda^{-1/2}) \) or larger. Especially this second approximation b) is worrisome, because on iteration of the integral equations we would not get all one-loop diagrams correctly. It also has been established that the approximation does not give exact Goldstone bosons where one expects them, because the phase transition is incorrectly predicted to be first order, instead of second order (in 3+1 D) or a cross over (1+1 D). There is a problem with renormalization in 3+1 dimensions [47] (but not in 1+1 D).

It will depend on the circumstances if these troublesome features of the Hartree approximation are numerically important.

### 2.2 Effective Hamiltonian and Conserved Charges

The equations of the Gaussian approximation derived in Section 2.1 are local in time and they may be derived from a conserved effective Hamiltonian. We shall present it here and exhibit its symmetries and accompanying conserved charges. We write

\[
\begin{align*}
  f_\alpha(x) &= \frac{1}{\sqrt{2}} \left[ f_{\alpha 1}(x) - i f_{\alpha 2}(x) \right], \\
  \xi_{\alpha a}(x) &= \left( \frac{1}{2} + n_0^a \right)^{1/2} f_{\alpha a}(x), \quad a = 1, 2. \\
  \eta_{\alpha a}(x) &= \partial_0 \xi_{\alpha a}(x), \quad \pi(x) = \partial_0 \phi(x).
\end{align*}
\]

In terms of the real canonical variables \( \phi, \pi, \xi_{\alpha a} \) and \( \eta_{\alpha a} \) the effective Hamiltonian takes the form

\[
H_{\text{eff}} = \int d^3x \left[ \frac{1}{2} \left( \pi^2 + \eta^2 + (\nabla \phi)^2 + (\nabla \xi)^2 \right) + \frac{1}{2} \mu^2 \left( \phi^2 + \xi^2 \right) + \frac{1}{4} \lambda \left( \phi^4 + 6\phi^2 \xi^2 + 3(\xi^2)^2 \right) \right],
\]

(2.22)
where
\[ \xi^2 = \sum_\alpha \left( \xi_{\alpha 1}^2 + \xi_{\alpha 2}^2 \right), \tag{2.23a} \]
\[ (\nabla \xi)^2 = \sum_\alpha \left[ (\nabla \xi_{\alpha 1})^2 + (\nabla \xi_{\alpha 2})^2 \right], \tag{2.23b} \]
\[ \eta^2 = \sum_\alpha \left( \eta_{\alpha 1}^2 + \eta_{\alpha 2}^2 \right). \tag{2.23c} \]

It is easy to check that the mean field equation (2.5) and the mode equations (2.9) are equivalent to the Hamilton equations
\[ \partial_0 \varphi = \pi, \quad \partial_0 \pi = -\frac{\delta H_{\text{eff}}}{\delta \varphi}, \quad \partial_0 \xi_{\alpha a} = \eta_{\alpha a}, \quad \partial_0 \eta_{\alpha a} = -\frac{\delta H_{\text{eff}}}{\delta \xi_{\alpha a}}. \tag{2.24} \]

It is also straightforward to show that \( H_{\text{eff}} \) is just the expectation value of the quantum Hamiltonian
\[ \hat{H}(t) = \int d^3x \left[ \frac{1}{2} \dot{\varphi}^2 + \frac{1}{2} (\nabla \varphi)^2 + \frac{1}{2} \mu^2 \varphi^2 + \frac{1}{4} \lambda \varphi^4 \right], \tag{2.25} \]
upon inserting the Gaussian approximation (2.10),
\[ H_{\text{eff}} = \langle \hat{H} \rangle. \tag{2.26} \]

The effective Hamiltonian has evidently a large symmetry, corresponding to rotations of the infinite dimensional vectors \( \xi_{\alpha a} \) and \( \eta_{\alpha a} \). For definiteness, let us assume a regularisation of the field theory such that there are \( M \) modes, \( \alpha = 1, \ldots, M \) (e.g. on an \( N^3 \) periodic lattice \( M = N^3 \)). Then the effective Hamiltonian has \( O(2M) \) symmetry, implying \( M(2M - 1) \) conserved generalised angular momenta of the general form
\[ L_{\alpha \alpha', \beta \beta'} = \int d^3x \left( \xi_{\alpha a} \eta_{\beta b} - \xi_{\beta b} \eta_{\alpha a} \right), \quad (\alpha, a) \neq (\beta, b). \tag{2.27} \]

Recalling the orthonormality relations for the mode functions, (2.11a) and (2.11b), we see that the conserved quantities are given in terms of the initial conditions as
\[ L_{\alpha 1, \alpha 2} = \frac{1}{2} + \eta_\alpha^0, \tag{2.28} \]
with all others vanishing.

It is interesting to compare with the effective Hamiltonian corresponding to the large \( n \) limit of the \( O(n) \) model [48], which may be obtained from \( H_{\text{eff}} \) above by the
replacing $3 \rightarrow 1$ (and $6 \rightarrow 2$). This has the effect of producing the combination $\lambda(\varphi^2 + \xi^2)^2$, so the symmetry enlarges to $O(2M+1)$. The additional $2M$ conserved generalised angular momenta depend on the initial conditions for $\varphi$ and $\pi$.\footnote{In \cite{48} the effective Hamiltonian for the homogeneous system was expressed in terms of the radial variable $\xi_\alpha = (\xi_{\alpha 1}^2 + \xi_{\alpha 2}^2)^{1/2}$ (modulo a factor of two), and the rotational symmetries mixing $\xi_{\alpha 1}$ and $\xi_{\alpha 2}$ are then absent. However, the corresponding equations of motion then suffer from numerical complications due to the angular momentum barriers.}

### 2.3 Equilibrium States

In a first exploration of the system and of the Gaussian approximation we study equilibrium states, i.e. stationary states with maximum entropy. This will give information on the phase structure and quasi-particle excitations as a function of temperature. From now on we will restrict to 1+1 dimensions, $x^\mu \rightarrow (t, x)$, and assume the system to be confined to a “volume” $L$ with periodic boundary conditions. The coupling $\lambda$ needs no renormalization while the bare mass parameter $\mu^2$ is only logarithmically divergent in the implicit cutoff.

We assume the equilibrium states to be homogeneous and time-independent, i.e. $\varphi(t, x) = v$ and $C(t; x; t; y) = C(0, x - y; 0, 0)$. Also the various time derivatives of $C$ evaluated at equal times are assumed to be time-independent. We shall seek solutions of the form (2.14) in which the mode functions are plane waves,

$$\varphi(t, x) = v, \quad f_k(t, x) = \frac{e^{ikx} - i\omega_k t}{\sqrt{2\omega_k L}}. \quad \text{(2.29a)}$$

Here the label $\alpha$ has become the wave number $k$ and we write $n_k$ for the corresponding (time independent) occupation numbers. With this ansatz the equations for the mean field and mode functions reduce to

\begin{align*}
(\mu^2 + 3\lambda C + \lambda v^2)v &= 0, \quad \text{(2.30)} \\
-\omega_k^2 + k^2 + \mu^2 + 3\lambda C + 3\lambda v^2 &= 0, \quad \text{(2.31)}
\end{align*}

where $C = C(t, x; t, x)$ is time-independent. In the infinite volume limit it is given by

$$C = \int \frac{dk}{2\pi} \left( n_k + \frac{1}{2} \right) \frac{1}{\omega_k}. \quad \text{(2.32)}$$

It follows that

$$\omega_k^2 = m^2 + k^2, \quad m^2 = \mu^2 + 3\lambda C + 3\lambda v^2. \quad \text{(2.33)}$$
To determine the $n_k$ we maximise the entropy $S$ subject to the constraint of fixed energy $U \equiv H_{\text{eff}} = E$, i.e. maximise $S + \beta (E - U)$, with Lagrange multiplier $\beta$. We shall write these equations in terms of the densities $s = S/L$, $u = U/L$, $\epsilon = E/L$ with $L \to \infty$. The (unrenormalized) energy density $u$ is given by

$$u = H_{\text{eff}}/L = \frac{1}{2} \mu^2 v^2 + \frac{1}{4} \lambda v^4 + \int \frac{dk}{2\pi} \left( n_k + \frac{1}{2} \right) \left( \frac{\omega_k^2 + k^2 + \mu^2 + 3\lambda v^2}{2\omega_k} + \frac{3}{4} \lambda C^2 \right),$$

and for our Gaussian density operator, $s$ can be written as

$$s = -\frac{1}{L} \text{Tr} \rho \log \rho = \int \frac{dk}{2\pi} \left[ (n_k + 1) \log (n_k + 1) - n_k \log n_k \right].$$

The maximisation equations read

$$0 = \frac{\delta [s + \beta (\epsilon - u)]}{\delta n_k} = \log \left( \frac{n_k + 1}{n_k} \right) - \beta \omega_k, \quad u = \epsilon,$$

with the solution

$$n_k = \frac{1}{e^{\beta \omega_k} - 1}$$

and $\beta$ such that $u = \epsilon$. So we found equilibrium states of the Hartree evolution corresponding to the Bose-Einstein distribution with temperature $T = \beta^{-1}$. All effects of the interaction are buried in the temperature dependent mass $m$ introduced in (2.33).

For simplicity of discussion, let us next use a simple momentum cutoff $|k| < \Lambda$ and define a renormalized mass parameter $\mu^2_r$ by combining the logarithmically divergent vacuum value of the mode sum (2.32) at the point $m^2 = \lambda$ with the bare mass parameter $\mu^2$:

$$\mu^2_r = \mu^2 + 3\lambda C (m^2 = \lambda, n_k = 0).$$

To leading order, $\mu^2_r$ is given by

$$\mu^2_r = \mu^2 + \frac{3\lambda}{4\pi} \log \frac{4\Lambda^2}{\lambda}.$$

and (2.33) takes the renormalized form

$$m^2 = \mu^2_r + \frac{3\lambda}{4\pi} \log \frac{\lambda}{m^2} + 3\lambda \int_0^\infty \frac{dk}{\pi} \frac{1}{\sqrt{m^2 + k^2}} \frac{1}{e^{\sqrt{m^2 + k^2}/T} - 1} + 3\lambda v^2.$$

At zero temperature the equilibrium state is the vacuum. For $v = 0$ there is one solution $m^2$ for every $\mu^2_r \in (-\infty, \infty)$

$$\mu^2_r = m^2 + \frac{3\lambda}{4\pi} \log \frac{m^2}{\lambda}.$$
For nonzero \( v \) we get, from (2.30), the relations
\[
m^2 = 2\lambda v^2, \quad \mu_r^2 = -\frac{1}{2} m^2 + \frac{3\lambda}{4\pi} \log \frac{m^2}{\lambda}.
\]
(2.42)

The right hand side of this equation has a maximum for \( m^2/\lambda = 3/(2\pi) \), meaning there are two solutions, provided
\[
\frac{\mu_r^2}{\lambda} < \frac{3}{4\pi} \left[ -1 + \log \left( \frac{3}{2\pi} \right) \right] \approx -0.415,
\]
(2.43)
otherwise there are none. To determine the true ground state we plot in Fig. 2.3a the effective potential \( u \) as a function of \( \varphi \) (i.e. with \( m^2 \) the solution of (2.40), with \( v \rightarrow \varphi \) and at \( T = 0 \), for various \( \mu_r \). The plot shows that there is a first order phase transition as a function of \( \mu_r^2 \), instead of the expected second order transition for a model in the universality class of the Ising model. This mis-representation of the phase transition is a well-known artifact of the Gaussian approximation (see, e.g. Ref. [47]).

Note that the second order transition would occur at strong coupling \( \lambda/m^2 \rightarrow \infty \), where the Gaussian approximation is suspect. In fact, the two masses at the transition also imply strong coupling: they are given by \( \lambda/m^2 \approx 10 \), for \( \varphi = 0 \) and \( \lambda/m^2 \approx 1.2 \) for \( \varphi = v_c \approx 0.65 \). To avoid fake first order effects we should evidently choose parameters away from the transition region. For this paper we mostly used \( \lambda/m^2 = 1/12 \) for which there is only one ground state at \( v^2 = 6 \), well away from \( v_c \approx 0.65 \).

Having determined the groundstate we define the renormalized energy \( H_{\text{eff},r} \) by subtracting from \( H_{\text{eff}} \) its value in the ground state, such that the vacuum energy is zero. It can be instructive to split the total energy into a classical (Gaussian mean field) part and a mode energy, \( H_{\text{eff},r} = H_{\text{mf}} + H_{\text{modes}} \). We define the mean field part as
\[
H_{\text{mf}} = \int dx \left[ \frac{1}{2} \pi^2 + \frac{1}{2} (\nabla \varphi)^2 + V_{\text{mf}}(\varphi) \right],
\]
(2.44a)
\[
V_{\text{mf}}(\varphi) = \begin{cases} 
\frac{1}{2} m^2 \varphi^2 + \frac{1}{4} \lambda \varphi^4, & v = 0, \\
\frac{1}{4} \lambda (\varphi^2 - v^2)^2, & v \neq 0,
\end{cases}
\]
(2.44b)
where \( m^2 \) and \( v^2 \) are the vacuum values (i.e. at \( T = 0 \)).

Consider now starting in the broken symmetry phase \( v \neq 0 \) at zero temperature and raising the temperature. In 1+1 dimensions there should be only a cross over and not a true phase transition. Fig. 2.3b shows the finite temperature effective potential (free energy density)
\[
f(\varphi) = u(\varphi) - T s(\varphi),
\]
(2.45)
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using the temperature \( T \) as independent variable instead of \( \mu_2^r \). Now \( m^2 = m^2(\varphi, T) \) is the solution of (2.40), \( v \rightarrow \varphi \), at finite \( T \). The parameters were chosen such that \( v^2 = m^2(v, 0)/2\lambda = 6 \) at \( T = 0 \). We see again a fake first order transition, at \( T_c \approx 1.79 \, m(v, 0) \), with \( v_c = 1.96 \). Its latent heat \( \ell \) and surface tension \( \sigma \) are given by

\[
\ell = \delta u = 0.39 \, m(v, 0)^2, \quad \sigma = \int_{0}^{v_c} d\varphi \, \sqrt{2f(\varphi)} = 0.295 \, m(v, 0). \tag{2.46}
\]

These are not particularly small values and we may not argue that the effects of the first order transition will be negligible under generic circumstances. However, in 1+1 dimensions, the critical size of a nucleating bubble is zero, so the bubble nucleation rate is not suppressed (\( \propto \exp(-2\sigma/T_c) \approx \exp(-0.17) \)) and supercooling will not be strong.

We end this section with some cautionary remarks. First, the fact that the equilibrium correlation function \( C(x, y) \) has the free form (i.e. eq. (2.47), below, with \( n_k \) given by the Bose-Einstein form (2.37)) is a result of the Gaussian approximation. The exact correlation function will have a more complicated form, although the corrections are expected to be small at weak coupling. We will check this explicitly by a Monte Carlo computation discussed in Section 2.7.1.

Second, it is not clear that the finite temperature equilibrium state found above will actually be approached at very large times. Any set of numbers \( n_k \) in conjunction with eqs. (2.29)–(2.34) gives a stationary solution to the Hartree equations.
Our derivation of the Bose-Einstein form for $n_k$, used the standard form (2.35) for the entropy, but we have not shown that this entropy is a large time result of the dynamics. Of course, this would be trivially the case if we choose the initial occupation numbers $n^0_\alpha = n_k$. But for a generic Gaussian initial state the correlation function may still approach a fixed point of the form just discussed ($t \approx t'$),

$$C(t, x; t', x') = \sum_\alpha \left[ (1 + n^0_\alpha) f_\alpha(t, x) f_\alpha^*(t', x') + n^0_\alpha f_\alpha^*(t, x) f_\alpha(t', x') \right]$$

$$\rightarrow \int \frac{dk}{2\pi} \left[ \frac{1 + n_k}{2\omega_k} e^{i k(x-x') - i \omega_k (t-t')} + \frac{n_k}{2\omega_k} e^{-i k(x-x') + i \omega_k (t-t')} \right], \quad (2.47)$$

where the $n_k$ are expected to correspond to maximum entropy in relation to the dynamics. Since the Hartree dynamics in terms of $H_{\text{eff}}$ is classical we may expect this entropy to take a classical form, which would lead to

$$n_k = \frac{T}{\omega_k}. \quad (2.48)$$

However, matters are complicated by the presence of the infinitely many conserved charges (2.28), which are determined by the initial conditions. Note that without these constraints one would expect $n_k + 1/2 = T/\omega_k$, instead of (2.48), which makes a big difference because equipartition suggests low $T = O(\epsilon/\lambda)$ and therefore small $n_k$. We elaborate on this in Appendix 2.B.

To study such matters numerically we now first introduce a coarse graining of the correlation function and define a corresponding time dependent distribution function $n_k(t)$.

### 2.4 Coarse grained particle numbers

The mode functions may be interpreted as representing particles which interact through the mean field. This is similar to electrons scattering off each other in classical electrodynamics, albeit that here the “particles” are treated quantum mechanically and their interaction is short ranged. Intuitively, such an interpretation supposes that the particles are localised, with a correspondingly fluctuating (and hence inhomogeneous) mean field taking the role of a classical field.

Within such a picture one expects the system to thermalize approximately. We would like such thermalization to be quantal, e.g. with particle distribution functions which are of the Bose-Einstein type. However, the fact that our equations of motion have the form of classical Hamilton equations in terms of $H_{\text{eff}}$ suggests otherwise, namely a distribution approaching a classical Boltzmann form $\exp(-\beta H_{\text{eff}})$, subject to the constraints set by the large number of conserved charges (2.27). But
this may take a very long time. In any case, one way to test the Gaussian approximation is to study its thermalization properties. This we do by looking at equal time correlation functions, which are coarse grained by averaging over a spacetime region. Assuming the system is weakly coupled we can compare such averages with a free field form in terms of quasi-particles with effective masses. If the system equilibrates locally in a quantum way, then the quasi-particle distribution \( n_k \) should approach the Bose-Einstein form. We define the correlation functions

\[
S(t, x, y) = \langle \hat{\phi}(t, x) \hat{\phi}(t, y) \rangle - \langle \hat{\phi}(t, x) \rangle \langle \hat{\phi}(t, y) \rangle,
\]

\[
T(t, x, y) = \frac{1}{2} \left[ \langle [\hat{\phi}(t, x) \hat{\pi}(t, y) + \hat{\pi}(t, y) \hat{\phi}(t, x)] \rangle \right] - \langle \hat{\phi}(t, x) \rangle \langle \hat{\pi}(t, y) \rangle,
\]

\[
U(t, x, y) = \langle \hat{\pi}(t, x) \hat{\pi}(t, y) \rangle - \langle \hat{\pi}(t, x) \rangle \langle \hat{\pi}(t, y) \rangle,
\]

where the overbar denotes the spacetime averaging as well as a possible average over initial conditions as in (1.5). Using (2.3a) and (2.8) we can express these quantities in terms of a "classical" (mean field) and a "quantum" contribution,

\[
S(t, x, y) = S^c(t, x, y) + S^q(t, x, y),
\]

\[
S^c(t, x, y) = \varphi(t, x) \varphi(t, y) - \varphi(t, x) \varphi(t, y),
\]

\[
S^q(t, x, y) = C(t, x; t, y),
\]

etc. Note that \( S^c \to 0 \) in case of averaging over initial conditions and/or spacetime. For simplicity the spatial average is performed over all of space. For example,

\[
\langle \hat{\phi}(t, x) \hat{\phi}(t, y) \rangle = \frac{1}{L^d} \int_{-\delta/2}^{t+\delta/2} dt' \int_0^L dz \langle \hat{\phi}(t', x + z) \hat{\phi}(t', y + z) \rangle.
\]

Because of the periodic boundary conditions \( S, T \) and \( U \) depend only on the difference between \( x \) and \( y \). Taking the Fourier transform

\[
S_k(t) = \frac{1}{L} \int_0^L dx \ dy \ e^{-ik(x-y)} S(x, y, t), \quad k = (0, \pm 1, \pm 2, \cdots) \frac{2\pi}{L},
\]

and similarly for \( T \) and \( U \), it is easy to see that \( S \) and \( U \) are symmetric and positive, i.e.

\[
S_k(t) = S_{-k}(t) \geq 0, \quad U_k(t) = U_{-k}(t) \geq 0,
\]

while \( T_k \) enjoys no such properties. For a free field with average occupation numbers \( \langle \hat{a}_k^\dagger \hat{a}_k \rangle = n_k \) and frequencies \( \omega_k \) the correlators are given by

\[
S_k = \frac{n_k + n_{-k} + 1}{2\omega_k}, \quad T_k = \frac{n_k - n_{-k}}{2}, \quad U_k = S_k \omega_k^2.
\]
Note that in this case $T$ is antisymmetric. We now define $\omega_k(t)$ and $n_k(t)$ for the interacting case by

$$ n_k(t) = n_k^s(t) + n_k^a(t), \quad n_k^s(t) = n_{-k}^s(t), \quad n_k^a(t) = -n_{-k}^a(t), \quad (2.55) $$

$S_k(t) = \left[ n_k^s(t) + \frac{1}{2} \right] \frac{1}{\omega_k(t)}$, \quad (2.56a)

$T_k^a(t) = \frac{1}{2} [T_k(t) - T_{-k}(t)] = n_k^a(t)$, \quad (2.56b)

$U_k(t) = \left[ n_k^s(t) + \frac{1}{2} \right] \omega_k(t)$. \quad (2.56c)

These equations can be easily solved in terms of $\omega_k$ and $n_k$:

$$ \omega_k = \omega_{-k} = \sqrt{U_k/S_k} \quad \quad n_k^s = \omega_k S_k - \frac{1}{2} = \sqrt{U_k S_k} - \frac{1}{2} \quad (2.57) $$

and $n_k$ follows by adding $T_k^a$. In practise $n_k$ is positive (it can be shown to be positive provided the symmetric correlation between $\phi$ and $\pi$ vanishes).

There is a more direct interpretation of these formulae in terms of the expectation value of a number operator $\hat{a}_k \hat{a}_k$. Suppose we define time dependent creation and annihilation operators as

$$ \hat{a}_k(t) = \frac{1}{\sqrt{2 \omega_k(t) L}} \int_0^L dx \ e^{-i k x} [\omega_k(t) \hat{\phi}(t, x) + i \hat{\pi}(t, x)], \quad (2.58a) $$

$$ \hat{a}_k^\dagger(t) = (\hat{a}_k(t))^\dagger. \quad (2.58b) $$

Then

$$ \langle \hat{a}_k^\dagger(t) \hat{a}_k(t) \rangle = n_k(t). \quad (2.59) $$

The problem with starting with (2.58) is that one does not know a priori how to choose the $\omega_k(t)$. This is especially so if some of the effective squared frequencies $\mu^2 + 3\lambda \varphi^2 + 3\lambda \chi$ in the equations for the mode functions turn negative. The line of reasoning leading to (2.55)–(2.56c) solves this problem, but we should keep in mind that this is by brute force, which can be misleading in extreme situations, e.g. when the spectral function is not dominated by a sufficiently narrow quasi-particle bump.

The quasi-particles can also be used to define an energy:

$$ E_{qp} = \sum_k n_k \omega_k \quad (2.60) $$

where $n_k$ can be obtained from the two-point functions of the mean field, of the mode functions, or of the sum of both. This definition can then be compared with the effective Hamiltonian.
2.5 Hartree Ensemble Approximation

Above we described the Hartree approximation. In the Hartree ensemble method this approximation is applied to each individual realisation \(|\varphi, \pi\rangle\langle \varphi, \pi|\) of the initial conditions as in (1.5). So in eq. (2.8) the Gaussian brackets stand for \(\langle \cdot \rangle = \langle \varphi, \pi| \cdot | \varphi, \pi \rangle\) and the average over \(\varphi, \pi\) is only taken in the evaluation of observables. Furthermore these states are pure, hence in (2.14), the initial particle density \(n^0_\alpha = 0\).

In this way we compute correlation functions with a generally non-Gaussian density operator \(\hat{\rho} = \sum_i p_i | \varphi_i^{(i)} \rangle \langle \varphi_i^{(i)} |\), as

\[
S_{xy} = \sum_i p_i [C_{xy}^{(i)} + \varphi_x^{(i)} \varphi_y^{(i)}] - \left( \sum_i p_i \varphi_x^{(i)} \right) \left( \sum_j p_j \varphi_y^{(j)} \right)
\]

(2.61)

The \(C_{xy}^{(i)}\) and \(\varphi_x^{(i)}\) are computed with Gaussian pure states as in (2.8). This means that in the time-evolution the Gaussian approximation is used, while expectation values are calculated using the more general initial density operator.

It should be stressed that for typical realisations the mean field \(\varphi_x^{(i)}\) is inhomogeneous in space, in contrast to the ensemble average \(\sum_i p_i \varphi_x^{(i)}\) which is in fact homogeneous for the initial conditions we shall employ.

2.6 Implementation on a Lattice

2.6.1 Quantum Mechanics

The discretization of the scalar field theory on a space-time lattice has some elegant features which we present briefly in this section; for fermions, see Ref. [20]. For simplicity we start with a simple quantum mechanical system of unit mass, with action

\[
S = a_0 \sum_t \left\{ \frac{[q(t + a_0) - q(t)]^2}{2a_0^2} - V[q(t)] \right\}
\]

(2.62)

where \(a_0\) is the time step, \(t = a_0 r\), with integer \(r\). We define the quantum system by means of the path integral. The discretized path integral

\[
Z = \int \left[ \prod_t dq(t) \right] e^{iS}
\]

(2.63)

corresponds to an evolution operator in Hilbert space that is a product of single step evolution operators given by

\[
\hat{U} = \hat{U}_p \hat{U}_q,
\]

(2.64)
with
\[ \hat{U}_p = e^{-ia_0 \hat{p}^2/2}, \quad \hat{U}_q = e^{-ia_0 V(\hat{q})}, \] (2.65)
where \( \hat{p} \) and \( \hat{q} \) are canonical operators satisfying \([\hat{q}, \hat{p}] = i\). A finite time-evolution then takes the “Trotter form”
\[ \hat{U}_q \hat{U}_r = \hat{U}_q \ldots \hat{U}_p \hat{U}_q \hat{U}_p \hat{U}_q \ldots \hat{U}_q, \] (2.66)

The Heisenberg operators
\[ \hat{p}(t) = \hat{U}_r^{\dagger} \hat{p} \hat{U}_r, \quad \hat{q}(t) = \hat{U}_r^{\dagger} \hat{q} \hat{U}_r, \quad t = a_0 r, \] (2.67)
satisfy the discretized equations of motion in leapfrog fashion,
\[ \hat{p}(t + a_0) = \hat{p}(t) - a_0 V'(\hat{q}(t)), \quad \hat{q}(t + a_0) = \hat{q}(t) + a_0 \hat{p}(t + a_0). \] (2.68a)
(2.68b)

With \( \hat{q}(t) \rightarrow q(t), \hat{p}(t) \rightarrow (q(t) - q(t - a_0))/a_0 \), the above equations (2.68) are identical in form to the classical equations obtained from the stationary action principle.

Making a unitary transformation
\[ \hat{T} = e^{-ia_0 V(\hat{q})/2} \hat{U} e^{ia_0 V(\hat{q})/2}, \] (2.69)
we get an equivalent operator \( \hat{T} \), that becomes the Hermitian and positive transfer operator upon analytically continuing to imaginary time (see e.g. Ref. [49]), writing \( a_0 = e^{-i\theta} |a_0|, \theta = 0 \rightarrow \pi/2, \)
\[ \hat{T} \rightarrow e^{-|a_0| V(\hat{q})/2} e^{-|a_0| \hat{p}^2/2} e^{-|a_0| V(\hat{q})/2}. \] (2.70)

Specialising to the harmonic case \( V(q) = \omega^2 q^2/2 \) we can diagonalize the time evolution in terms of creation and annihilation operators \( \hat{c}^{\dagger} \) and \( \hat{c} \),
\[ \hat{T} \hat{c} \hat{T}^{\dagger} = e^{ia_0 \omega^{(e)}(e)} \hat{c}, \quad \hat{T} \hat{c}^{\dagger} \hat{T}^{\dagger} = e^{-ia_0 \omega^{(e)}(e)} \hat{c}^{\dagger}, \] (2.71)
with
\[ \hat{c} = \frac{1}{\sqrt{2\omega^{(n)}}} (\omega^{(n)} \hat{q} + i\hat{p}), \] (2.72)
and
\[ \cos(a_0 \omega^{(e)}) = 1 - \frac{1}{2} a_0^2 \omega^2, \] (2.73a)
\[ \omega^{(n)} = \frac{1}{a_0} \sin(a_0 \omega^{(e)}) = \omega \sqrt{1 - \frac{1}{4} a_0^2 \omega^2}, \] (2.73b)
and the conjugate relation for $\hat{c}^\dagger$. The creation and annihilation operators satisfy the standard commutation relation $[\hat{c}, \hat{c}^\dagger] = 1$. The superscripts $e$ and $n$ distinguish the “exponent omega” (eigenvalue omega) $\omega^{(e)}$ from the “normalisation omega” (eigenvector omega) $\omega^{(n)}$, and both go over to the “original omega” $\omega$ in the continuous time limit $a_0 \to 0$. The ground state is given by

$$\hat{c}|0\rangle = 0, \quad \langle q|0\rangle = \nu e^{-\omega^{(n)} q^2/2}, \quad (2.74)$$

with $\nu$ a normalisation constant and

$$\hat{T}(\hat{c}^\dagger)^n|0\rangle = e^{-i(n+1/2)a_0 \omega^{(e)}} (\hat{c}^\dagger)^n|0\rangle. \quad (2.75)$$

The evolution becomes unstable when $a_0^2 \omega^2 > 4$, for which $\omega^{(e)}_k$ is imaginary. The eigenvalues of $\hat{T}$ are then no longer phase factors and its eigenfunctions no longer normalisable, despite its formally unitary form. This is of course avoided by taking $a_0$ sufficiently small. The discretization errors in $\omega^{(e)}$ and $\omega^{(n)}$ are of order $a_0^2$.

It is natural to identify the Hamiltonian $\hat{H}$ from $\hat{T} = e^{ia_0 V(\hat{q})/2}$, but this leaves a modulo $2\pi/a_0$ ambiguity for the eigenvalues of $\hat{H}$ (the imaginary time version is unambiguous). To pin down $\hat{H}$ more precisely we can use the Baker-Campbell-Hausdorff series for combining the exponents in $\hat{T}$, which gives $\hat{H} = \hat{p}^2/2 + V(\hat{q}) + O(a_0^3)$. We shall neglect the corrections of order $a_0^2$. The exact $\hat{H}$ is time-independent. In practise, the expectation value of the approximate $\hat{H}$ is constant in time up to small fluctuations, as expected for a leapfrog algorithm.

### 2.6.2 Field Theory: Hartree Approximation

For the application to the Hartree approximation it will be more convenient for us to work with the unitarily-related creation and annihilation operators that diagonalize the operator $\hat{U}$,

$$\hat{a} = e^{ia_0 V(\hat{q})/2} \hat{c} e^{-ia_0 V(\hat{q})/2} = \frac{1}{\sqrt{2\omega^{(n)}}} \left( 1 - e^{-ia_0 \omega^{(e)}} \frac{i\hat{q} + i\hat{p}}{ia_0} \right), \quad (2.76a)$$

$$\hat{U} \hat{a} \hat{U}^\dagger = e^{ia_0 \omega^{(e)}} \hat{a}, \quad (2.76b)$$

for $V = \omega^2 q^2/2$. Note that $\hat{a} \to \hat{c}$ in the limit $a_0 \to 0$.

The generalisation of the above quantum mechanical model to our scalar field is straightforward. The lattice action on a space-time lattice with spatial/temporal...
The lattice distance $a/a_0$ is given by

$$S[\varphi] = a_0 a \sum_{x,t} \left\{ \frac{[\varphi(x, t + a_0) - \varphi(t, x)]^2}{2a_0^2} - \frac{[\varphi(x + a, t) - \varphi(t, x)]^2}{2a^2} \right. \\
- \left. \frac{1}{2} \mu^2 \varphi(t, x)^2 - \frac{1}{4} \lambda \varphi(t, x)^4 \right\},$$

(2.77)

where we assume a periodic physical size $L = Na$. The operator description in Hilbert space follows from the lattice regularised path integral. In the Hartree approximation we write the operator fields in terms of a complete set of mode functions,

$$\hat{\varphi}(t, x) = \varphi(t, x) + \sum_k [\hat{b}_k f_k(t, x) + \hat{b}_k^\dagger f_k^*(t, x)],$$

(2.78a)

$$\hat{\pi}(t, x) = \pi(t, x) + \sum_k [\hat{b}_k \dot{f}_k(t, x) + \hat{b}_k^\dagger \dot{f}_k^*(t, x)],$$

(2.78b)

where the use of

$$f(t, x) = \frac{f(t, x) - f(x, t - a_0)}{a_0},$$

(2.79)

is inspired by equation (2.68b) (using instead the forward derivative $\dot{f}_k(t, x) = [f(x, t + a_0) - f(t, x)]/a_0$ gives equivalent results). Imposing canonical commutation relations for both $\hat{\varphi}, \hat{\pi}$ and $\hat{b}_k, \hat{b}_k^\dagger$, leads to the orthonormality and completeness relations

$$a \sum_{x} [i\dot{f}_k(t, x) f_k^*(t, x) - if_k(t, x) \dot{f}_k^*(t, x)] = \delta_{kl},$$

(2.80a)

$$\sum_{k} [i\dot{f}_k^*(t, x) \dot{f}_k(y, t) - if_k(t, x) \dot{f}_k^*(y, t)] = \delta_{xy} \frac{a}{a}. $$

(2.80b)

The time-independence of the orthonormality conditions corresponds to Noether charges of symmetries of the effective action on the lattice, as explained in Section 2.2. We use the static solutions of the Hartree equations in constructing the set of mode functions. Their equation of motion

$$\frac{f_k(x, t + a_0) - 2f_k(t, x) + f_k(x, t - a_0)}{a_0^2} = \frac{\dot{f}_k(x + a, t) - 2\dot{f}_k(t, x) + \dot{f}_k(x - a, t)}{a^2} - m^2 f_k(t, x),$$

(2.81)
can be written in the leapfrog form (2.68). The solution of the recursion relation (2.81) can be written as

\[ f_k(t, x) = \frac{e^{ikx-i\omega_k^{(e)}t}}{\sqrt{2\omega_k^{(n)}L}}, \quad k = \frac{2\pi j}{L}, \quad j = -\frac{N}{2} + 1, \ldots, \frac{N}{2}, \]  

(2.82)
giving

\[ -\frac{2 - 2\cos(\omega_k^{(e)}a_0)}{a_0^2} + \frac{2 - 2\cos(ka)}{a^2} + m^2 = 0. \]  

(2.83)

Defining a lattice \( \omega_k^{(a)} \) as

\[ \omega_k^{(a)} = \sqrt{m^2 + \frac{2 - 2\cos(ka)}{a^2}}, \]  

(2.84)
we find the analogue of (2.73a),

\[ \cos(a_0 \omega_k^{(e)}) = 1 - \frac{1}{2} a_0^2 (\omega_k^{(a)})^2, \]  

(2.85)
which has real \( \omega_k^{(e)} \) solutions for \( a/a_0 \geq \sqrt{4 + a^2m^2} \). In simulations we used \( a/a_0 \geq 10 \), which amply secured the stability. The normalisation in (2.82) is fixed by the orthonormality relation (2.80a), which gives the analogue of (2.73b)

\[ \omega_k^{(n)} = \frac{\sin(a_0 \omega_k^{(e)})}{a_0} = \omega_k^{(a)} \sqrt{1 - \frac{1}{4} a_0^2 (\omega_k^{(a)})^2}, \]  

(2.86)
The completeness relation (2.80b) is then also satisfied. When the mode functions have the form (2.82), the \( \hat{a}_k \) defined by

\[ \hat{\phi} = \sum_k \hat{a}_k f_k + \text{h.c.}, \quad \hat{\pi} = \sum_k \hat{a}_k \dot{f}_k + \text{h.c.}, \]  

(2.87)
are related to \( \hat{\phi} \) and \( \hat{\pi} \) as in the quantum mechanical case (2.76a). Note that \( \omega_k^{(n)} \), \( \omega_k^{(e)} \to \omega_k^{(a)} \) in the limit \( a_0 \to 0 \), and \( \omega_k^{(a)} \to \sqrt{m^2 + k^2} \) as \( a \to 0 \).

2.6.3 PARTICLE NUMBER

We end this section with a properly discretized version of the instantaneous particle number \( n_k \), using the stationary solution (2.82) and the two-point functions (2.49). Suppose the mean field is zero and

\[ \langle \hat{b}_k \hat{b}_k \rangle = n_k^0 = n_{-k}^0. \]  

(2.88)
Then

\[ S_k(t) = \left(n_k^0 + \frac{1}{2}\right) \frac{1}{\omega_k^{(n)}} \]

(2.89a)

\[ U_k(t) = \left(n_k^0 + \frac{1}{2}\right) \left(\frac{\omega_k^{(a)}}{\omega_k^{(n)}}\right)^2, \]

(2.89b)

where we used

\[ \dot{f}_k(t, x) \dot{f}_k^*(y, t) = \left(\omega_k^{(a)}\right)^2 f_k(t, x) f_k^*(y, t). \]

(2.90)

Inverting (2.89) we find that our definition of the instantaneous particle energy \(\omega_k(t)\) does not need discretization corrections,

\[ \omega_k^{(a)} = \sqrt{U_k(t) S_k(t)} \equiv \omega_k(t). \]

(2.91)

On the other hand, compared to (2.57) the definition of instantaneous particle number needs important corrections for large \(\omega_k\):

\[ n_k^0 + \frac{1}{2} = \sqrt{U_k S_k} \frac{\omega_k^{(n)}}{\omega_k^{(a)}} = \sqrt{U_k (S_k - \frac{1}{4}a_0^2 U_k)} \equiv n_k(t) + \frac{1}{2}, \]

(2.92)

using (2.86) and (2.91).

For larger energies the corrections can become quite important. Denoting the uncorrected particle number by \(\tilde{n}_k = \sqrt{U_k S_k} - 1/2\), we find

\[ \frac{\tilde{n}_k - n_k}{n_k} = \frac{n_k + \frac{1}{2}}{n_k} \left(\frac{1}{\sqrt{1 - \frac{1}{4}(a_0 \omega_k^{(a)})^2}} - 1\right), \]

(2.93)

\[ \approx \frac{n_k + \frac{1}{2}}{n_k} \frac{1}{8} \left(a_0 \omega_k^{(a)}\right)^2. \]

Using a Bose-Einstein distribution at \(T = m\) and the typical value \(a_0 m = 1/80\) we find that the relative difference becomes unity for \(\omega_k/m = 7.5\). At the lower temperature \(T/m = 0.5\) this is the case already for \(\omega_k/m = 4.3\).

### 2.7 Numerical results

#### 2.7.1 Monte Carlo check

In this section we will first check the expectation, that for weakly coupled fields the equilibrium particle densities, defined according to (2.56), indeed have a Bose-Einstein distribution, while the energies will have a free quasi-particle dispersion.
Towards Equilibrium

Figure 2.4: Dispersion relation computed from a Monte Carlo simulation of the Euclidean time version of the model. The model parameters are: $\lambda/m^2 = 1/2v^2 = 1/4$, $Lm = 25.6$, $1/am = 10$ and $T/m = 1$, with 20 steps in the Euclidean time direction. Here $k$ is the lattice momentum $\sqrt{2 - 2\cos(ak)/a}$. The statistical error bars are smaller than the symbols.

relation, approximately,

$$n_k = \frac{1}{e^{\omega_k/T} - 1}, \quad \omega_k^2 = m(T)^2 + \frac{2 - 2\cos(ak)}{a^2}. \quad (2.94)$$

The effective mass $m(T)$ of the quasi-particles is temperature dependent. In the following we shall use the zero temperature mass $m \equiv m(T = 0)$ to scale dimensionful quantities.

To substantiate this expectation (2.94), we have performed several Monte Carlo simulations of the Euclidean time version of our model at parameter values in the same range as we will use for the Hartree simulations. In Fig. 2.4 we show the dispersion relation computed from such a Monte Carlo simulation. We chose a temperature $T/m = 1$ and measured $S_{xy}$. We stress that such a Monte Carlo simulation gives the exact (up to statistical errors) results for the finite temperature Green function. Making the assumption that $n_k$ has the BE form, we computed the $\omega_k$ from $S_{xy}$ using (2.56). As can be seen from the figure, the free form (2.94) for the quasi-particle dispersion relation holds very well, with $m(T)/m \approx 0.43$. This value is close to that found with the effective potential calculations in the Hartree approximation, as described in Section 2.3, which gives $m(T)/m \approx 0.41$ at $T/m = 1$. The
effects of the temperature and interactions show up almost exclusively in the value of the effective mass \( m(T) \).

### 2.7.2 Hartree Ensemble Approximation: Initial Conditions

We will now describe some Hartree simulations we used for obtaining the particle numbers \( n_k(t) \). The mass and coupling parameters were chosen such that the system at zero temperature is in the “broken symmetry phase”. The coupling was weak, \( \nu^2 = m^2/2\lambda = 6 \). Here and in the following \( m \) is the mass of the particles at zero temperature.

The system is discretized on a space-time lattice with spatial (temporal) lattice distance \( a(a_0) \), with \( a_0/a = 0.1 \). The number of spatial lattice sites, equal to the number of independent complex mode functions, will be denoted with \( N = L/a \). The discretized Lagrangian gives rise to second order difference equations, with a time evolution which is equivalent to a first order leapfrog algorithm for \( \pi_x(t) \equiv \left[ \phi_x(t + a_0) - \phi_x(t) \right]/a_0 \) and \( \phi_x(t) \).

The initialisation is similar to that used in [16, 17],

\[
\varphi_x^{(i)} = v, \quad \pi_x^{(i)} = A m \sum_{j=1}^{j_{\text{max}}} \cos(2\pi j x/L - \psi_j^{(i)}),
\]

with random phases \( \psi_j \) uniformly distributed in \([0, 2\pi]\). The modes are initialised with the equilibrium form at zero temperature: the \( n_0^k \) are all zero and the modes \( f_k(x, 0), \dot{f}_k(x, 0) \) are given by the plane waves (2.82) and their time derivative at \( t = 0 \), together with the definitions (2.85) and (2.86). The density operator is thus a superposition of coherent pure states as in (1.5).

### 2.7.3 Towards Equilibrium

We first describe a simulation for which \( \lambda/m^2 = 1/12, N = 256, mL = 32, j_{\text{max}} = 4, A = 1/\sqrt{2} \), such that the energy density is given by \( E/Lm^2 = A^2 j_{\text{max}}/4 = 0.5 \). A Bose-Einstein distribution describing particles with such an energy density would have a temperature \( T/m \approx 1.08 \), well below the phase transition at \( T/m \approx 1.8 \), as calculated from the finite temperature effective potential. We also chose these parameters so that the system may end up in a low temperature quantum regime and not in a classical regime with \( T/m \gg 1 \). A boring consequence is that the volume averaged mean field typically just oscillates around one of the two minima, we did not encounter an initial condition for which it crossed the barrier after \( t m > 50 \).
Initially the mean field carries all the energy in its low momentum modes $0 < k/m \leq \pi/4$ (zero momentum mode excluded). Due to interaction with the inhomogeneous mean field, the modes will not keep the vacuum form, but get excited. Fig. 2.5 shows the time dependence of the energy density for one of the members of the ensemble. The total energy is conserved up to a numerical accuracy of about 0.2%. The energy in the mean field (cf. (2.44) for its definition), initially equal to the total energy, is decreasing rapidly and after a time $t_m \approx 100$ about 50% has been transferred to the modes. The mean field continues losing energy after that time but at a time $t_m$ of the order 20 000 some 15% is still left.

The development of the particle numbers $n_k(t)$ at early times is shown in Fig. 2.6a, including the mean field contribution, cf. (2.50a)–(2.50c).\(^3\) Initially the mean field gives the main contribution since $n_k^0 = 0$ for the modes, but then the mode contribution rapidly takes over. Because the mean field contribution fluctuates strongly we used as many as 500 initial conditions for these early times, without coarsening over time. Fig. 2.6b shows the mode contribution to $n_k$ as a function of $\omega$ (40 initial conditions were used for the data at $t_m > 200$, with no coarsening over time). It starts out identically zero, rises rapidly and then appears to stabilise. The figure also shows a fit to the Bose-Einstein distribution with chemical potential $\mu$ at time $t_m = 990$. A chemical potential is expected to develop temporarily at weak coupling, since elastic scattering dominates over processes like $2 \leftrightarrow 4$ scattering. The fitted temperature ($\beta m = 1.08$) is already approaching the earlier estimate

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\(^3\)In this and following figures an average is taken over $k = \pm |k|$. The distributions $n_k$ for positive and negative $k$ are equal within fluctuations.
2.7 Numerical results

$T/m \approx 1.1$ based on the energy density. The complete distribution function (including the mean field contribution) reaches much larger values at these early times (by a factor $3 - 4$) and the curves appear closer together. However the plots are noisier, due to the strongly fluctuating mean field.

To study the tail of the distribution more easily, a plot of $\log(1 + 1/n)$ is shown in Fig. 2.7a. This function is linear in $\omega$ for a Bose-Einstein distribution with slope equal to the inverse temperature $\beta$ and offset equal to the $\beta \mu$. We indeed see linear Bose-Einstein behaviour developing at low momenta with gradual participation of the higher momentum modes. Including the contribution of the mean field, shown in Fig. 2.7b, a more rapid convergence and higher occupation numbers can be seen, giving a higher fitted temperature and smaller chemical potential, compared to the data in Fig. 2.7a. The trend seen in Figs. 2.7a and 2.7b continues at larger times, as shown in Fig. 2.8 for the contribution of the modes only. A plot where the mean field contribution is included looks similar. For this simulation an average is taken over a time interval $t_m = 24$, approximately 3.5 oscillation periods, and only 10 initial configurations. The straight line is a Bose-Einstein fit with zero chemical potential at $t_m = 6200$ in the region $\omega/m < 1.8$. We see that the slope is roughly constant in time and that the thermalized part of the distribution is extending to higher values of $\omega$, roughly linear in $\log t_m$.

In Fig. 2.9a a plot is made of the Bose-Einstein temperatures from the fits (modes only) as a function of time. For times $t_m < 3000$ the fit is made over the interval $\omega/m < 1.4$ while for later times this is increased to $\omega/m < 1.8$. The figure shows an anti-correlation between $T$ and $\mu$ which would be meaningful, i.e. not just a fitting artifact, if the particle density $n = \sum_k n_k/L$ is constant, or has evidently smaller fluctuations. This seems to be the case indeed: as shown in Fig. 2.9b, the density $n$
Figure 2.7: Particle number \( \log(1 + 1/n_k) \) versus \( \omega_k \) for early times. The straight line is a Bose-Einstein fit for the latest time, over \( \omega/m < 1.2 \).

corresponding to the modes only is quite constant for times \( t_m > 100 \), and in fact continues to remain so up to times of over 5000. On a larger time scale of order 10000 or so it drops somewhat. The initial approach of \( n/m \) (modes only) to the value \( \approx 0.34 \) can be fitted to an exponential, which yields an equilibration time scale \( \tau_m = 15 \text{–} 20 \), depending on the fitting range.

We have to be careful, however, that our \( \mu \) is not an artifact of the fitting procedure. We believe this to be the case for the larger times \( t_m \gtrsim 40000 \) where \( \mu \) becomes negative. As can be seen (with difficulty) in Fig. 2.8, the distribution starts to deviate at low \( \omega \) upwards from the straight line, corresponding to a suppression of \( n_k \) compared to the Bose-Einstein form. We interpret this as a contamination by classical behaviour \( n_k \approx T_{cl}/\omega_k \), cf. (2.48), as will be argued later in this section.

Let us now make a comparison with analytical results derived from the equilibrium finite temperature effective potential (2.45). Around time \( t_m = 15000 \text{–} 20000 \) the temperature measured in the simulation is \( T/m = 1.1 \). The effective potential then gives for the thermal mass \( m(T = 1.1)/m = v(T = 1.1)/v = 0.93 \). We derive the thermal mass in the simulation from the dispersion relation of measured \( \omega_k \). It is in very good agreement with a free form: \( \omega_k^2 = m^2(T) + k^2 \). A straight line fit of \( \omega^2 \) versus \( k^2 \) over the interval \( t_m = 15000 \text{–} 20000 \) gives a slope 1.00 and an offset \( m(T = 1.1)/m = 0.908 \). This is also in good agreement with the volume averaged value of the mean field, which is 0.91. These values are somewhat lower than the position of the minimum in the effective potential because of its asymmetric shape. However the difference is small because of the small amplitude of the mean field oscillations around this minimum.

The quasi-particle aspect can be investigated further by looking at the energy
Figure 2.8: The particle numbers (modes only) at later times.

\[ \sum_k n_k \omega_k \], as plotted in Fig. 2.5. We have made a distinction between the particle number as derived from the mean field, quantum and total two-point function. We see that the total energy in the particles (mean field + modes) is only a few percent lower than the total energy is the system, as may be expected for a weakly coupled system. It is also interesting to note that, while the quantum modes initially carry only a small fraction of the total energy, they thermalize with the same temperature 1.1m the system would have if all energy would be distributed according to a Bose-Einstein distribution with zero chemical potential.

\[ \frac{T}{m} \]  

\[ \frac{\mu}{m} \]

a: Bose-Einstein temperature. The smoother lines are drawn to guide the eye.

b: Particle densities \( n/m = \sum_k n_k / Lm \)

Figure 2.9: Bose-Einstein temperature and particle densities \( n/m = \sum_k n_k / Lm \).
2.7.4 Late Time Behaviour

We now turn to the very long time behaviour of the system, where we expect Bose-Einstein behaviour to be replaced by classical equipartition according to the effective Hamiltonian (2.22). The numerical computation of the equilibrium distribution functions in this regime is very difficult as it changes exceedingly slowly (cf. the slow log t-like population of the high momentum modes in Fig. 2.8). We therefore have carried out simulations in a smaller system at stronger coupling and at larger energy densities in order to make time scales a lot shorter. Here we present data for \( N = 16, L_m = 1, \lambda/m^2 = 1 \) and \( E/L_m^2 = 36 \), for which the system is in the “symmetric phase”. In Fig. 2.10 we plotted \( n_k \omega_k \) (modes + mean field) versus the integer \( kL/2\pi = k/2\pi m \), for different times. Note that it was necessary to initially also excite the highest momentum modes, otherwise the system would not reach final equilibrium sufficiently closely even after a time of \( 12 \cdot 10^6 \). Classical equipartition suggests \( n_k \omega_k = T_{cl} \), giving a straight horizontal line in the plot. We see indeed flat behaviour, with lower momentum modes tending to have somewhat smaller occupation numbers, except for the zero mode. Runs at small coupling \( \lambda/m^2 = 1/12 \) in larger volumes \( L_m = 4 \) and \( L_m = 16 \) in the “broken phase” showed similar results, except that the zero modes were less exceptional.

So we do find approximate classical \( n_k = T_{cl} / \omega_k \) behaviour at very large times. Classical equipartition leads to small temperatures \( T_{cl} = O(1/N) \). If this behaviour sets in first for the low momentum modes, then these will appear to be under-occupied compared to the Bose-Einstein distribution at temperature \( T > T_{cl} \). This is indeed the trend noticed earlier in Fig. 2.8, where the low momentum data at times
\( t_m > 20000 \) lie above the straight line going through the data at larger momenta.

2.8 Discussion

In this chapter we introduced the Hartree approximation and explained how its thermalization properties can be improved, by extending it with an initial ensemble average, thus allowing for the simulation of systems which are non-Gaussian.

We presented results of simulations mainly for a weakly coupled system in the broken symmetry phase. For such a weakly coupled system a near equilibrium description in terms of quasi-particles is expected to be reasonable, which we checked and confirmed in a Monte Carlo simulation.

Starting with distributions which are initially far out of equilibrium, in which only low momentum modes \( k \lesssim m \) of the classical field were excited with low energy density, we observed approximate thermalization with a particle distribution function approaching the Bose-Einstein form. After a fairly rapid initial thermalization at low momenta, the gradual adjustment of progressively higher momentum modes is very slow. The energy in the mean field gets transferred to the two-point function and one might think that the system behaves as if the mean field were constant. However, this is not the case: up to large times \( t_m = 80000 \) the mean field keeps fluctuating in space and time and carries a non-negligible fraction of the total energy.

It is hard to assign a time scale for the gradual adjustment of the distribution at higher momenta, however it appears to be at least two orders of magnitude larger than the equilibration time \( \tau m \approx 20 \) for the particle density, found at early times \( (t_m = O(10)) \). Slow thermalization was also found in a recent study of the fully nonlinear classical system in the symmetric phase [18]. Using our parameter combination \( \lambda T/m^3 \approx 1.1/12 \) in their empirical fit \( 1/\tau m = 5.8 \times 10^{-6} (6\lambda T/m^3)^{1.39} \) would give \( \tau m \approx 4 \times 10^5 \).

On a large time scale, perhaps of the order of \( t_m = 10000 \) or more, the distribution moves away from the quantum (Bose-Einstein) form towards classical equipartition. We never reached this classical equipartition for the weak coupling and low temperature used in this study, because of the very long computer time this would take. Only the use of very small systems, at high energy density and/or coupling enabled us to reach a situation resembling classical equipartition.

We have carried out many more simulations at higher energy densities, and larger couplings, in which the approximate quantum nature of the distribution at intermediate times was also evident. With higher energy density and/or larger coupling the effective coupling strength \( n_k \lambda / m^2 \) increases. Things then go quicker and the time scales of quantum versus classical equilibration get closer and might even get blurred. Furthermore, the Bose-Einstein distribution, on which we based
our analysis, might get distorted by non-perturbative effects. We may have seen such effects already in a significant enhancement of $n_k$ at low momenta, in simulations at larger volume.

Summarising, on the one hand our intuitive expectation that there may be quantal thermalization in the Gaussian approximation, due to scattering of the mode particles via the arbitrary inhomogeneous mean field, appears to be validated, but on the other hand it is not clear how useful this approximation can be for equilibrium physics, e.g. at finite density. It is possible that starting closer to quantum thermal equilibrium the time to reach thermalization is reduced and the intermediate time regime of quantal equilibrium can be stretched to do useful computations. Then it will be interesting to compare the Gaussian approximation with the classical approximation and see which one fares best. We will address these aspects in the next chapter. In that chapter we will also investigate the possibility of using fewer mode functions, in order to save on the numerical cost of the inhomogeneous Gaussian approximation, which is substantial: for an $N^d$ spatial lattice, the computational time scales like $N^{2d+1}$.

### 2.A Diagonal Coherent State Representation

To derive the representation (1.5) consider first a quantum mechanical system of two degrees of freedom with canonical variables $p$ and $q$. Let $|pq\rangle$ be a normalised coherent state, such that

$$\hat{a}|pq\rangle = \frac{1}{\sqrt{2\omega}} (\omega q + ip)|pq\rangle, \quad \hat{a} \equiv \frac{1}{\sqrt{2\omega}} (\omega \hat{q} + i\hat{p}),$$

$$\langle p'q'|pq\rangle = \exp\left\{ \frac{i}{2} (pq' - p'q) - \frac{1}{4\omega} [\omega^2 (q - q')^2 + (p - p')^2] \right\}$$

$$\int \frac{dp \, dq}{2\pi} |pq\rangle \langle pq| = \hat{1}. \tag{2.96c}$$

where $\omega > 0$ is arbitrary. As is well known, the coherent states form a (over) complete set, so it should be possible to represent an arbitrary operator $\hat{\rho}$ in the form

$$\hat{\rho} = \int \frac{dp \, dq}{2\pi} \rho(p, q) |pq\rangle \langle pq|.$$ \tag{2.97}

In our application $\hat{\rho}$ is a density operator, for which

$$\int \frac{dp \, dq}{2\pi} \rho(p, q) = 1. \tag{2.98}$$
Taking matrix elements of the above equation with $|p', q'angle$ and $\langle -p', -q'| \hat{\rho} |p', q'\rangle$ gives
\[ e^{(\omega^2 q'^2 + p'^2)/2\omega} \langle -p', -q'| \hat{\rho} |p', q'\rangle = \int \frac{dp \, dq}{2\pi} e^{i(p'q - p'q')} e^{-(\omega^2 q^2 + p^2)/2\omega} \rho(p, q), \] (2.99)
from which follows that the function $\rho(p, q)$ is given by the inverse Fourier transform
\[ \rho(p, q) = e^{(\omega^2 q^2 + p^2)/2\omega} \int \frac{dp' \, dq'}{2\pi} e^{-i(p'q - p'q')} e^{(\omega^2 q'^2 + p'^2)/2\omega} \langle -p', -q'| \hat{\rho} |p', q'\rangle. \] (2.100)

A trivial example is a coherent state centred about $(p_1, q_1)$, for which $\rho(p, q) = 2\pi\delta(p - p_1)\delta(q - q_1)$. Another simple example is given by the thermal density operator of the harmonic oscillator with Hamiltonian $H = (\omega^2 q^2 + p^2)/2$,
\[
\hat{\rho} = \frac{1}{Z} \exp \left[ -\beta \omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \right],
\] (2.101)
with $Z$ the partition function, such that $\text{Tr} \hat{\rho} = 1$. Choosing the $\omega$ in the definition of the coherent states equal to the $\omega$ appearing in this $\hat{\rho}$, it follows that
\[
\langle -p', -q'| \hat{\rho} |p', q'\rangle = \frac{1}{Z} \exp \left[ -\left( e^{-\beta \omega} - 1 \right) \frac{1}{2\omega} (\omega^2 q'^2 + p'^2) - \frac{1}{2} \beta \omega \right],
\] (2.102)
and
\[
\rho(p, q) = \frac{1}{Z} \exp \left[ -\left( e^{\beta \omega} - 1 \right) \frac{1}{2\omega} (\omega^2 q^2 + p^2) + \frac{1}{2} \beta \omega \right].
\] (2.103)
We recognise the inverse Bose-Einstein distribution, $\exp(\beta \omega) - 1$, in the exponent. For large temperatures, $\beta \omega \ll 1$, $\rho(p, q)$ approaches the classical Boltzmann distribution $\exp(-\beta H)$. In the limit of zero temperature we get the distribution representing the ground state,
\[
\rho(p, q) = 2\pi\delta(p)\delta(q).
\] (2.104)
More examples can be found in Ref. [39, 40]. The generalisation to the scalar field is straightforward.

2.B EQUIPMENT?

The effective Hamiltonian $H_{\text{eff}}[\varphi, \pi, \xi, \eta]$ of the Gaussian approximation is conserved in time. So one may expect that after very large times the system reaches
classical equilibrium. Assuming ergodicity, time averages will then correspond to the Boltzmann distribution \( \exp(-H_{\text{eff}}/T) \), under the constraints of the conserved generalised angular momenta \( L_{\alpha \alpha', \beta \beta'} \), cf. (2.27). We shall now derive an approximate form for the particle distribution function \( n_k \), corresponding to this classical equilibration.

In our derivation we assume the system to be weakly coupled, such that we may approximate \( H_{\text{eff}} \) in the Boltzmann distribution by a free field form (possibly after having shifted \( \varphi \) by its equilibrium value such that \( \langle \varphi \rangle = 0 \)),

\[
H_{\text{free}} = \int dx \left[ \frac{1}{2} \pi^2 + \frac{1}{2} (\partial \varphi)^2 + \frac{1}{2} m^2 \varphi^2 + \sum_{\alpha} (|\eta_{\alpha}|^2 + |\partial \xi_{\alpha}|^2 + m^2 |\xi_{\alpha}|^2) \right],
\]

(2.105)

where \( m \) is an effective mass. For convenience we use a complex formalism for the mode functions, \( \xi_{\alpha} = (\xi_{\alpha 1} - i \xi_{\alpha 2}) / \sqrt{2} = \sqrt{n_0^\alpha + 1/2} f_{\alpha} \), cf. (2.21). The generalised angular momenta are just the naturally conserved charges of the complex fields,

\[
Q_{\alpha} = i \int dx (\xi_{\alpha}^* \eta_{\alpha} - \eta_{\alpha} \xi_{\alpha}) = L_{\alpha 1, \alpha 2} = n_0^\alpha + \frac{1}{2}.
\]

(2.106)

We take them into account by introducing chemical potentials \( \mu_{\alpha} \), such that the average charges are equal to their values set by the initial conditions, \( Q_{\alpha} = n_0^\alpha + 1/2 \). It is not immediately clear that this procedure is correct, because these initial values are not extensive and therefore relative fluctuations will be large, but the emerging formulae below look reasonable. Imposing the constraints exactly appears to be quite cumbersome, except for \( N = 1 \). Recall that \( N \) is the number of complex mode functions, which in the lattice regularisation is equal to the number of lattice sites: \( N = \sum_k = \sum_{\alpha} \). Here we shall assume a sharp momentum cutoff \( |k| < \Lambda \), for simplicity.

The classical grand canonical average will be indicated by an over-bar:

\[
\overline{F} = \frac{1}{Z_c} \int [d\varphi \, d\pi] \prod_{\alpha} d\xi_{\alpha} \, d\eta_{\alpha} \exp \left[ -\frac{1}{T} \left( H_{\text{free}} - \sum_{\alpha} \mu_{\alpha} Q_{\alpha} \right) \right] F,
\]

(2.107)

with \( Z_c \) the partition function such that \( \overline{T} = 1 \). Our approximation for \( n_k \) is now given by (\( \omega_k = \sqrt{m^2 + k^2} \))

\[
S(x, y) = \sum_k e^{i k(x-y)} \frac{n_k + 1/2}{\omega_k},
\]

\[
= \varphi(x) \varphi(y) + \sum_{\alpha} \left[ \frac{n_0^\alpha + 1}{n_0^\alpha + 1/2} \xi_{\alpha}^*(x) \xi_{\alpha}(y) + \frac{n_0^\alpha}{n_0^\alpha + 1/2} \xi_{\alpha}^*(x) \xi_{\alpha}(y) \right].
\]

(2.108)

\footnote{We added a superscript 0 to \( n_{\alpha} \) to indicate that these are the initial values at time \( t = 0 \), in order to avoid possible confusion with the \( n_k \).}
The calculation is a straightforward free field exercise. Introducing the classical analogues of the creation and annihilation operators,

\[ \varphi(x) = \sum_k \frac{e^{ikx}}{\sqrt{2\omega_k L}} (a_k + a^*_k), \quad \xi_{\alpha} = \sum_k \frac{e^{ikx}}{\sqrt{2\omega_k L}} (a_{\alpha k} + b^*_{\alpha -k}), \]

(2.109)

and accordingly for the canonical momenta \( \pi \) and \( \eta_{\alpha} \), we get

\[ H_{\text{free}} = \sum_k \left( |a_k|^2 + \sum_{\alpha} |a_{\alpha k}|^2 + |b_{\alpha k}|^2 \right) \omega_k, \]

(2.110a)

\[ Q_\alpha = \sum_k |a_{\alpha k}|^2 - |b_{\alpha k}|^2. \]

(2.110b)

It follows that

\[ n_k + \frac{1}{2} = \frac{|a_k|^2 + \sum_{\alpha} |a_{\alpha k}|^2 + |b_{\alpha k}|^2}{\omega_k} \]

\[ = \frac{T}{\omega_k} + \sum_{\alpha} \left( \frac{T}{\omega_k - \mu_\alpha} + \frac{T}{\omega_k + \mu_\alpha} \right). \]

(2.111)

The \( \mu_{\alpha} \) are to be determined by the conditions

\[ n_0^\alpha + \frac{1}{2} = Q_{\alpha} = \sum_k \left( |a_{\alpha k}|^2 - |b_{\alpha k}|^2 \right) \]

\[ = \sum_k \left( \frac{T}{\omega_k - \mu_\alpha} - \frac{T}{\omega_k + \mu_\alpha} \right). \]

(2.112)

Before turning to the case \( n_0^\alpha = 0 \) used mostly in this paper, we comment on the properties of the above equations. Suppose there is only one complex mode function (“quantum mechanics”): \( N = 1 \). Then the solution of the equations is given by

\[ \mu = \sqrt{\omega^2 + \frac{T^2}{(n^0 + 1/2)^2} - \frac{T}{n^0 + 1/2}}, \]

(2.113a)

\[ n + \frac{1}{2} = \sqrt{\left( n^0 + \frac{1}{2} \right)^2 + \frac{T^2}{\omega^2} + \frac{T}{\omega}}, \]

(2.113b)

for which \( n \geq n^0 \). We see that \( \mu \to \omega, n \to n^0 \) as \( T \to 0 \), and \( \mu \to 0, n \to \infty \) as \( T \to \infty \).
For finite \( N \), eq. (2.112) for \( \mu_\alpha \) can be rewritten as a polynomial equation of degree \( 2N \) by multiplying the LHS and RHS by \( \prod_k (\omega_k^2 - \mu_\alpha^2) \). So there are in principle \( 2N \) solutions for each \( \mu_\alpha \). For \( T \to 0 \) we have a solution in which \( \alpha \leftrightarrow k \) (as in (2.29b), behaving as

\[
\mu_k = \omega_k - T/(n_k^0 + 1/2) + \cdots, \quad n_k = n_k^0 + \cdots. \tag{2.114}
\]

For the case \( n_\alpha^0 \equiv 0 \) it is natural to look for a solution in which all the chemical potentials are equal, \( \mu_\alpha = \mu \). Eq. (2.112) then reduces to

\[
\frac{1}{2} = 2T\mu \sum_k \frac{1}{\omega_k^2 - \mu^2} \approx 2TL\mu \int_0^\Lambda \frac{dk}{\pi} \frac{1}{m^2 + k^2 - \mu^2}
\]

\[
\approx \frac{TL\mu}{\sqrt{m^2 - \mu^2}},
\]

for large volumes \( mL \gg 1 \) and large momentum cutoff \( \Lambda/m \gg 1 \) (the integral converges for \( \Lambda \to \infty \)). It follows that

\[
\mu \approx \frac{m}{\sqrt{1 + 4T^2L^2}}. \tag{2.115}
\]

On the other hand, we have from (2.111),

\[
n_k + \frac{1}{2} = \frac{T}{\omega_k} + 2NT\omega_k,
\]

which depends explicitly on the number of modes \( N \). We see that \( n_k + 1/2 \) falls roughly like \( 1/\omega_k \), and there is a danger that \( n_k \) may get negative for large \( \omega_k \), which should not happen.

In fact, in our numerical simulations we always found the \( n_k \) to be positive, however it did not follow the distribution (2.117) for all \( k \). Even after very large times we usually find that only a limited number of modes are able to thermalize approximately classically, except for small systems such as in Fig. 2.10.

If we approximate

\[
N = \sum_k \approx L \int_0^\Lambda \frac{dk}{\pi} = L\Lambda/\pi, \quad \omega_\Lambda \approx \Lambda, \tag{2.118}
\]

the condition

\[
n_\Lambda + 1/2 \approx 2TN/\Lambda \geq 1/2 \tag{2.119}
\]

leads to

\[
LT \geq \pi/4. \tag{2.120}
\]
If this condition is not satisfied, more complicated solutions for the chemical potentials may be needed in which $\mu_k \approx \omega_k$, as in (2.114). We have explored such solutions on the lattice, using Mathematica. Despite ambiguities (e.g. funny behaviour of the alternating lattice modes), such solutions indicate that $n_k \omega_k$ is quite constant (but apparently not exactly), i.e. approximate equipartition.

So we tentatively conclude that, approximately, $n_k \approx T_{cl}/\omega_k$ is the predicted form for the particle distribution at very large times.