Eur. Phys. J. C 38, 135–143 (2004)
Digital Object Identifier (DOI) 10.1140/epjc/s2004-02007-0

THE EUROPEAN PHYSICAL JOURNAL C

Particle number in kinetic theory

B. Garbrecht[a], T. Prokopec[b], M. G. Schmidt[c]

Institut für Theoretische Physik, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany

Received: 18 May 2004 / Revised version: 27 August 2004
Published online: 20 October 2004 –

Abstract. We provide a derivation for the particle number densities on phase space for scalar and fermionic fields in terms of Wigner functions. Our expressions satisfy the desired properties: for bosons the particle number is positive, for fermions it lies in the interval between *zero* and *one*, and both are consistent with thermal field theory. As applications we consider the Bunch–Davies vacuum and fermionic preheating after inflation.

1 Introduction

The notion of particles is very intuitive, and at the classical level, in statistical physics, the dynamics is very successfully described by the classical Boltzmann equation for particle densities in phase space. In quantum physics however, the uncertainty principle seems to prohibit the use of phase space densities, and they are replaced by their closest analogues, the Wigner functions [1,2]. Yet, strictly speaking they can neither be interpreted as particle numbers nor as probability distributions on phase space, since they may acquire negative values. Attempts have been made to define particle number in relativistic quantum kinetic theory [3], but so far there exists no result that would be applicable to general situations.

In spite of those difficulties, the dynamics of quantum fields and particle numbers in the presence of temporally varying background fields has been extensively studied and is well understood [4–6]. The particle number operator can be calculated by a Bogolyubov transformation rotating the Fock space to a new basis, which mixes positive and negative frequency solutions.

In the analysis presented in this paper we show that the Wigner function, which we here take as an expectation value with respect to the ground state of the original basis, provides the necessary information about the rotated basis to calculate the particle number produced by the coupling to time-dependent external fields.

2 Scalars

As the first model case we consider a massive scalar field minimally coupled to gravity, such that in a conformal space-time, with the metric of the form $g_{\mu\nu} = a^2\eta_{\mu\nu}$, the Lagrangean is given by

$$\sqrt{-g}\mathcal{L}_{\Phi} = \frac{1}{2}a^2\eta^{\mu\nu}(\partial_\mu\Phi)(\partial_\nu\Phi) - \frac{1}{2}a^4 m_\phi^2\Phi^2, \qquad (1)$$

where $\eta^{\mu\nu} = \mathrm{diag}[1,-1,-1,-1]$ is the Minkowski (flat) metric, and $a = a(\eta)$ is the scale factor. For example, in inflation $a = -1/(H\eta)$ $(\eta < 0)$, while in the radiation-matter era, $a = a_r\eta + a_m\eta^2$. Here η denotes conformal time, a_r and a_m are constants.

We quantize the theory (1) by promoting $\Phi(x)$ to an operator,

$$\Phi(x) \equiv \frac{\varphi}{a} = \frac{1}{aV}\sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\Big(\varphi_{\mathbf{k}}(\eta)a_{\mathbf{k}} + \varphi^*_{-\mathbf{k}}(\eta)a^\dagger_{-\mathbf{k}}\Big),$$

where V denotes the comoving volume. The mode functions obey the Klein–Gordon equation

$$\big(\partial_\eta^2 + \omega_{\mathbf{k}}^2 - a''/a\big)\varphi_{\mathbf{k}} = 0, \qquad (2)$$

where $' \equiv \mathrm{d}/\mathrm{d}\eta$, $\omega_{\mathbf{k}}^2 = \mathbf{k}^2 + a^2 m_\phi^2(\eta)$ defines the single particle (comoving) energy, and we take for the Wronskian

$$\varphi^*_{\mathbf{k}}\varphi'_{\mathbf{k}} - \varphi^{*\prime}_{\mathbf{k}}\varphi_{\mathbf{k}} = \mathrm{i}. \qquad (3)$$

Throughout this paper we assume that the modes $\varphi_{\mathbf{k}} = \varphi_k$ $(k \equiv |\mathbf{k}|)$ are homogeneous, which is justified when the mass is varying slowly in space, such that we can ignore its gradients. The field $\varphi = a\Phi$ obeys the canonical commutation relation,

$$[\varphi(\mathbf{x},\eta), \partial_\eta\varphi(\mathbf{x}',\eta)] = \mathrm{i}\delta^3(\mathbf{x}-\mathbf{x}'), \qquad (4)$$

which implies $[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}$.

The fundamental quantity of quantum kinetic theory is the two-point Wightman function, which we here write

[a] e-mail: B.Garbrecht@thphys.uni-heidelberg.de
[b] e-mail: T.Prokopec@thphys.uni-heidelberg.de
[c] e-mail: M.G.Schmidt@thphys.uni-heidelberg.de

for the ground state $|0\rangle$ annihilated by $a_{\mathbf{k}}$, $a_{\mathbf{k}}|0\rangle = 0$. With the rescaling suitable for conformal space-times, it reads

$$\mathrm{i}\bar{G}^{<}(u,v) \equiv a(u)\mathrm{i}G^{<}(u,v)a(v) = \langle 0|\varphi(v)\varphi(u)|0\rangle\,, \quad (5)$$

and its Wigner transform is defined as

$$\mathrm{i}G^{<}(k,x) = \int \mathrm{d}^4 r \mathrm{e}^{\mathrm{i}k\cdot r}\mathrm{i}G^{<}(x+r/2, x-r/2)\,,$$

which satisfies the Klein–Gordon equation [7,8]

$$\left(-\mathrm{i}k_0\partial_\eta + \frac{1}{4}\partial_\eta^2 - k^2 + \bar{m}_\phi^2(\eta)\mathrm{e}^{-\frac{\mathrm{i}}{2}\overleftarrow{\partial}_\eta \partial_{k_0}}\right)\mathrm{i}\bar{G}^{<} = 0, \quad (6)$$

where $\bar{m}_\phi^2 = a^2 m_\phi^2 - a''/a$. It is then useful to define the nth moments of the Wigner function,

$$f_n(\mathbf{k},x) \equiv \int \frac{\mathrm{d}k_0}{2\pi} k_0^n \mathrm{i}\bar{G}^{<}(k,x). \quad (7)$$

Taking the 1st (0th) moment of the imaginary (real) part of (6) yields [7,8]

$$f_2' - \frac{1}{2}(\bar{m}_\phi^2)' f_0 = 0, \qquad \frac{1}{4}f_0'' - f_2 + \bar{\omega}_{\mathbf{k}}^2 f_0 = 0, \quad (8)$$

with $\bar{\omega}_{\mathbf{k}}^2 = \mathbf{k}^2 + \bar{m}_\phi^2$. Eliminating f_2 from (8) yields [8]

$$f_0''' + 4\bar{\omega}_{\mathbf{k}}^2 f_0' + 2(\bar{\omega}_{\mathbf{k}}^2)' f_0 = 0. \quad (9)$$

This can be integrated once to give

$$\bar{\omega}_{\mathbf{k}}^2 f_0^2 + \frac{1}{2}f_0'' f_0 - \frac{1}{4}{f_0'}^2 = \frac{1}{4}\,, \quad (10)$$

where the integration constant is obtained by making use of $f_0 = |\varphi_{\mathbf{k}}|^2$ (cf. (27) below), (2) and the Wronskian (3).

2.1 Bogolyubov transformation

The Hamiltonian density corresponding to the Lagrangean (1) reads

$$H = \frac{1}{2V}\sum_{\mathbf{k}}\left\{\Omega_{\mathbf{k}}(a_{\mathbf{k}}a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}^\dagger a_{\mathbf{k}}) + (\Lambda_{\mathbf{k}}a_{\mathbf{k}}a_{-\mathbf{k}} + \mathrm{h.c.})\right\},$$
$$\Omega_{\mathbf{k}} = |\varphi_k' - (a'/a)\varphi_k|^2 + \omega_{\mathbf{k}}^2|\varphi_k|^2\,,$$
$$\Lambda_{\mathbf{k}} = \left(\varphi_k' - \frac{a'}{a}\varphi_k\right)^2 + \omega_{\mathbf{k}}^2\varphi_k^2. \quad (11)$$

Consider now the homogeneous Bogolyubov transformation

$$\begin{pmatrix}\hat{a}_{\mathbf{k}} \\ \hat{a}_{-\mathbf{k}}^\dagger\end{pmatrix} = \begin{pmatrix}\alpha_k & \beta_k^* \\ \beta_k & \alpha_k^*\end{pmatrix}\begin{pmatrix}a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger\end{pmatrix}, \quad (12)$$

with the norm

$$|\alpha_k|^2 - |\beta_k|^2 = 1\,, \quad (13)$$

upon which $\Lambda_{\mathbf{k}}$ and $\Omega_{\mathbf{k}}$ transform as

$$\Lambda_{\mathbf{k}}' = -2\alpha_k^*\beta_k\Omega_{\mathbf{k}} + (\alpha_k^*)^2\Lambda_{\mathbf{k}} + \beta_k^2\Lambda_{\mathbf{k}}^* \quad (14)$$

$$\Omega_{\mathbf{k}}' = (|\alpha_k|^2 + |\beta_k|^2)\Omega_{\mathbf{k}} - \alpha_k^*\beta_k^*\Lambda_{\mathbf{k}} - \alpha_k\beta_k\Lambda_{\mathbf{k}}^*. \quad (15)$$

In terms of real and imaginary parts, these equations can be recast as

$$\begin{aligned}&2|\alpha_k||\beta_k|\Omega_{\mathbf{k}} + |\Lambda_{\mathbf{k}}'|\cos(\phi_\lambda + \phi_\alpha - \phi_\beta)\\ &\quad - (|\alpha_k|^2 + |\beta_k|^2)|\Lambda_{\mathbf{k}}|\cos(\phi_\Lambda - \phi_\alpha - \phi_\beta)\\ &\quad = 0, \end{aligned} \quad (16)$$

$$\begin{aligned}&|\Lambda_{\mathbf{k}}'|\sin(\phi_{\Lambda'} + \phi_\alpha - \phi_\beta)\\ &\quad - |\Lambda_{\mathbf{k}}|\sin(\phi_\Lambda - \phi_\alpha - \phi_\beta)\\ &\quad = 0,\end{aligned} \quad (17)$$

$$\begin{aligned}&\Omega_{\mathbf{k}}' - (|\alpha_k|^2 + |\beta_k|^2)\Omega_{\mathbf{k}}\\ &\quad + 2|\alpha_k|\,|\beta_k|\,|\Lambda_{\mathbf{k}}|\cos(\phi_\Lambda - \phi_\alpha - \phi_\beta)\\ &\quad = 0,\end{aligned} \quad (18)$$

with $|\alpha_k| = \sqrt{1 + |\beta_k|^2}$, and where we have introduced the phases

$$\Lambda_{\mathbf{k}}' = |\Lambda_{\mathbf{k}}'|\exp(\mathrm{i}\phi_{\Lambda'})\,, \quad \Lambda_{\mathbf{k}} = |\Lambda_{\mathbf{k}}|\exp(\mathrm{i}\phi_\Lambda) \quad (19)$$
$$\alpha_k = |\alpha_k|\exp(\mathrm{i}\phi_\alpha)\,, \quad \beta_k = |\beta_k|\exp(\mathrm{i}\phi_\beta)\,. \quad (20)$$

Equations (16) and (18) can be combined to give

$$\cos(\phi_\lambda + \phi_\alpha - \phi_\beta) = \frac{(|\alpha_k|^2 + |\beta_k|^2)\Omega_{\mathbf{k}} - \Omega_{\mathbf{k}}'}{2|\alpha_k|\,|\beta_k|\,|\Lambda_{\mathbf{k}}|}\,, \quad (21)$$

while (18) gives an expression for $\cos(\phi_\Lambda - \phi_\alpha - \phi_\beta)$. Upon squaring (17) and making use of $\sin^2(\zeta) = 1 - \cos^2(\zeta)$, we find that

$$\Omega_{\mathbf{k}}^2 - |\Lambda_{\mathbf{k}}|^2 = {\Omega_{\mathbf{k}}'}^2 - |\Lambda_{\mathbf{k}}'|^2 \quad (22)$$

is an invariant of the Bogolyubov transformations (12).

Next we solve (18) for $n_{\mathbf{k}} \equiv |\beta_k|^2$ to find

$$n_{\mathbf{k}\pm} = \frac{\Omega_{\mathbf{k}}\Omega_{\mathbf{k}}' \pm \sqrt{|\Lambda_{\mathbf{k}}|^2 x^2({\Omega_{\mathbf{k}}'}^2 - \Omega_{\mathbf{k}}^2 + |\Lambda_{\mathbf{k}}|^2 x^2)}}{2(\Omega_{\mathbf{k}}^2 - |\Lambda_{\mathbf{k}}|^2 x^2)} - \frac{1}{2}, \quad (23)$$

where $x \equiv \cos(\varphi_\Lambda - \varphi_\alpha - \varphi_\beta)$. Upon extremizing this with respect to x^2, one can show that a maximum is formally reached for $x_{\max}^2 = \Omega_{\mathbf{k}}^2/|\Lambda_{\mathbf{k}}|^2$, which must be greater than one if the Hamiltonian (11) is to be diagonalizable. Taking account of $x^2 \le 1$, one gets that the maximum for $n_{\mathbf{k}\pm}$ is reached when $x^2 = 1$, for which

$$n_{\mathbf{k}\pm} = \frac{\Omega_{\mathbf{k}}\sqrt{\Omega_{\mathbf{k}}^2 - |\Lambda_{\mathbf{k}}|^2 + |\Lambda_{\mathbf{k}}'|^2} \pm |\Lambda_{\mathbf{k}}|\,|\Lambda_{\mathbf{k}}'|}{2(\Omega_{\mathbf{k}}^2 - |\Lambda_{\mathbf{k}}|^2)} - \frac{1}{2}\,. \quad (24)$$

Since $n_{\mathbf{k}-} = 0$ when $|\Lambda_{\mathbf{k}}'| = |\Lambda_{\mathbf{k}}|$, the physical branch corresponds to $n_{\mathbf{k}} = n_{\mathbf{k}-}$. Furthermore, when considered as a function of $|\Lambda_{\mathbf{k}}'|$, $n_{\mathbf{k}} \equiv n_{\mathbf{k}-}$ monotonically increases as $|\Lambda_{\mathbf{k}}'|$ decreases, reaching a maximum when $|\Lambda_{\mathbf{k}}'| = 0$ (see Fig. 1), for which the particle number

$$n_{\mathbf{k}} = \langle 0|\hat{a}_{\mathbf{k}}^\dagger\hat{a}_{\mathbf{k}}|0\rangle = \frac{\Omega_{\mathbf{k}}}{2\omega_{\mathbf{k}}} - \frac{1}{2}\,, \quad (25)$$

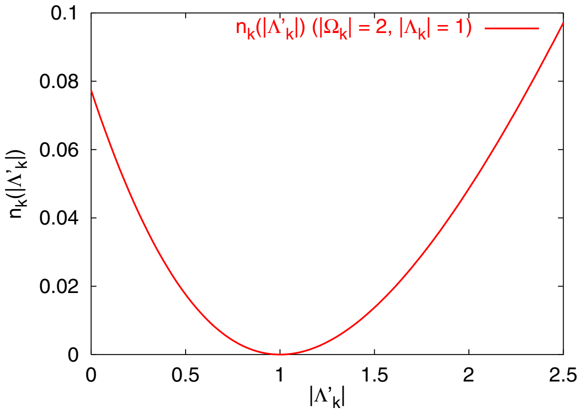

Fig. 1. Particle number $n_{\mathbf{k}}$ as a function of $|\Lambda'_{\mathbf{k}}|$ for $|\Omega_{\mathbf{k}}| = 2$, $|\Lambda_{\mathbf{k}}| = 1$. Provided $|\Lambda'_{\mathbf{k}}| \leq |\Lambda_{\mathbf{k}}|$, $n_{\mathbf{k}}$ maximizes at $|\Lambda'_{\mathbf{k}}| = 0$

where $\omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + a^2 m_\phi^2}$. This definition, which corresponds to the (constrained) maximum possible particle number a detector can observe, we shall be using as our definition for particle number on phase space. Moreover, note that, in terms of the thus transformed creation and annihilation operators $\hat{a}^\dagger_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$, the Hamiltonian is diagonal

$$H = \frac{1}{2V}\sum_{\mathbf{k}} \omega_{\mathbf{k}}(\hat{a}_{\mathbf{k}}\hat{a}^\dagger_{\mathbf{k}} + \hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}}), \quad [\hat{a}_{\mathbf{k}}, \hat{a}^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}, \tag{26}$$

such that our definition agrees with the one advocated, for example, in [4, 9].

2.2 Particle number in scalar kinetic theory

It is now a simple matter to calculate the particle number in terms of Wigner functions. Making use of (5) and (7) we find

$$|\varphi_k|^2 = f_0, \qquad |\varphi'{}_k|^2 = \frac{1}{2}f_0'' + \bar{\omega}^2_{\mathbf{k}} f_0, \tag{27}$$

from which it follows that

$$\Omega_{\mathbf{k}} = 2\left(\omega^2_{\mathbf{k}} f_0 + \frac{1}{4}f_0''\right) - \frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{a'}{a}f_0\right). \tag{28}$$

We then insert (28) into (25) to get

$$n_{\mathbf{k}} = \omega_{\mathbf{k}} f_0 + \frac{1}{4\omega_{\mathbf{k}}}f_0'' - \frac{1}{2} - \frac{1}{2\omega_{\mathbf{k}}}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{a'}{a}f_0\right). \tag{29}$$

This is our main result for scalars, which is positive, simply because $n_{\mathbf{k}} \equiv |\beta_k|^2 \geq 0$ (see (25)). Equation (29) is of course not a unique definition of particle number. Indeed, any Bogolyubov transformation (12) and (13) corresponds to some particle number definition. Our definition (29) is however a special one, in that it corresponds to the detector with the best possible resolution, i.e. which measures the maximum number of particles, as we showed in Sect. 2.1.

We now apply (29) to the Chernikov–Tagirov [10] (Bunch–Davies [11]) vacuum,

$$\varphi_k = \frac{1}{\sqrt{2k}}\left(1 - \frac{\mathrm{i}}{k\eta}\right)\mathrm{e}^{-\mathrm{i}k\eta}, \tag{30}$$

which corresponds to the mode functions of a minimally coupled massless scalar field in de Sitter inflation, $a = -1/H\eta$ (cf. (2)), for which $f_0 = (2k)^{-1}\big(1 + 1/(k\eta)^2\big)$, leading to the particle number

$$n_{\mathbf{k}} = \frac{1}{4k^2\eta^2} = a^2\left(\frac{H}{2k}\right)^2. \tag{31}$$

This is to be compared with [12], which finds $n_{\mathbf{k}} \sim (-k\eta)^{-3}$ $(-k\eta \ll 1)$.

We suspect that the difference is due to the approximate methods used in [12]. On the other hand, when considering the transition from de Sitter inflation to radiation, one finds that the spectrum $n_{\mathbf{k}} \sim (-k\eta_0)^{-4}$ $(-k\eta_0) \gg 1$ (η_0 denotes conformal time at the end of inflation) is produced [13].

As a consistency check, we now apply (29) to thermal equilibrium, where the Wigner function is (cf. [14])

$$\mathrm{i}G^< = 2\pi \mathrm{sign}(k_0)\delta(k^2 - m_\phi^2)\frac{1}{\mathrm{e}^{\beta k_0} - 1}. \tag{32}$$

By making use of (7) and (29) we obtain the standard Bose–Einstein distribution, $n_{\mathbf{k}} = 1/(\mathrm{e}^{\beta\omega_{\mathbf{k}}} - 1)$.

Recently, an interesting particle number definition has been proposed in [15], according to which (expanding space-times are not considered)

$$\left(\tilde{n}_{\mathbf{k}} + \frac{1}{2}\right)^2 = |\phi_k|^2\,|\phi_k'|^2 = f_0\left(\frac{1}{2}f_0'' + \bar{\omega}^2_{\mathbf{k}} f_0\right). \tag{33}$$

Note that in the adiabatic domain, in which $f_0'' \to 0$, (33) and (29) both reduce to $n_{\mathbf{k}} \to \omega_{\mathbf{k}} f_0 - 1/2$, such that for example in thermal equilibrium of a free scalar theory (32), both definitions yield the Bose–Einstein distribution. According to the authors of [15], the definition (33) should be applicable to general situations (whenever there is a reasonably accurate quasiparticle picture of the plasma), and it is obtained as a consistency requirement on the energy conservation, and quasiparticle current relation, respectively,

$$\frac{\omega^2_{\mathbf{k}}}{2}|\phi_k|^2 + \frac{1}{2}|\phi_k'|^2 = \omega_{\mathbf{k}}\left(\frac{1}{2} + \tilde{n}_{\mathbf{k}}\right), \quad \omega_{\mathbf{k}}|\phi_k|^2 = \frac{1}{2} + \tilde{n}_{\mathbf{k}}. \tag{34}$$

The consistency is reached when the kinetic and potential energies are equal, in which case a generalized quasiparticle energy is given by $\omega^2_{\mathbf{k}} = |\phi_k'|^2/|\phi_k|^2$.

In order to make a non-trivial comparison, consider now a pure state of a scalar theory interacting only weakly with a classical background field (which can be described by a time-dependent mass term). The WKB form for the mode functions can be recast as

$$\phi_k = \frac{1}{\sqrt{2\epsilon_{\mathbf{k}}}}\left(\alpha_0 \mathrm{e}^{-\mathrm{i}\int^\eta \epsilon_{\mathbf{k}}(\eta')\mathrm{d}\eta'} + \beta_0 \mathrm{e}^{\mathrm{i}\int^\eta \epsilon_{\mathbf{k}}(\eta')\mathrm{d}\eta'}\right), \tag{35}$$

$$\phi_k' = -\mathrm{i}\sqrt{\frac{\epsilon_{\mathbf{k}}}{2}}\left(\alpha_0 \mathrm{e}^{-\mathrm{i}\int^\eta \epsilon_{\mathbf{k}}(\eta')\mathrm{d}\eta'} - \beta_0 \mathrm{e}^{\mathrm{i}\int^\eta \epsilon_{\mathbf{k}}(\eta')\mathrm{d}\eta'}\right) - \frac{1}{2}\frac{\epsilon_{\mathbf{k}}'}{\epsilon_{\mathbf{k}}}\phi_k, \quad (36)$$

where $\epsilon_{\mathbf{k}}$ satisfies $\epsilon_{\mathbf{k}}^2 = \omega_{\mathbf{k}}^2 - (1/2)\epsilon_{\mathbf{k}}''/\epsilon_{\mathbf{k}} + (3/4)(\epsilon_{\mathbf{k}}'/\epsilon_{\mathbf{k}})^2$. In a free theory $|\alpha_0|^2 - |\beta_0|^2$ is conserved, and it is usually normalized to *one*. In an interacting theory however, the single particle description breaks down, and consequently $|\alpha_0|^2 - |\beta_0|^2$ is not conserved. For the purpose of this example, we assume that the interactions are weak enough, such that $|\alpha_0|^2 - |\beta_0|^2$ is changing sufficiently slowly, and the subsequent discussion applies. In the adiabatic limit $\epsilon_{\mathbf{k}} \to \omega_{\mathbf{k}} \to$ constant, the particle number (25) and (29) of the state (36) is simply $n_{\mathbf{k}}^{(0)} = |\beta_0|^2$.

On the other hand, when applied to the state (36), the definition (33) yields an oscillating particle number even in the adiabatic regime,

$$\left(\tilde{n}_{\mathbf{k}} + \frac{1}{2}\right)^2 \approx \frac{1}{4} + (1 + |\beta_0|^2)\,|\beta_0|^2 \sin^2(2\epsilon_{\mathbf{k}}\eta - \chi_\alpha + \chi_\beta)\,, \quad (37)$$

where $\alpha_0 = |\alpha_0|\mathrm{e}^{\mathrm{i}\chi_\alpha}, \beta_0 = |\beta_0|\mathrm{e}^{\mathrm{i}\chi_\beta}$, which is positive and bounded from above by[1] $\tilde{n}_{\mathbf{k}} \le |\beta_0|^2 \equiv n_{\mathbf{k}}^{(0)}$. Hence, for the state (36) our particle number definition (29) provides an upper limit for (33). This was to be expected, considering that (29) was derived in Sect. 2.1 by an extremization procedure over the Bogolyubov transformations (12). We expect that a similar behavior pertains in other situations.

3 Fermions

Provided the fields are rescaled as $a^{3/2}\psi \to \psi$ and the mass as $am \to m$, the fermionic Lagrangean reduces to the standard Minkowski form,

$$\sqrt{-g}\mathcal{L}_\psi \to \bar{\psi}\,\mathrm{i}\partial\!\!\!/\,\psi - \bar{\psi}(m_R + \mathrm{i}\gamma^5 m_{\mathrm{I}})\psi,$$

where, for notational simplicity, we omitted the rescaling of the fields and absorbed the scale factor in the mass term. Note that the complex mass term $m = m_R(\eta) + \mathrm{i}m_I(\eta)$ may induce CP-violation (cf. [16]).

The fermionic Wigner function,

$$\mathrm{i}S^<(k,x) = -\int \mathrm{d}^4 r \mathrm{e}^{\mathrm{i}k\cdot r}\langle 0|\bar{\psi}(x - r/2)\psi(x + r/2)|0\rangle,$$

satisfies the corresponding Dirac equation which, in the Wigner representation, reads

$$\left(k\!\!\!/ + \frac{\mathrm{i}}{2}\gamma^0\partial_t - (m_R + \mathrm{i}\gamma^5 m_I)\mathrm{e}^{-\frac{\mathrm{i}}{2}\overleftarrow{\partial_t}\partial_{k_0}}\right)\mathrm{i}S^< = 0, \quad (38)$$

where $(\mathrm{i}\gamma^0 S^<)^\dagger = \mathrm{i}\gamma^0 S^<$ is hermitean. The helicity operator in the Weyl representation $\hat{h} = \hat{\mathbf{k}}\cdot\gamma^0\boldsymbol{\gamma}\gamma^5$ commutes with the Dirac operator in (38), such that we can make the helicity block-diagonal ansatz for the Wigner function (cf. [16])

$$\mathrm{i}S^< = \sum_{h=\pm}\mathrm{i}S_h^<\,, \qquad -\mathrm{i}\gamma_0 S_h^< = \frac{1}{4}\big(1 + h\hat{\mathbf{k}}\cdot\boldsymbol{\sigma}\big)\otimes\rho^a g_{ah}, \quad (39)$$

where $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$ and σ^a, ρ^a $(a = 0,1,2,3)$ are the Pauli matrices. Taking the traces of $\{1, -h\gamma^i\gamma^5, -\mathrm{i}h\gamma^i, -\gamma^5\}$ times the real part of (38), and integrating over k_0, yields the kinetic equations for the 0th moments of g_{ah},

$$\dot{f}_{0h} = 0, \quad (40)$$

$$\begin{aligned}
&\dot{f}_{1h} + 2h|\mathbf{k}|f_{2h} - 2m_I f_{3h} = 0,\\
&\dot{f}_{2h} - 2h|\mathbf{k}|f_{1h} + 2m_R f_{3h} = 0,\\
&\dot{f}_{3h} - 2m_R f_{2h} + 2m_I f_{1h} = 0,
\end{aligned} \quad (41)$$

where

$$\begin{aligned}
f_{0h} &\equiv \mathrm{Tr}\left[(1P_h)\int\frac{\mathrm{d}k_0}{2\pi}(-\mathrm{i}\gamma^0 S^<)\right],\\
f_{1h} &\equiv \mathrm{Tr}\left[(-h\hat{\mathbf{k}}\cdot\boldsymbol{\gamma}\gamma^5 P_h)\int\frac{\mathrm{d}k_0}{2\pi}(-\mathrm{i}\gamma^0 S^<)\right],\\
f_{2h} &\equiv \mathrm{Tr}\left[(-\mathrm{i}h\hat{\mathbf{k}}\cdot\boldsymbol{\gamma}P_h)\int\frac{\mathrm{d}k_0}{2\pi}(-\mathrm{i}\gamma^0 S^<)\right],\\
f_{3h} &\equiv \mathrm{Tr}\left[(-\gamma^5 P_h)\int\frac{\mathrm{d}k_0}{2\pi}(-\mathrm{i}\gamma^0 S^<)\right],
\end{aligned} \quad (42)$$

and $P_h = (1/2)[1 + h\hat{\mathbf{k}}\cdot\gamma^0\boldsymbol{\gamma}\gamma^5]$ denotes the helicity projector. Equation (40) expresses the conservation of the Noether vector current. The traces of the imaginary parts of (38) decouple from (41) at tree level, and hence are of no importance for the analysis presented here. The moments f_{ah} can be related to the positive and negative frequency mode functions, $u_h(\mathbf{k},t)$ and $v_h(\mathbf{k},t) = -\mathrm{i}\gamma^2(u_h(\mathbf{k},t))^*$, respectively. They form a basis for the Dirac field,

$$\psi(x) = \frac{1}{V}\sum_{\mathbf{k}h}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\big(u_h a_{\mathbf{k}h} + v_h b_{-\mathbf{k}h}^\dagger\big), \quad u_h = \begin{pmatrix} L_h \\ R_h \end{pmatrix}\otimes\xi_h,$$

where ξ_h is the helicity two-eigenspinor, $\hat{h}\xi_h = h\xi_h$. The Dirac equation then decomposes into

$$\begin{aligned}
&\mathrm{i}\partial_0 L_h - h|\mathbf{k}|L_h = m_R R_h + \mathrm{i}m_I R_h,\\
&\mathrm{i}\partial_0 R_h + h|\mathbf{k}|R_h = m_R L_h - \mathrm{i}m_I L_h.
\end{aligned} \quad (43)$$

Note that these equations incorporate CP-violation and thus generalize the analysis of [5, 6, 17]. Now, from (43)

[1] Note that the definition of the quasiparticle energy, $\omega_{\mathbf{k}} \equiv |\phi_k'|/|\phi_k|$, oscillates even in the adiabatic limit, with the minimum and maximum values given by $\omega_{\mathbf{k},\min} = \epsilon_{\mathbf{k}}(|\alpha_0| - |\beta_0|)/(|\alpha_0| + |\beta_0|)$ and $\omega_{\mathbf{k},\max} = \epsilon_{\mathbf{k}}^2/\omega_{\mathbf{k},\min}$, respectively, such that $\omega_{\mathbf{k}} \ne \epsilon_{\mathbf{k}}$ in general. This indicates that imposing instantaneous equality of the potential and kinetic energies may not be appropriate in general situations. When particle number is understood as an average over the characteristic oscillation period however, imposing equality of the potential and kinetic energy may lead to a reasonable definition for the particle number density.

one can derive (40) and (41) by multiplying with L_h and R_h and employing

$$f_{0h} = |L_h|^2 + |R_h|^2, \quad f_{3h} = |R_h|^2 - |L_h|^2,$$
$$f_{1h} = -2\Re(L_h R_h^*), \quad f_{2h} = 2\Im(L_h^* R_h). \tag{44}$$

The Hamiltonian density reads

$$H = \frac{1}{V}\sum_{\mathbf{k}h}\Big\{\Omega_{\mathbf{k}h}\left(a^\dagger_{\mathbf{k}h}a_{\mathbf{k}h} + b^\dagger_{-\mathbf{k}h}b_{-\mathbf{k}h}\right) + (\Lambda_{\mathbf{k}h}b_{-\mathbf{k}h}a_{\mathbf{k}h} + \mathrm{h.c.})\Big\},$$

where

$$\Omega_{\mathbf{k}h} = hk\left(|L_h|^2 - |R_h|^2\right) + mL_h^*R_h + m^*L_hR_h^*,$$
$$\Lambda_{\mathbf{k}h} = 2kL_hR_h - hm^*L_h^2 + hmR_h^2, \tag{45}$$

with $\{\hat{a}_{\mathbf{k}h}, \hat{a}^\dagger_{\mathbf{k}'h'}\} = \delta_{h,h'}\delta_{\mathbf{k},\mathbf{k}'}$, $\{\hat{b}_{\mathbf{k}h}, \hat{b}^\dagger_{\mathbf{k}'h'}\} = \delta_{h,h'}\delta_{\mathbf{k},\mathbf{k}'}$. We now use the Bogolyubov transformation

$$\begin{pmatrix}\hat{a}_{\mathbf{k}h}\\ \hat{b}^\dagger_{-\mathbf{k}h}\end{pmatrix} = \begin{pmatrix}\alpha_{kh} & \beta_{kh}\\ -\beta^*_{kh} & \alpha^*_{kh}\end{pmatrix}\begin{pmatrix}a_{\mathbf{k}h}\\ b^\dagger_{-\mathbf{k}h}\end{pmatrix},$$

to diagonalize the Hamiltonian, where α_{kh} and β_{kh} are

$$\frac{1}{2}\left(\left|\frac{\alpha_{kh}}{\beta_{kh}}\right| - \left|\frac{\beta_{kh}}{\alpha_{kh}}\right|\right) = \frac{\Omega_{\mathbf{k}h}}{|\Lambda_{\mathbf{k}h}|}, \quad |\alpha_{kh}|^2 + |\beta_{kh}|^2 = 1, \tag{46}$$

leading to the particle number density on phase space,

$$n_{\mathbf{k}h} = |\beta_{kh}|^2 = \frac{1}{2} - \frac{\Omega_{\mathbf{k}h}}{2\omega_{\mathbf{k}}}, \tag{47}$$

where now $\omega_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + |m|^2}$.

To construct the initial mode functions in the adiabatic domain, $\eta \to -\infty$, we use the positive frequency solution and its charge conjugate,

$$\psi_{\mathbf{k}} \to \begin{pmatrix}\alpha_0 L_h^+ + \beta_0 L_h^-\\ \alpha_0 R_h^+ + \beta_0 R_h^-\end{pmatrix}, \qquad |\alpha_0|^2 + |\beta_0|^2 = 1.$$

From the Dirac equation under adiabatic conditions it follows that

$$L_h^+ = \sqrt{\frac{\omega_{\mathbf{k}} + hk}{2\omega_{\mathbf{k}}}}, \quad L_h^- = -\mathrm{i}\frac{m}{|m|}\sqrt{\frac{\omega_{\mathbf{k}} - hk}{2\omega_{\mathbf{k}}}},$$
$$R_h^+ = \frac{m^*}{\sqrt{2\omega_{\mathbf{k}}(\omega_{\mathbf{k}} + hk)}}, \quad R_h^- = \mathrm{i}\frac{|m|}{\sqrt{2\omega_{\mathbf{k}}(\omega_{\mathbf{k}} - hk)}}.$$

These mode functions correspond to an initial particle number $n^{(0)}_{\mathbf{k}} = |\beta_0|^2$. We now make use of (44) to express $\Omega_{\mathbf{k}h}$ in terms of the Wigner functions,

$$\Omega_{\mathbf{k}h} = -(hkf_{3h} + m_R f_{1h} + m_I f_{2h}), \tag{48}$$

which implies our main result for fermions,

$$n_{\mathbf{k}h} = \frac{1}{2\omega_{\mathbf{k}}}\left(hkf_{3h} + m_R f_{1h} + m_I f_{2h}\right) + \frac{1}{2}. \tag{49}$$

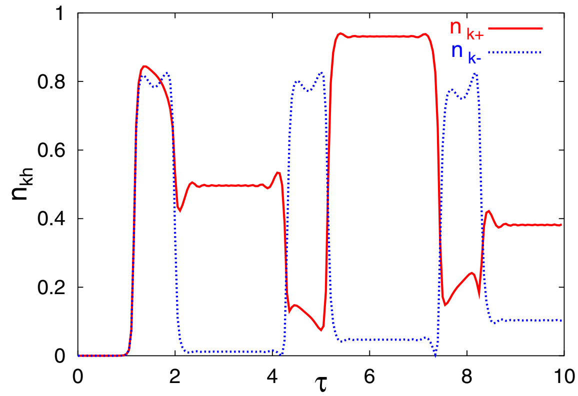

Fig. 2. The number of produced fermions as a function of time with helicity $h = +$ (solid) and $h = -$ (dotted), mass $m/\omega_{\mathrm{I}} = 10 + 15\cos(2\tau) - \mathrm{i}\sin(2\tau)$, $|\mathbf{k}| = \omega_{\mathrm{I}}$, $\tau = \omega_{\mathrm{I}} t$, where ω_{I} denotes the frequency of the inflaton oscillations

Note that in the limit $m \to 0$, this expression reduces to the phase space density of axial particles. Moreover, $0 \leq n_{\mathbf{k}h} \equiv |\beta_{kh}|^2 = 1 - |\alpha_{kh}|^2 \leq 1$ (see (46)–(47)).

As an application of (49) we consider particle production at preheating [9,17], in which the fermionic mass is generated by an oscillating inflaton condensate. Assuming that the inflaton oscillates as a cosine function results in the fermion production shown in Fig. 2. Observe that, even for a relatively small imaginary (pseudoscalar) mass term, particle production of the opposite helicity states is completely different, implying a non-perturbative enhancement of a CP-violating particle density, $n_{\mathbf{k}+} - n_{\mathbf{k}-}$, which may be of relevance for baryogenesis.

When applied to thermal equilibrium, where (cf. [14])

$$\mathrm{i}S^< = -(\not{k} + m_R - \mathrm{i}\gamma_5 m_I)\delta(k^2 - |m|^2)\frac{2\pi\mathrm{sign}(k_0)}{\mathrm{e}^{\beta k_0} + 1}, \tag{50}$$

we find

$$f_{0h} = 1,$$
$$f_{1h} = (2m_R/\omega_{\mathbf{k}})[\{\exp(\beta\omega_{\mathbf{k}}) + 1\}^{-1} - 1/2],$$
$$f_{2h} = (2m_I/\omega_{\mathbf{k}})[\{\exp(\beta\omega_{\mathbf{k}}) + 1\}^{-1} - 1/2],$$
$$f_{3h} = (2hk/\omega_{\mathbf{k}})[\{\exp(\beta\omega_{\mathbf{k}}) + 1\}^{-1} - 1/2],$$

such that (49) yields the Fermi–Dirac distribution, $n_{\mathbf{k}h} = 1/(\mathrm{e}^{\beta\omega_{\mathbf{k}}} + 1)$.

4 Multiflavor case

We now generalize the definition of particle number in terms of two-point functions to the case of several species, mixing through a mass matrix. While in the single-flavor case always an equal number of particles and antiparticles is produced, we will here encounter the creation of a charge asymmetry when the mass matrix is non-symmetric. Because of this charge violation, the orthogonality of particle modes with respect to antiparticle modes is not preserved under time evolution, and it is thus impossible to expand the field operators in terms of an orthogonal basis.

Hence, the use of the basis-independent two-point functions is advantageous. We can either calculate the time evolution of the system in terms of these quantities or measure them, since they correspond to physical charge and current densities. When finally the mass matrix is diagonal and only adiabatically slowly evolving, there exists a well-defined basis, in terms of which the Hamiltonian is diagonal. We use this basis to define the particle number operators and construct their expectation values out of the two-point functions.

4.1 Fermions

Since Dirac spinors naturally include particle and antiparticle modes, we here first discuss the fermionic case. We decompose the mass matrix M into a hermitean and an antihermitean part,

$$M_H = \frac{1}{2}(M + M^\dagger), \quad M_A = \frac{1}{2\mathrm{i}}(M - M^\dagger), \tag{51}$$

such that the Dirac equation reads

$$\left[\mathrm{i}\partial\!\!\!/ - M_H - \mathrm{i}\gamma^5 M^A\right]_{ij} \psi_j = 0. \tag{52}$$

One can then attempt to proceed as in the single-flavor case and construct the field operators as

$$\begin{aligned} &\psi_i(x) \qquad (53)\\ &= \sum_{\mathbf{k}\tilde{h}j} \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{V}\Big[U_{\tilde{h}\,ij}(\mathbf{k},t)a_{\tilde{h}\,j}(\mathbf{k}) + V_{\tilde{h}\,ij}(\mathbf{k},t)b^\dagger_{\tilde{h}\,j}(-\mathbf{k})\Big],\\ &\psi_i^\dagger(x)\\ &= \sum_{\mathbf{k}\tilde{h}j} \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{V}\Big[a^\dagger_{\tilde{h}\,j}(\mathbf{k})U^\dagger_{\tilde{h}\,ji}(\mathbf{k},t) + b_{\tilde{h}\,j}(-\mathbf{k})V^\dagger_{\tilde{h}\,ji}(\mathbf{k},t)\Big], \end{aligned}$$

with the mode function

$$U_{h\,ij} = \begin{pmatrix} L_{h\,ij} \\ R_{h\,ij} \end{pmatrix} \otimes \xi_h \tag{54}$$

and its charge conjugate

$$V_{h\,ij} = -\mathrm{i}\gamma^2 (U_{h\,ij})^* = C U_{h\,ij} C^{-1} = \begin{pmatrix} -hR^*_{h\,ij} \\ hL^*_{h\,ij} \end{pmatrix} \otimes \xi_{-h}. \tag{55}$$

This procedure, however, fails, when M is not a symmetric matrix, which can easily be seen by plugging $U_{h\,ij}$ into (52)

$$\begin{aligned} \{\mathrm{i}\partial_0 - h|\mathbf{k}|\}\, L_{h\,ij} &= M^H_{il} R_{h\,lj} + \mathrm{i}M^A_{il} R_{h\,lj}, \\ \{\mathrm{i}\partial_0 + h|\mathbf{k}|\}\, R_{h\,ij} &= M^H_{il} L_{h\,lj} - \mathrm{i}M^A_{il} L_{h\,lj}, \end{aligned} \tag{56}$$

and $V_{h\,ij}$, respectively,

$$\begin{aligned} \{\mathrm{i}\partial_0 - h|\mathbf{k}|\}\, L_{h\,ij} &= M^{H*}_{il} R_{h\,lj} + \mathrm{i}M^{A*}_{il} R_{h\,lj}, \\ \{\mathrm{i}\partial_0 + h|\mathbf{k}|\}\, R_{h\,ij} &= M^{H*}_{il} L_{h\,lj} - \mathrm{i}M^{A*}_{il} L_{h\,lj}, \end{aligned} \tag{57}$$

where summation over the repeated index l is implied.

Obviously, when M is not symmetric, (56) and (57) are inconsistent. In particular, for non-symmetric M, the orthogonality condition

$$U^\dagger_{r\,il} V_{s\,lj} = 0 \tag{58}$$

is not preserved at all times, and hence, the expansion of the field operators (53) is not suitable. This complication can however lead to the generation of a net charge stored in the produced particles, because the operation of charge conjugation becomes time dependent, an effect which may be of relevance for baryogenesis [18].

The construction of an appropriate Bogolyubov transformation for the case of a symmetric mass matrix is discussed in [19]. In comparison with the single-flavor case this procedure is fairly complicated. For the general case, we therefore refrain from a computation of a Bogolyubov transformation and the time evolution of Heisenberg creation and annihilation operators.

It is more convenient to calculate the time evolution of the initial state in terms of two-point functions. We straightforwardly generalize the formalism for the single-flavor Wigner functions to the multiflavor case by defining

$$\mathrm{i}S^<_{ij}(k,x) = -\int \mathrm{d}^4 r\, \mathrm{e}^{\mathrm{i}k\cdot r} \langle \bar{\psi}_j(x - r/2)\psi_i(x + r/2)\rangle, \tag{59}$$

where i, j are flavor indices. These obey the equation of motion

$$\left(k\!\!\!/ + \frac{\mathrm{i}}{2}\gamma^0\partial_t - (M_H + \mathrm{i}\gamma^5 M_A)\mathrm{e}^{-\frac{\mathrm{i}}{2}\overleftarrow{\partial_t}\partial_{k_0}}\right)_{il} \mathrm{i}S^<_{lj} = 0\,. \tag{60}$$

As described for the single-flavor case in Sect. 3, this can be simplified and yields

$$\begin{aligned} &\dot{f}_{0h} + \mathrm{i}\,[M_H, f_{1h}] + \mathrm{i}\,[M_A, f_{2h}] = 0, \\ &\dot{f}_{1h} + 2h|\mathbf{k}|f_{2h} + \mathrm{i}\,[M_H, f_{0h}] - \{M_A, f_{3h}\} = 0, \\ &\dot{f}_{2h} - 2h|\mathbf{k}|f_{1h} + \{M_H, f_{3h}\} + \mathrm{i}\,[M_A, f_{0h}] = 0, \\ &\dot{f}_{3h} - \{M_H, f_{2h}\} + \{M_A, f_{1h}\} = 0. \end{aligned} \tag{61}$$

As already noted in [18], we can infer from these equations as a necessary condition for the non-conservation of the charge density f_{0h} that M must not be symmetric, in accordance with our discussion above.

Now assume that, after some time evolution, M has become symmetric and slowly varying. Then, it is possible to expand the field operators as in (53) and to define the expectation values of the number of particles

$$n^+_{\mathbf{k}h\,i} = \langle a^\dagger_{h\,i}(\mathbf{k}) a_{h\,i}(\mathbf{k})\rangle$$

and antiparticles

$$n^-_{\mathbf{k}h\,i} = \langle b^\dagger_{h\,i}(\mathbf{k}) b_{h\,i}(\mathbf{k})\rangle.$$

Moreover, we choose this basis such that the Hamilton operator is diagonal and reads

$$H = \frac{1}{V}\sum_{\mathbf{k}hij} \Big(h|\mathbf{k}| L^\dagger_h L_h + L^\dagger_h \left[M^H + \mathrm{i}M^A\right] R_h$$

$$- h|\mathbf{k}|R_h^\dagger R_h + R_h^\dagger \left[M^H - \mathrm{i}M^A\right] L_h\Big)_{ij} \times \left(a_{hi}^\dagger(\mathbf{k})a_{hj}(\mathbf{k}) - b_{hi}(\mathbf{k})b_{hj}^\dagger(\mathbf{k})\right). \quad (62)$$

We can now also express the functions $f_{\mu h}^{ij}$ employing this basis. Explicitly, they read

$$\begin{aligned}
f_{0h}^{ij}(x,\mathbf{k}) &= -\int \mathrm{d}^4 r\, \mathrm{e}^{\mathrm{i}k\cdot r} \langle \bar\psi_{hj}(x-r/2)\gamma^0\psi_{hi}(x+r/2)\rangle \\
&= \left(L_h^{il*}L_h^{jl'} + R_h^{il*}R_h^{jl'}\right) \\
&\quad \times \left\langle a_{hl'}^\dagger(\mathbf{k})a_{hl}(\mathbf{k}) + b_{hl'}(\mathbf{k})b_{hl}^\dagger(\mathbf{k})\right\rangle, \\
f_{1h}^{ij}(x,\mathbf{k}) &= -\int \mathrm{d}^4 r\, \mathrm{e}^{\mathrm{i}k\cdot r} \langle \bar\psi_{hj}(x-r/2)\psi_{hi}(x+r/2)\rangle \\
&= -2\Re\left(L_h^{il}R_h^{jl'*}\right) \\
&\quad \times \left\langle a_{hl'}^\dagger(\mathbf{k})a_{hl}(\mathbf{k}) + b_{hl'}(\mathbf{k})b_{hl}^\dagger(\mathbf{k})\right\rangle, \\
f_{2h}^{ij}(x,\mathbf{k}) &= -\int \mathrm{d}^4 r\, \mathrm{e}^{\mathrm{i}k\cdot r} \langle \bar\psi_{hj}(x-r/2)(-\mathrm{i}\gamma^5)\psi_{hi}(x+r/2)\rangle \\
&= 2\Im\left(L_h^{il*}R_h^{jl'}\right) \times \left\langle a_{hl'}^\dagger(\mathbf{k})a_{hl}(\mathbf{k}) + b_{hl'}(\mathbf{k})b_{hl}^\dagger(\mathbf{k})\right\rangle, \\
f_{3h}^{ij}(x,\mathbf{k}) &= -\int \mathrm{d}^4 r\, \mathrm{e}^{\mathrm{i}k\cdot r} \langle \bar\psi_{hj}(x-r/2)\gamma^0\gamma^5\psi_{hi}(x+r/2)\rangle \\
&= \left(L_h^{il*}L_h^{jl'} - R_h^{il*}R_h^{jl'}\right) \\
&\quad \times \left\langle a_{hl'}^\dagger(\mathbf{k})a_{hl}(\mathbf{k}) + b_{hl'}(\mathbf{k})b_{hl}^\dagger(\mathbf{k})\right\rangle.
\end{aligned}$$

By comparing with the expression (62), we obtain

$$\langle H\rangle = -\frac{1}{V}\sum_{\mathbf{k}hi}\left(h|\mathbf{k}|f_{3h\,ii} + M_{ii}^H f_{1h,ii} + M_{ii}^A f_{2h\,ii}\right). \quad (63)$$

We define $\omega_i(\mathbf{k}) = (\mathbf{k}^2 + |M_{ii}|^2)^{1/2}$, and since we assumed diagonality of the Hamiltonian, this has to equal

$$\begin{aligned}
\langle H\rangle &= \frac{1}{V}\sum_{\mathbf{k}hi}\omega_i(\mathbf{k})\langle a_{h\,i}^\dagger(\mathbf{k})a_{h\,i}(\mathbf{k}) - b_{h\,i}(\mathbf{k})b_{h\,i}^\dagger\rangle \\
&= \frac{1}{V}\sum_{\mathbf{k}hi}\omega_i(\mathbf{k})\left(n_{\mathbf{k}hi}^+ + n_{\mathbf{k}h\,i}^- - 1\right), \quad (64)
\end{aligned}$$

while the charge is

$$f_{0h\,ii} = \langle a_{h\,i}^\dagger(\mathbf{k})a_{h\,i}(\mathbf{k}) + b_{h\,i}(\mathbf{k})b_{h\,i}^\dagger\rangle = n_{\mathbf{k}h\,i}^+ - n_{\mathbf{k}h\,i}^- + 1. \quad (65)$$

We thus find the following generalization of (49):

$$n_{\mathbf{k}hi}^+ = \frac{h|\mathbf{k}|f_{3hii} + M_{ii}^H f_{1hii} + M_{ii}^A f_{2hii}}{2\omega_i(\mathbf{k})} + \frac{1}{2}f_{0hii}, \quad (66)$$

$$n_{\mathbf{k}hi}^- = \frac{h|\mathbf{k}|f_{3hii} + M_{ii}^H f_{1hii} + M_{ii}^A f_{2hii}}{2\omega_i(\mathbf{k})} - \frac{1}{2}f_{0hii} + 1, \quad (67)$$

which is of course the anticipated result, since the number of particles is just the half of the total particle number (particles plus antiparticles) plus half of the total charge (particles minus antiparticles).

4.2 Scalars

Consider now a complex scalar field Φ_i describing N flavors, which we expand into its hermitean and antihermitean parts as follows:

$$\Phi_i = \frac{1}{\sqrt{2}}(\Phi_i^1 + \mathrm{i}\Phi_i^2), \quad (68)$$

such that the multiflavor field operator is

$$\begin{aligned}
\Phi_i &= \frac{\varphi_i}{a} \quad (69) \\
&= \frac{1}{aV}\sum_{\mathbf{k}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\left(\varphi_{ij}^1(\mathbf{k},\eta)a_j^1(\mathbf{k}) + \mathrm{i}\varphi_{ij}^2(\mathbf{k},\eta)a_j^2(\mathbf{k})\right. \\
&\quad \left. + \varphi_{ij}^{1\dagger}(-\mathbf{k},\eta)a_j^{1\dagger}(-\mathbf{k}) + \mathrm{i}\varphi_{ij}^{2\dagger}(-\mathbf{k},\eta)a_j^{2\dagger}(-\mathbf{k})\right),
\end{aligned}$$

where the rescaled fields obey the generalized Klein–Gordon equation

$$\left\{\partial_\eta^2 + \mathbf{k}^2 + a^2M^2 - \frac{a''}{a}\right\}_{il}\varphi_{lj}^\alpha = 0. \quad (70)$$

Note that this is independent of whether $\alpha = 1$ or $\alpha = 2$, which is just as in the fermionic case, where the functions U and V both satisfy the Dirac equation. The individual components Φ_i^1 and Φ_i^2 are imposed to be hermitean. Therefore, $\sum_j(\varphi_{ij}(\mathbf{k}) + \varphi_{ij}(-\mathbf{k}))$ has to be real, which can in general be satisfied only if M^2 is real or, more precisely, real symmetric.

Let us therefore assume again, that we are in a final state with diagonal and only non-adiabatically varying M. We define

$$a(\mathbf{k}) = \frac{1}{\sqrt{2}}\left[a^1(\mathbf{k}) + \mathrm{i}a^2(\mathbf{k})\right]$$

and

$$b(\mathbf{k}) = \frac{1}{\sqrt{2}}\left[a^1(\mathbf{k}) - \mathrm{i}a^2(\mathbf{k})\right]. \quad (71)$$

Then, we find the charge operator to be

$$Q_i(\mathbf{k}) = \langle a_i^\dagger(\mathbf{k})a_i(\mathbf{k}) - b_i^\dagger(\mathbf{k})b_i(\mathbf{k})\rangle \quad (72)$$

and the Hamiltonian

$$H = \frac{1}{V}\sum_{\mathbf{k}}\Omega_i(\mathbf{k})\left(a_i^\dagger(\mathbf{k})a_i(\mathbf{k}) + b_i^\dagger(\mathbf{k})b_i(\mathbf{k}) + 1\right), \quad (73)$$

where $\Omega_i(\mathbf{k}) = |\varphi_i'(\mathbf{k}) - (a'/a)\varphi_i(\mathbf{k})|^2 + \omega_i(\mathbf{k})^2|\varphi_i(\mathbf{k})|^2$, $\omega_i^2(\mathbf{k}) = \mathbf{k}^2 + a^2M_{ii}^2$.

We define the multiflavor Wightman function as

$$\mathrm{i}\bar{G}^{<}_{ij} = \langle \varphi^{\dagger}_{j}(u)\varphi_{i}(v)\rangle \tag{74}$$

and adapt straightforwardly the definition of the momenta from the single-flavor case. These then satisfy the system of equations

$$\frac{1}{4}f_0'' - f_2 + \frac{1}{2}\left\{a^2M^2, f_0\right\} + \left(\mathbf{k}^2 - \frac{a''}{a}\right) f_0 = 0, \tag{75}$$

$$f_1' - \frac{\mathrm{i}}{2}\left[a^2M^2, f_0\right] = 0, \tag{76}$$

$$f_2' - \frac{\mathrm{i}}{2}\left[a^2M^2, f_1\right] - \frac{1}{4}\left\{(\mathbf{k}^2 + a^2M^2 - a''/a)', f_0\right\} = 0. \tag{77}$$

We find $Q_i(\mathbf{k}) = f_{1\,ii}(x,\mathbf{k}) + 1$, which is also in accordance with the $U(1)$-Noether charge. Together with the identities (27), this leads us to

$$n^{+}_{\mathbf{k}\,i} = \omega_i f_{0\,ii} + \frac{f''_{0\,ii}}{4\omega_i} - \frac{1}{2\omega_i}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{a'}{a}f_{0\,ii}\right) + \frac{1}{2}f_{1\,ii}, \tag{78}$$

$$n^{-}_{\mathbf{k}\,i} = \omega_i f_{0\,ii} + \frac{f''_{0\,ii}}{4\omega_i} - \frac{1}{2\omega_i}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\frac{a'}{a}f_{0\,ii}\right) - \frac{1}{2}f_{1\,ii} - 1, \tag{79}$$

where $n^{+}_{\mathbf{k}\,i}$ is the number of particles, $n^{-}_{\mathbf{k}\,i}$ the number of antiparticles, and the same simple interpretation as in the fermionic case applies.

5 Discussion

We have derived general expressions for the particle number densities on phase space for single scalars (29) and fermions (49) in terms of the appropriate Wigner functions. We have then generalized our analysis to the case of mixing scalars, (78) and (79), and fermions, (66) and (67). All of these expressions are positive, and moreover, the number of fermions is bounded from above by *unity*, as required by the Pauli principle. In order to incorporate the effect of the self-energy into (29) and (49), one needs to include this correction into the dispersion relation, $\omega = \omega(\mathbf{k},x) \to \omega + \Sigma_H(\mathbf{k},x)$, where $\Sigma_H(\mathbf{k},x) \equiv \int[\mathrm{d}k_0/(2\pi)](1/2)[\Sigma^r(k,x) + \Sigma^a(k,x)]$, and Σ^r and Σ^a denote the retarded and advanced self-energies, respectively [20]. When the single particle picture breaks down it is not clear whether a sensible definition of particle number can be constructed. Our analysis can be quite straightforwardly extended to include (time-varying) gauge fields by coupling them canonically to scalars and fermions.

The kinetic theory definition of the particle number is of course by construction identical with the definition in terms of Bogolyubov transformations. The number of individual particles is the total energy of the system divided by the energy of an individual particle. Taking the point of view of kinetic theory proves advantageous when considering statistical systems, such as the thermal equilibrium, or the multiflavor case.

While the fermionic particle number definition (49) is generally applicable, the scalar one (29) fails however when $\omega^2_{\mathbf{k}} = \mathbf{k}^2 + a^2m^2_{\phi} < 0$, which can happen at phase transitions. Then $\Omega_{\mathbf{k}} < |\Lambda_{\mathbf{k}}|$ in (11), and the Bogolyubov transformation (12) does not have a solution. Nevertheless, even in this case, the energy density on phase space $\Omega_{\mathbf{k}}$ in (28) is well defined and should be considered as a fundamental quantity of kinetic theory. Another important quantity is $\Lambda^{*}_{\mathbf{k}} = \langle \mathbf{k}, -\mathbf{k}|H|0\rangle$, the transition amplitude for particle pair creation with the momenta $\{\mathbf{k}, -\mathbf{k}\}$; and likewise $\Lambda_{\mathbf{k}}$ is the transition amplitude for pair annihilation. The appropriate description in this case is in terms of squeezed states. For an account of the inverted harmonic oscillator in terms of squeezed states, see e.g. [22].

Our definition of particle number can be used for studies of the quantum-to-classical transition, decoherence and entropy calculations of e.g. cosmological perturbations [22–24]. Moreover, when suitably normalized, the particle density $n_{\mathbf{k}}$ can be used to define a density matrix on phase space, $\varrho_{\mathbf{k}} = n_{\mathbf{k}}/\sum_{\mathbf{k}'} n_{\mathbf{k}'}$.

In the derivation of our results, we considered pure quantum states, yet showed explicitly their applicability to thermal states. More generally, our definitions are valid if one requires the density matrix ϱ to satisfy $\langle a_{\mathbf{k}}a_{\mathbf{k}}\rangle_{\varrho} = \langle a^{\dagger}_{\mathbf{k}}a^{\dagger}_{\mathbf{k}}\rangle_{\varrho} = 0$. These relations hold e.g. for eigenstates of the particle number operator $\hat{N}_{\mathbf{k}} \equiv a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}$, and, as pointed out in [21], for random phase states, a special case of which is the canonical ensemble. States of this kind can be treated as a linear superposition of the particle number eigenstates which we considered above.

Finally, we note that after the first version of this article appeared, an out-of-equilibrium investigation of the dynamics of chiral fermions coupled to scalars was studied in [25]. In order to show that at late times the system thermalizes to the Fermi–Dirac equilibrium, the authors used the particle number definition which can be in our notation written as

$$\tilde{n}_{\mathbf{k}} = \frac{1}{2}\sum_{h=\pm}\tilde{n}_{\mathbf{k}h}\,, \qquad \tilde{n}_{\mathbf{k}h} = \frac{1}{2}\left(1 + hf_{3h}\right)\,. \tag{80}$$

This definition corresponds to the massless fermion limit, $m \to 0$, of our definition (49).

Acknowledgements. We would like to acknowledge discussions with Jürgen Berges, Dietrich Bödeker, Kimmo Kainulainen and Julien Serreau.

References

1. E.P. Wigner, Phys. Rev. **40**, 749 (1932)
2. M. Hillery, R.F. O'Connell, M.O. Scully, E.P. Wigner, Phys. Rept. **106**, 121 (1984)
3. Y. Kluger, E. Mottola, J.M. Eisenberg, Phys. Rev. D **58**, 125015 (1998) [hep-ph/9803372]
4. L. Parker, Phys. Rev. **183**, 1057 (1969)
5. S.G. Mamaev, V.M. Mostepanenko, V.M. Frolov, Sov. J. Nucl. Phys. **23**, 592 (1976)

6. D.J. Chung, E.W. Kolb, A. Riotto, I.I. Tkachev, Phys. Rev. D **62**, 043508 (2000) [hep-ph/9910437]
7. P. f. Zhuang, U.W. Heinz, Phys. Rev. D **57**, 6525 (1998) [hep-ph/9801221].
8. D. Bödeker, K. Kainulainen, T. Prokopec (unpublished)
9. L. Kofman, A.D. Linde, A.A. Starobinsky, Phys. Rev. D **56**, 3258 (1997) [hep-ph/9704452]
10. N.A. Chernikov, E.A. Tagirov, Annales Poincaré Phys. Theor. A **9**, 109 (1968)
11. T.S. Bunch, P.C. Davies, Proc. Roy. Soc. Lond. A **360**, 117 (1978)
12. M. Mijić, Phys. Rev. D **57**, 2138 (1998) [gr-qc/9801 094]
13. L.H. Ford, Phys. Rev. D **35**, 2955 (1987)
14. M. Le Bellac, Thermal field theory (Cambridge University Press 1996)
15. G. Aarts, J. Smit, Phys. Rev. D **61**, 025002 (2000) [hep-ph/9906538]; M. Salle, J. Smit, J.C. Vink, Phys. Rev. D **64**, 025016 (2001) [hep-ph/0012346]; G. Aarts, J. Berges, Phys. Rev. D **64**, 105010 (2001) [hep-ph/0103049]
16. K. Kainulainen, T. Prokopec, M.G. Schmidt, S. Weinstock, Phys. Rev. D **66**, 043502 (2002) [hep-ph/0202177]; JHEP **0106**, 031 (2001) [hep-ph/0105295]
17. M. Peloso, L. Sorbo, JHEP **0005**, 016 (2000) [hep-ph/0003045]
18. B. Garbrecht, T. Prokopec, M.G. Schmidt, Phys. Rev. Lett. **92**, 061303 (2004) hep-ph/0304088
19. H.P. Nilles, M. Peloso, L. Sorbo, JHEP **0104**, 004 (2001) [hep-th/0103202]
20. T. Prokopec, M.G. Schmidt, S. Weinstock, Transport equations for chiral fermions to order h-bar and electroweak baryogenesis: Part I [hep-ph/0312110] and Part II [hep-ph/0406140], Annals of Physics (to be published)
21. H.E. Kandrup, Phys. Rev. D **38**, 1773 (1988)
22. A. Albrecht, P. Ferreira, M. Joyce, T. Prokopec, Phys. Rev. D **50**, 4807 (1994) [astro-ph/9303001]
23. D. Polarski, A.A. Starobinsky, Class. Quant. Grav. **13**, 377 (1996) [gr-qc/9504030]
24. R.H. Brandenberger, V. Mukhanov, T. Prokopec, Phys. Rev. Lett. **69**, 3606 (1992) [astro-ph/9206005]
25. J. Berges, S. Borsanyi, J. Serreau, Nucl. Phys. B **660**, 51 (2003) [hep-ph/0212404]