Institute of Physics Publishing Journal of Physics: Conference Series **35** (2006) 390–397
doi:10.1088/1742-6596/35/1/036 Progress in Nonequilibrium Green's Functions III

Comparing Boltzmann vs. Kadanoff-Baym

Markus Michael Müller

Physik-Department T30d, Technische Universität München
James-Franck-Straße, 85748 Garching, Germany

Max-Planck-Institut für Physik (Werner-Heisenberg-Institut)
Föhringer Ring 6, 80805 München, Germany

E-mail: `Markus_Michael_Mueller AT ph.tum.de`

Abstract. (Classical) Boltzmann equations suffer from several shortcomings as compared to their quantum mechanical generalizations, the so-called Kadanoff-Baym equations. Nevertheless, in practical calculations approximations to Boltzmann equations are widely used. A prominent example is the computation of the baryon asymmetry of the universe. In this work, we present a detailed comparison between the Kadanoff-Baym and Boltzmann equations in the framework of a scalar Φ^4 quantum field theory. We solve the Kadanoff-Baym and the Boltzmann equations numerically in 3+1 dimensions and compare their predictions on the evolution of systems out of thermal equilibrium for various initial conditions. The obtained numerical solutions reveal significant discrepancies between both types of equations. Most notably, the universality respected by Kadanoff-Baym equations is severely restricted in the case of Boltzmann equations.

1. Introduction

One of the most attractive frameworks to explain the matter-antimatter asymmetry of the universe is furnished by the so-called leptogenesis mechanism [1, 2]. Here, lepton number violating processes generate a lepton asymmetry which afterwards is converted to the observed baryon asymmetry by certain standard model processes called sphalerons. For the dynamical generation of the lepton asymmetry it is necessary, that the universe was in a state out of thermal equilibrium [3]. Classical statistical systems out of thermal equilibrium can be described by corresponding Boltzmann equations. They find their quantum mechanical generalization in the so-called Kadanoff-Baym equations [4, 5]. Although the process of leptogenesis involves elementary particles, which certainly obey the laws of quantum mechanics, the standard method to describe leptogenesis makes use of Boltzmann equations.

In order to derive Boltzmann equations from Kadanoff-Baym equations, among other approximations one has to employ the quasi-particle (or on-shell) approximation [5–7]. As a consequence, the conservation of momentum and energy prevents Boltzmann equations from describing thermalization in $1+1$ space-time dimensions. In contrast to this, it has been shown in the framework of a scalar Φ^4 quantum field theory that this is feasible with the Kadanoff-Baym equations [8]. The reason for this qualitative discrepancy is that the Kadanoff-Baym equations take off-shell effects into account [9], while these are neglected in the Boltzmann equation. Of course, in 3+1 dimensions both types of equations are capable of describing thermalization. However, in the case of leptogenesis the on-shell character of the Boltzmann equation leads to a

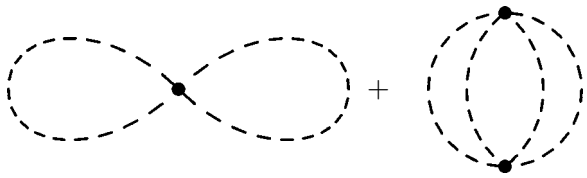

Figure 1. Two- and three-loop contribution to $i\Gamma_2[G]$. The lines represent the full connected Schwinger-Keldysh propagator $G(x,y)$.

further inconsistency: All leptogenesis scenarios share the fact that some heavy particles decay out of thermal equilibrium into the particles which we observe in the universe today. The spectral function of a particle that can decay into other particles is given by a Breit-Wigner curve with a non-vanishing width. By employing the quasi-particle approximation we reduce this decay width of the particles to zero, ie. a Boltzmann equation can only describe systems consisting of stable, or at least very long-lived, particles. After all, how does the on-shell character of the Boltzmann equation affect the description of quantum fields out of thermal equilibrium in $3+1$ dimensions?

When applying the Boltzmann equation to the description of leptogenesis, the standard technique to construct the collision integral — before employing further approximations — is to take the usual bosonic and fermionic statistical gain and loss terms multiplied with the S-matrix element for the respective reaction [10, 11]. These S-matrix elements are computed in vacuum, and one may wonder of which significance they are for a statistical quantum mechanical system.

These shortcomings of the Boltzmann equation lead to the conclusion that one should perform a detailed comparison between the Boltzmann and the Kadanoff-Baym equations in order to explicitely see how large the quantum mechanical corrections are [6, 12–15]. Due to the large complexity of the problem, we restrict ourselves for the moment to a scalar Φ^4 quantum field theory in $3+1$ dimensions. Of course, this theory cannot describe the phenomenon of leptogenesis, but nevertheless it allows to present a detailed comparison of the Boltzmann and Kadanoff-Baym equations and may well be a starting point for further investigations.

2. Kadanoff-Baym Equations

We consider a real scalar quantum field in the symmetric regime (i.e. $\langle\Phi(x)\rangle = 0$) whose dynamics is determined by the Lagrangian density

$$\mathscr{L} = -\frac{1}{2}\Big(\partial_\mu\Phi\Big)\Big(\partial^\mu\Phi\Big) - \frac{1}{2}m_B^2\Phi^2 - \frac{\lambda}{4!}\Phi^4 \,.$$

For Gaussian initial conditions the 2PI effective action can be parameterized in the form [8, 16]

$$\Gamma[G] = \frac{i}{2}\,\mathrm{tr}_{\mathcal{C}}\log_{\mathcal{C}}\left[G^{-1}\right] - \frac{1}{2}\,\mathrm{tr}_{\mathcal{C}}\left[G_0^{-1}G\right] + \Gamma_2[G] + const\,,$$

where G_0^{-1} is the inverse free propagator. The index $\mathcal{C}$ indicates that integrations have to be taken along the closed real-time path [17, 18]. $i\Gamma_2[G]$ is the sum of all two-particle irreducible vacuum diagrams, where internal lines represent the full connected Schwinger-Keldysh propagator $G(x,y)$. In this work, we apply the loop expansion of the 2PI effective action up to three-loop order. The diagrams contributing to $i\Gamma_2[G]$ in this approximation are shown in Fig. 1. The equation of motion for the full propagator reads [16]

$$\frac{\delta\Gamma[G]}{\delta G(y,x)} = 0 \quad\Longleftrightarrow\quad G^{-1}(x,y) = iG_0^{-1}(x,y) - \Pi(x,y)\,, \tag{1}$$

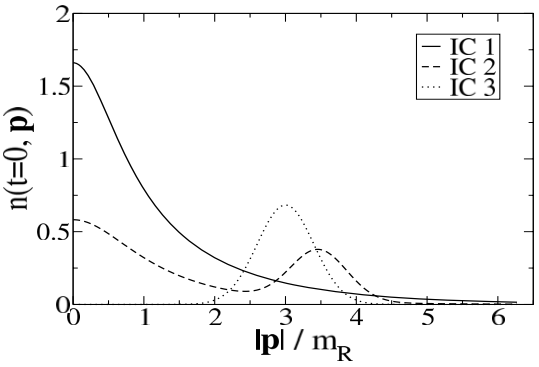

Figure 2. Initial conditions. Here we plotted the initial particle number densities, for which we numerically solved the Boltzmann and Kadanoff-Baym equations, against the absolute momenta. These particle number densities can immediately be fed into the numerics for the Boltzmann equation. In order to obtain the initial values of the propagators as needed by the numerics for the Kadanoff-Baym program we follow Refs. [8, 19].

where the proper self-energy is given by

$$\Pi\left(x,y\right)=2i\frac{\delta\Gamma_2\left[G\right]}{\delta G\left(y,x\right)}=-i\delta_{\mathcal{C}}\left(x-y\right)\Pi^{(local)}\left(x\right)+\Pi^{(nonlocal)}\left(x,y\right)\ .$$

The local part of the self energy leads to an effective mass [8]

$$M^2\left(x\right)=m_B^2+\Pi^{(local)}\left(x\right)=m_B^2+\frac{\lambda}{2}G_F\left(x,x\right)\ . \tag{2}$$

The propagator and the nonlocal part of the self energy can be decomposed into statistical and spectral parts according to [8]

$$G\left(x,y\right)=G_F\left(x,y\right)-\frac{i}{2}\mathrm{sign}_{\mathcal{C}}\left(x^0-y^0\right)G_\varrho\left(x,y\right)$$

and

$$\Pi^{(nonlocal)}\left(x,y\right)=\Pi_F\left(x,y\right)-\frac{i}{2}\mathrm{sign}_{\mathcal{C}}\left(x^0-y^0\right)\Pi_\varrho\left(x,y\right)\ .$$

When we insert all these definitions into the Schwinger-Dyson equation (1), we observe that it splits into two complementary real-valued evolution equations for the statistical propagator and the spectral function, respectively [8]. These are the Kadanoff-Baym equations:

$$\left(-\partial_{x^\mu}\partial_{x_\mu}+M^2\left(x\right)\right)G_F\left(x,y\right)=\int_0^{y^0}d^4z\ \Pi_F\left(x,z\right)G_\varrho\left(z,y\right)-\int_0^{x^0}d^4z\ \Pi_\varrho\left(x,z\right)G_F\left(z,y\right) \tag{3}$$

and

$$\left(-\partial_{x^\mu}\partial_{x_\mu}+M^2\left(x\right)\right)G_\varrho\left(x,y\right)=-\int_{y^0}^{x^0}d^4z\ \Pi_\varrho\left(x,z\right)G_\varrho\left(z,y\right)\ . \tag{4}$$

For a spatially homogeneous system we can Fourier transform the full propagator with respect to the spatial relative coordinates. One can then define an effective kinetic energy density $\omega\left(t,\mathbf{p}\right)$ and an effective particle number density $n\left(t,\mathbf{p}\right)$ according to [19]:

$$\omega^2\left(t,\mathbf{p}\right)=\left(\frac{\partial_{x^0}\partial_{y^0}G_F\left(x^0,y^0,\mathbf{p}\right)}{G_F\left(x^0,y^0,\mathbf{p}\right)}\right)_{x^0=y^0=t} \tag{5}$$

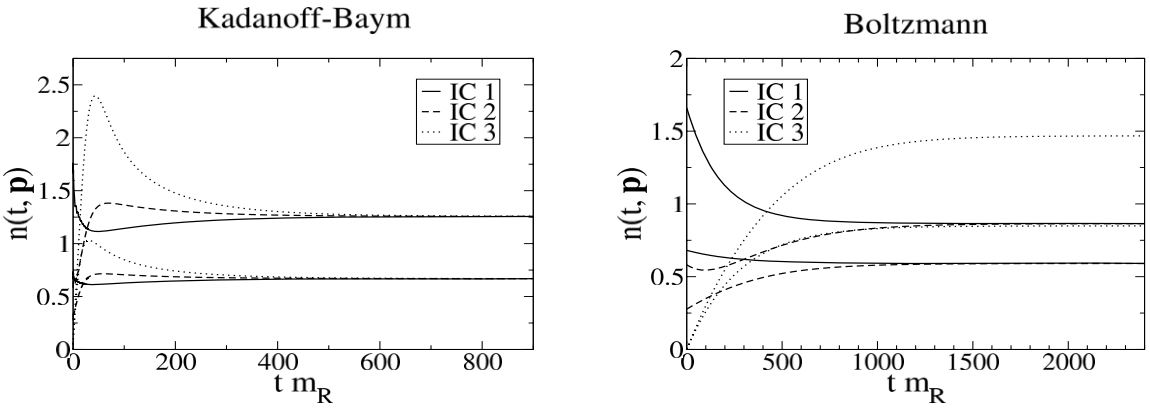

Figure 3. Evolution of the particle number densities. These plots show the time evolution of the particle number densities for two different momentum modes ($|\mathbf{p}| = 0$ and $|\mathbf{p}| = 1.16 m_R$) and all initial conditions (cf. Fig. 2) as determined by the Boltzmann and the Kadanoff-Baym equations, respectively. The left plot shows that the Kadanoff-Baym equations respect full universality, whereas in the case of the Boltzmann equation only a restricted universality is maintained, cf. Fig. 4.

and

$$n\left(t,\mathbf{p}\right) = \omega\left(t,\mathbf{p}\right) G_F\left(t,t,\mathbf{p}\right) - \frac{1}{2}\,. \tag{6}$$

However, we stress that the Kadanoff-Baym equations are self-consistent evolution equations for the full propagator of our system, and that one has to follow the evolution of the two-point function throughout the whole x^0-y^0-plane (of course, constrained to the part with $x^0 \geq 0$ and $y^0 \geq 0$). One can then follow the evolution of the effective particle number density along the bisecting line of this plane.

3. Boltzmann Equation

Employing a first-order gradient expansion and a Wigner transformation, one can derive quantum kinetic equations from the Kadanoff-Baym equations [5–7]. The kinetic equation for the statistical propagator reads [20]:

$$\begin{aligned}
&\left(2k^\mu \partial_{X^\mu} + \left(\partial_{X^\mu} M^2\left(X\right)\right)\partial_{k_\mu}\right)\tilde{G}_F\left(X,k\right) \\
&\quad = \tilde{G}_F\left(X,k\right)\tilde{\Pi}_\varrho\left(X,k\right) - \tilde{G}_\varrho\left(X,k\right)\tilde{\Pi}_F\left(X,k\right) \\
&\qquad + \left\{\tilde{\Pi}_F\left(X,k\right), \mathrm{Re}\left(\tilde{G}_R\left(X,k\right)\right)\right\}_{PB} + \left\{\mathrm{Re}\left(\tilde{\Pi}_R\left(X,k\right)\right), \tilde{G}_F\left(X,k\right)\right\}_{PB}\,.
\end{aligned}$$

After we have discarded the Poisson brackets, we employ the Kadanoff-Baym ansatz [5–7]

$$\tilde{G}_F\left(X,k\right) = \tilde{G}_\varrho\left(X,k\right)\left(\tilde{n}\left(X,k\right) + \frac{1}{2}\right) \tag{7}$$

and the quasi-particle approximation [5–7]:

$$\tilde{G}_\varrho\left(X,k\right) = \frac{\pi}{E\left(X,\mathbf{k}\right)}\left(\delta\left(k^0 - E\left(X,\mathbf{k}\right)\right) - \delta\left(k^0 + E\left(X,\mathbf{k}\right)\right)\right)\,. \tag{8}$$

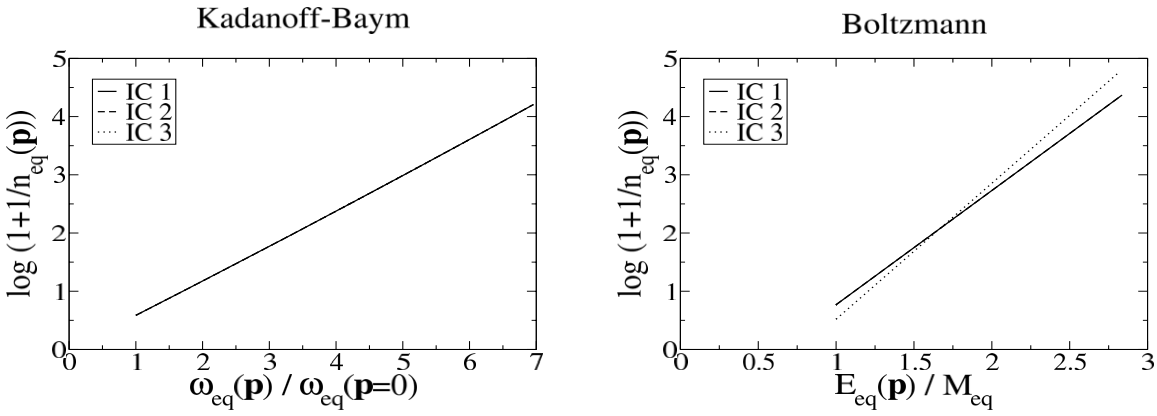

Figure 4. Equilibrium particle number densities. Here, we plotted the particle number densities, obtained for times when thermal equilibrium has effectively been reached, against the corresponding thermal energy densities. For a given initial condition, the inverse temperature β is given by the slope of the line and the chemical potential is obtained from the y-axis intercept divided by $-\beta$. Supplementing Fig. 3 we observe full (restricted) universality in the case of the Kadanoff-Baym (Boltzmann) equations.

The quasi-particle energy and number density are given by

$$E\left(X,\mathbf{k}\right)=\sqrt{M^{2}\left(X\right)+\mathbf{k}^{2}}\qquad\text{and}\qquad n\left(X,\mathbf{k}\right)=\tilde{n}\left(X,\mathbf{k},E\left(X,\mathbf{k}\right)\right)\ .$$

Eventually, we arrive at a Boltzmann equation for the quasi-particles. For a spatially homogeneous and isotropic system it reads [15]:

$$\partial_{t}n\left(t,k\right)=\frac{\lambda^{2}}{96\pi^{4}}\int_{0}^{\infty}dp\int_{0}^{\infty}dq\Bigg[\Theta\left(r_{0}^{2}\right)\frac{pqD\left(k,p,q,r_{0}\right)}{E_{k}E_{p}E_{q}}\times\Big(\left(1+n_{k}\right)\left(1+n_{p}\right)n_{q}n_{r_{0}}-n_{k}n_{p}\left(1+n_{q}\right)\left(1+n_{r_{0}}\right)\Big)\Bigg]\ . \tag{9}$$

where, we used the abbreviations $k=|\mathbf{k}|$, $E_{k}=\sqrt{M^{2}\left(t\right)+\mathbf{k}^{2}}$ and $n_{k}=n\left(t,|\mathbf{k}|\right)$. For a spatially homogeneous system the effective mass depends only on time, and, according to Eqs. (2), (7) and (8), is given by the following gap equation:

$$M^{2}\left(t\right)=m_{B}^{2}+\frac{\lambda}{2}\int\frac{d^{3}p}{\left(2\pi\right)^{3}}\left[\frac{2n\left(t,p\right)+1}{\sqrt{M^{2}\left(t\right)+\mathbf{p}^{2}}}\right]\ . \tag{10}$$

r_{0} and D are the following auxiliary functions [15]:

$$D\left(k,p,q,r\right)=\int_{0}^{\infty}d\xi\ \frac{1}{k\xi^{2}}\ \sin\left(k\xi\right)\ \sin\left(p\xi\right)\ \sin\left(q\xi\right)\ \sin\left(r\xi\right)\ ,$$

$$r_{0}=r_{0}\left(t,k,p,q\right)=\sqrt{\left(E_{k}+E_{p}-E_{q}\right)^{2}-M^{2}\left(t\right)}\ .$$

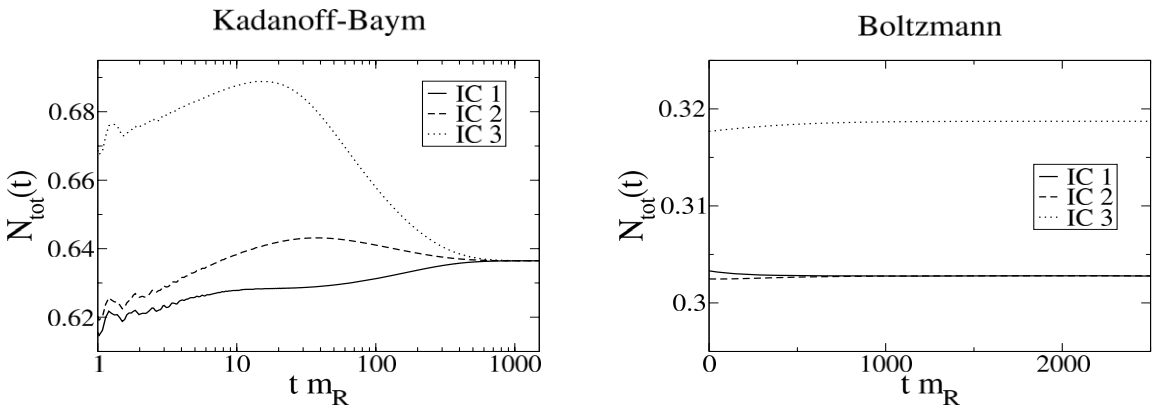

Figure 5. Evolution of the total particle numbers. As expected from Ref. [9], the Kadanoff-Baym equations include off-shell particle creation and annihilation. As a result the total particle number may change with time. In contrast to this, the total particle number is strictly conserved in the case of the Boltzmann equation. Concerning our simulations, of course, this only holds up to numerical errors ($< 0.4\%$).

4. Comparing Boltzmann and Kadanoff-Baym

In order to solve the Kadanoff-Baym equations numerically, we employ a standard lattice discretization on a lattice with $500^2 \times 32^3$ points [8, 15, 19]. We renormalize the mass perturbatively on the one-loop level and use the renormalized vacuum mass m_R to set the scale. The lattice spacings are $a_t m_R = 0.06$ and $a_s m_R = 0.5$. For the Boltzmann equation we use a manifestly isotropic discretization with 500 momentum modes and the same cutoff as for the Kadanoff-Baym equations. In order to advance in time we use a fourth order Runge-Kutta-Cash-Karp method with adaptive step-size control [15].

We consider initial conditions which correspond to the same average energy density, but different initial particle number densities. We choose the initial particle number densities according to Fig. 2. These particle number densities can immediately be fed into the numerics for the Boltzmann equation. In order to obtain the initial conditions for the Kadanoff-Baym equations, we follow Refs. [8, 19] and invert Eqs. (5) and (6).

Figs. 3 and 4 show the evolution of the particle number densities for two different momentum modes and the corresponding equilibrium particle number densities, respectively, for all initial conditions. In the left plots we can see, that the Kadanoff-Baym equations lead to a universal equilibrium particle number density. In particular the predicted temperature, given by the inverse slope of the line in Fig. 4, is the same for all initial conditions. However, the right plots reveal that, in general, this will not be the case for the Boltzmann equation. In contrast to the Kadanoff-Baym equations, the Boltzmann equation respects only a restricted universality. The reason for this can be extracted from Fig. 5: The Boltzmann equation conserves the total particle number, whereas the Kadanoff-Baym equations let it approach a universal equilibrium value. Of course, in the case of the Boltzmann equation this additional constant of motion severely restricts the evolution of the particle number density. Only initial conditions for which the average energy density and the total particle number agree from the very beginning, lead to the same equilibrium results.

In this context it is important to recall that we consider real (neutral) scalar quantum fields with a quartic self interaction. Thus the dynamics of our theory comprises processes which

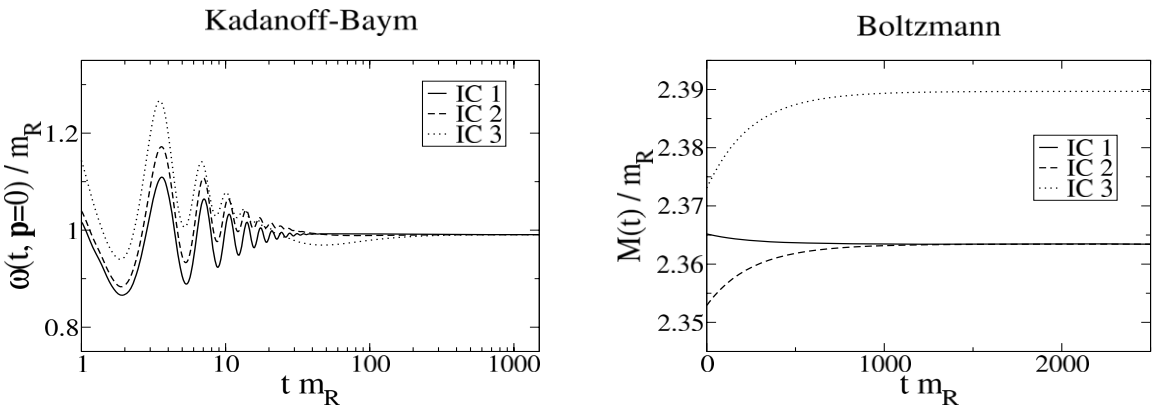

Figure 6. Evolution of the thermal masses. Again, for the Kadanoff-Baym (Boltzmann) equations we find full (restricted) universality. The late time values of the thermal (effective) masses are used to set the scale in Fig. 4.

can change the total particle number, such as eg. the decay of one particle into three, or the corresponding recombination process. However, due to the conservation of energy and momentum these processes can only occur off the mass shell. In Ref. [9], it has been shown that the Kadanoff-Baym equations indeed include these processes into their description of thermalization. In contrast to this, due to the quasi-particle approximation, these processes are neglected by the Boltzmann equation. As a consequence, the Boltzmann equation predicts significantly larger thermalization times as compared to the Kadanoff-Baym equations, cf. Fig. 3. Furthermore, for a system allowing for creation and annihilation of particles, the chemical potential of particles, whose total number is not restricted by any conserved quantity, must vanish in thermodynamical equilibrium. The chemical potential is given by the y-axis intercept extracted from Fig. 4 divided by $-\beta$. Using a ruler the reader might convince himself that the Kadanoff-Baym equations indeed lead to a universally vanishing chemical potential. In contrast to this, the Boltzmann equation, in general, will lead to a non-vanishing chemical potential [14].

Eventually, Fig. 6 exhibits the evolution of the thermal masses. In the case of the Kadanoff-Baym equations, the thermal mass is given by the zero mode of the effective kinetic energy density (5). On the other hand, the thermal mass appearing in the Boltzmann equation is given by the tadpole-corrected effective mass (10). Again, for the Kadanoff-Baym equations full universality is respected and a common equilibrium value approached, while for the Boltzmann equation only the restricted universality is preserved.

5. Conclusions

Starting from the 2PI effective action for a scalar Φ^4 quantum field theory, we briefly reviewed the derivation of the Kadanoff-Baym equations and the approximations which are necessary to eventually arrive at a Boltzmann equation. We solved the Boltzmann and Kadanoff-Baym equations numerically in 3+1 dimensions for spatially homogeneous and isotropic systems and compared their predictions on the evolution of systems out of thermal equilibrium.

We have shown that the Kadanoff-Baym equations respect universality [19]: For systems with equal average energy density the late-time behavior coincides independently of the details of the initial conditions. In particular, the particle number densities, temperatures and thermal masses predicted for times, when equilibrium has effectively been reached, coincide. Furthermore, the

chemical potentials also coincide and vanish.

In contrast to the Kadanoff-Baym equations, the Boltzmann equation only respects a restricted universality. The reason for this is the fact that the Boltzmann equation conserves not only the average energy density, but also the total particle number. Thus the late-time results can only agree for systems for which both of these quantities agree from the very beginning.

Furthermore, in Ref. [15] we could show that the Kadanoff-Baym equations separate the time scales for kinetic and chemical thermalization. Due to the lack of chemical equilibration, this separation of time scales is absent in the case of the Boltzmann equation.

Some of the approximations that lead from the Kadanoff-Baym equations to the Boltzmann equation are clearly motivated by equilibrium considerations. Taking the observed restriction of universality into account, it seems that one can safely apply the Boltzmann equation only to systems which are sufficiently close to equilibrium. Accordingly, for a system far from equilibrium the results given by the Boltzmann equation should be treated with care.

Acknowledgments

TripleM would like to thank Jürgen Berges and Manfred Lindner for many fruitful discussions and collaboration on related work, and Sigurd Köhler for interesting discussions during this workshop. This work was supported by "Sonderforschungsbereich 375 für Astroteilchenphysik der Deutschen Forschungsgemeinschaft".

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