

Comparison of Boltzmann kinetics with quantum dynamics for a chiral Yukawa model far from equilibrium

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Boltzmann equations are often used to describe the nonequilibrium time-evolution of many-body systems in particle physics. Prominent examples are the computation of the baryon asymmetry of the universe and the evolution of the quark-gluon plasma after a relativistic heavy ion collision. However, Boltzmann equations are only a classical approximation of the quantum thermalization process, which is described by so-called Kadanoff-Baym equations. This raises the question how reliable Boltzmann equations are as approximations to the complete Kadanoff-Baym equations. Therefore, we present in this article a detailed comparison of the Boltzmann and the Kadanoff-Baym equations in the framework of a chirally invariant Yukawa-type quantum field theory including fermions and scalars. The obtained numerical results reveal significant differences between both types of equations. Apart from quantitative differences, on a qualitative level the late-time universality respected by the Kadanoff-Baym equations is severely restricted in the case of the Boltzmann equations. Furthermore, the Kadanoff-Baym equations strongly separate the time scales between kinetic and chemical equilibration. In contrast to this standard Boltzmann equations cannot describe the process of quantum-chemical equilibration, and consequently also cannot feature the above separation of time scales.

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I. INTRODUCTION

This article is an extension of our previous studies [1], where we performed a detailed comparison of Boltzmann and Kadanoff-Baym equations in the framework of a real scalar Φ^4 quantum field theory. The motivation for these studies is a better understanding of processes like leptogenesis or preheating in the early universe [2–5], or the evolution of the quark-gluon plasma after relativistic heavy-ion collisions [6–9]. All these phenomena require the description of many-particle systems out of thermal equilibrium. The standard means to deal with this nonequilibrium situation are Boltzmann equations. However, it is well known that (classical) Boltzmann equations suffer from several shortcomings as compared to their quantum mechanical generalizations, so-called Kadanoff-Baym equations. This motivates a comparison of Boltzmann and Kadanoff-Baym equations in order to assess the reliability of quantitative predictions based on standard Boltzmann techniques. In the present work we generalize our previous results to the case of a chirally invariant Yukawa-type quantum field theory coupling fermions with scalars. More precisely, we consider a globally $SU(2) \times SU(2) \times U(1)$ symmetric quantum field theory, which offers two interpretations for the particle content: On one hand, in the context of leptogenesis one might think of a single generation of leptons and a Higgs bidoublet [10]. On the other hand, this theory is equivalent to the linear σ -model [11–13], which can be used to describe low-energy quark-meson dynamics in two-flavor QCD. In

any case, this work can be regarded as a further step to approach more realistic theories, which can be used to describe the phenomena motivating our studies.

What are the shortcomings of Boltzmann equations? Originally, Boltzmann equations have been designed for the description of the nonequilibrium time-evolution of dilute gases of classical particles. As such, their range of validity must be scrutinized once quantum effects become relevant. This is certainly the case for elementary particles playing the central role in phenomena-like leptogenesis or the quark-gluon plasma. As already indicated above, the quantum dynamics of such systems is described by so-called Kadanoff-Baym equations. Employing a sequence of approximations, Boltzmann equations can be derived from Kadanoff-Baym equations [14–18]. However, it is important to note that these approximations might be neither justifiable nor controllable, and sometimes even inconsistent. After all, standard Boltzmann equations take only on-shell processes into account, feature spurious constants of motion, and introduce irreversibility by implying the assumption of molecular chaos (“Stoßzahlansatz”) [19–22]. In contrast to this, Kadanoff-Baym equations are time-reversal invariant and take memory and off-shell effects into account [23–26]. Therefore, one should perform a detailed comparison of Boltzmann and Kadanoff-Baym equations [1,24,25,27–30].

Because of the complexity of the problem, in a first step we restricted ourselves to a real scalar Φ^4 quantum field theory in 3 + 1 space-time dimensions [1]. Of course, in this framework one can neither describe the phenomenon of leptogenesis nor thermalization of the quark-gluon plasma after a relativistic heavy ion collision. Nevertheless, it certainly allowed us to perform a detailed

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comparison of the Boltzmann and Kadanoff-Baym equations, which revealed interesting phenomena to be investigated in more realistic theories. We found considerable differences in the results furnished by the Boltzmann and Kadanoff-Baym equations: On a quantitative level, we found that the Boltzmann equation predicts significantly larger thermalization times than the corresponding Kadanoff-Baym equations. On a qualitative level we could verify that Kadanoff-Baym equations respect full late-time universality [23,31] and strongly separate the time scales between kinetic and chemical equilibration [32]. In the case of a real scalar Φ^4 quantum field theory the Boltzmann equation includes only two-particle scattering processes, which conserve the total particle number. This spurious constant of motion severely constrains the evolution of the particle number distribution. As a result, the Boltzmann equation respects only a restricted universality, fails to describe the process of quantum-chemical equilibration, and does not separate any time scales.

In the present work we extend our comparison of Boltzmann and Kadanoff-Baym equations to a chirally invariant Yukawa-type quantum field theory coupling fermions with scalars. We start from the 2PI effective action [33,34] and derive the Kadanoff-Baym equations by requiring that the 2PI effective action be stationary with respect to variations of the complete connected two-point functions [35,36]. First, this guarantees that the Kadanoff-Baym equations conserve the average energy density as well as global charges [37–39], and second, the 2PI effective action has proven to be an efficient and reliable tool for the description of quantum fields out of thermal equilibrium in numerous previous treatments [23,36,40–43]. In order to derive the corresponding Boltzmann equations, subsequently one has to employ a first-order gradient expansion, a Wigner transformation, the Kadanoff-Baym ansatz, and the quasiparticle approximation [14–18]. While Boltzmann equations describe the time evolution of particle number distributions, Kadanoff-Baym equations describe the evolution of the complete quantum mechanical two-point functions of the system. However, one can define effective particle number distributions, which can be obtained from the complete propagators and their time derivatives evaluated at equal times [36,40]. Finally, we solve the Boltzmann and the Kadanoff-Baym equations numerically for highly symmetric systems in $3 + 1$ space-time dimensions and compare their predictions on the evolution of these systems for various initial conditions.

II. 2PI EFFECTIVE ACTION

We consider a globally $SU(2)_L \times SU(2)_R \times U(1)_{B-L}$ symmetric quantum field theory with one generation of chiral leptons and a Higgs bidoublet with Dirac-Yukawa interactions [10]. The Dirac fields are denoted with $\Psi_l^\alpha(x)$, where α is a Dirac index and $l \in \{\nu, e\}$ denotes the type of

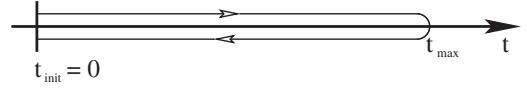


FIG. 1. Closed real-time path \mathcal{C} . This time path was invented by Schwinger [53] and applied to nonequilibrium problems by Keldysh [54]. In order to avoid the doubling of the degrees of freedom, we use the form presented in Ref. [15].

the leptons. Using the Pauli matrices, the (complex) Higgs bidoublet can be parametrized by real scalar fields denoted with $\Phi_a(x)$, where $a \in \{0, \dots, 3\}$. In this notation the Lagrangian density takes the form¹

$$\mathcal{L} = -\bar{\Psi}\not{\partial}\Psi - \frac{1}{2}(\partial_\mu\Phi_a)(\partial^\mu\Phi_a) - \frac{1}{2}m_B^2\Phi_a\Phi_a - \lambda(\Phi_a\Phi_a)^2 - i\eta\bar{\Psi}\Phi_a(\sigma_a P_R - \sigma_a^\dagger P_L)\Psi.$$

Although we refer to the scalar fields as Higgs fields, we would like to note that this theory is equivalent to the linear σ -model [11–13], which can be used to describe low-energy quark-meson dynamics in two-flavor QCD. This and a similar model have been considered in a related context in Refs. [32,36].

Since we will compute the evolution of the two-point Green's functions for nonequilibrium initial conditions, already the classical action has to be defined on the closed Schwinger-Keldysh real-time contour, shown in Fig. 1. The free inverse propagators can then be read off the free part of the classical action:

$$I_0 = - \int_{\mathcal{C}} d^4x d^4y \left[\bar{\Psi}_l(x) S_{0,lm}^{-1}(x, y) \Psi_m(y) + \frac{1}{2} \Phi_a(x) G_{0,ab}^{-1}(x, y) \Phi_b(y) \right],$$

where the inverse free propagators are given by

$$G_{0,ab}^{-1}(x, y) = (\partial_{x^\mu} \partial_{y_\mu} + m_B^2) \delta_{\mathcal{C}}(x - y) \delta_{ab} \quad (1)$$

and

$$S_{0,lm}^{-1}(x, y) = \not{\partial}_x \delta_{\mathcal{C}}(x - y) \delta_{lm}. \quad (2)$$

We consider a system without symmetry breaking, i. e. $\langle \Phi_a(x) \rangle = 0$. In this case the full connected Schwinger-Keldysh propagators are given by

$$G_{ab}(x, y) = \langle T_{\mathcal{C}} \{ \Phi_a(x) \Phi_b(y) \} \rangle \quad (3)$$

and

$$S_{lm}^{\alpha\beta}(x, y) = \langle T_{\mathcal{C}} \{ \Psi_l^\alpha(x) \bar{\Psi}_m^\beta(y) \} \rangle, \quad (4)$$

so that the 2PI effective action can be written in the form

¹The form of the kinetic term indicates that we use the Minkowski metric where the time-time component is negative. σ_1, σ_2 and σ_3 are the usual Pauli matrices, while $\sigma_0 = i\mathbb{1}$. In addition to the Dirac γ matrices we will frequently use $\beta = i\gamma^0$, and $P_L = \frac{1}{2}(\mathbb{1} + \gamma_5)$ and $P_R = \frac{1}{2}(\mathbb{1} - \gamma_5)$.

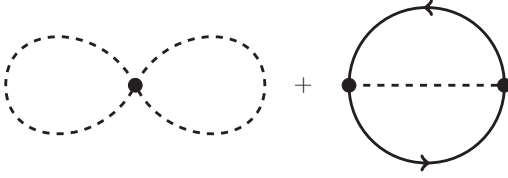


FIG. 2. Two-loop contribution to $\Gamma_2[G, S]$. Full (dashed) lines represent the complete connected lepton (Higgs) propagator S (G).

$$\Gamma[G, S] = \frac{i}{2} \text{tr}_C \log_C[G^{-1}] - \frac{1}{2} \text{tr}_C[G_0^{-1}G] - i \text{tr}_C \log_C[S^{-1}] + \text{tr}_C[S_0^{-1}S] + \Gamma_2[G, S] + \text{const.} \quad (5)$$

The square brackets indicate that the trace, the logarithm, and the product of the propagators have to be taken in the functional sense, and the subscript C reminds us that integrals over time are running along the closed real-time contour. $i\Gamma_2[G, S]$ is the sum of all two-particle irreducible vacuum diagrams, where internal lines represent the complete connected propagators S and G . In this work we apply the loop expansion of the 2PI effective action up to two-loop order. The diagrams contributing to Γ_2 in this approximation are shown in Fig. 2. Using the abbreviation

$$H_{a,lm}^{\alpha\beta} = i\eta[(\sigma_a)_{lm}P_R^{\alpha\beta} - (\sigma_a^\dagger)_{lm}P_L^{\alpha\beta}]$$

we find

$$\begin{aligned} \Gamma_2[G, S] = & -\lambda \int_C d^4x [G_{aa}(x, x)G_{bb}(x, x) \\ & + 2G_{ab}(x, x)G_{ab}(x, x)] - \frac{i}{2} \\ & \times \int_C d^4x d^4y G_{ab}(x, y) \text{tr}(H_a S(x, y)H_b S(y, x)), \end{aligned}$$

where the trace runs over Dirac and lepton type indices.

III. KADANOFF-BAYM EQUATIONS

The equations of motion for the complete propagators read

$$\frac{\delta\Gamma[G, S]}{\delta G_{ba}(y, x)} = 0 \quad \text{and} \quad \frac{\delta\Gamma[G, S]}{\delta S_{ml}^{\beta\alpha}(y, x)} = 0. \quad (6)$$

They are equivalent to the corresponding self-consistent Schwinger-Dyson equations

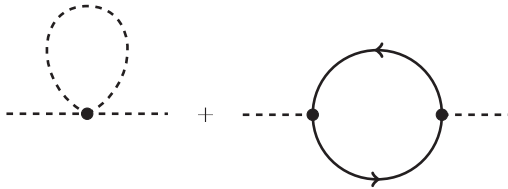


FIG. 3. One-loop contribution to the Higgs self-energy.



FIG. 4. One-loop contribution to the lepton self-energy.

$$G_{ab}^{-1}(x, y) = iG_{0,ab}^{-1}(x, y) - \Pi_{ab}(x, y) \quad (7)$$

and

$$S_{lm}^{-1}(x, y) = iS_{0,lm}^{-1}(x, y) - \Sigma_{lm}(x, y), \quad (8)$$

where the proper self-energies are given by (cf. Figs. 3 and 4)

$$\begin{aligned} \Pi_{ab}(x, y) = & 2i \frac{\delta\Gamma_2[G, S]}{\delta G_{ba}(y, x)} \\ = & -4\lambda i \delta_C(x - y)(G_{dd}(x, x)\delta_{ab} + 2G_{ab}(x, x)) \\ & + \text{tr}(H_a S(x, y)H_b S(y, x)) \end{aligned} \quad (9)$$

and

$$\begin{aligned} \Sigma_{lm}^{\alpha\beta}(x, y) = & -i \frac{\delta\Gamma_2[G, S]}{\delta S_{ml}^{\beta\alpha}(y, x)} \\ = & -H_{a,lk}^{\alpha\gamma} H_{b,nm}^{\delta\beta} S_{kn}^{\gamma\delta}(x, y)G_{ab}(x, y). \end{aligned} \quad (10)$$

Next, we define the spectral function²

$$G_{\varrho,ab}(x, y) = i\langle[\Phi_a(x), \Phi_b(y)]_-\rangle$$

and the statistical propagator³

$$G_{F,ab}(x, y) = \frac{1}{2}\langle[\Phi_a(x), \Phi_b(y)]_+\rangle$$

for the Higgs bosons, so that we can write the complete Higgs propagator as

$$G(x, y) = G_F(x, y) - \frac{i}{2} \text{sign}_C(x^0 - y^0)G_{\varrho}(x, y). \quad (11)$$

In the case of real scalar fields the spectral function and the statistical propagator are real-valued quantities [40]. In a similar way, we also define the spectral function⁴

$$S_{\varrho,lm}^{\alpha\beta}(x, y) = i\langle[\Psi_l^\alpha(x), \bar{\Psi}_m^\beta(y)]_+\rangle \quad (12)$$

and the statistical propagator⁵

²From the definition of the Higgs spectral-function we see that it is antisymmetric in the sense that $G_{\varrho,ba}(y, x) = -G_{\varrho,ab}(x, y)$. Furthermore, the canonical equal-time commutation relations give $(G_{\varrho,ab}(x, y))_{x^0=y^0} = 0$ and $(\partial_{y^0}G_{\varrho,ab}(x, y))_{x^0=y^0} = -\delta_{ab}\delta^3(\mathbf{x} - \mathbf{y})$.

³In contrast to the spectral function, the statistical Higgs-propagator is symmetric in the sense that $G_{F,ba}(y, x) = G_{F,ab}(x, y)$.

⁴The adjoint of the lepton spectral function is given by $S_{\varrho,lm}^\dagger(x, y) = -\beta S_{\varrho,ml}(y, x)\beta$. Furthermore, the canonical equal-time anticommutation relations give $(S_{\varrho,lm}(x, y))_{x^0=y^0} = i\beta\delta(\mathbf{x} - \mathbf{y})\delta_{lm}$.

⁵The adjoint of the statistical lepton-propagator is given by $S_{F,lm}^\dagger(x, y) = \beta S_{F,ml}(y, x)\beta$.

$$S_{F,lm}^{\alpha\beta}(x, y) = \frac{1}{2}[\Psi_l^\alpha(x), \bar{\Psi}_m^\beta(y)]_- \quad (13)$$

for the leptons, so that we can decompose the complete lepton propagator according to

$$S(x, y) = S_F(x, y) - \frac{i}{2} \text{sign}_C(x^0 - y^0) S_\varrho(x, y). \quad (14)$$

Then, using Eqs. (11) and (14), we can decompose the Higgs self-energy (9) as well as the lepton self-energy (10) according to:

$$\begin{aligned} \Pi(x, y) &= -i\delta_C(x - y)\Pi^{\text{(local)}}(x) + \Pi_F(x, y) \\ &\quad - \frac{i}{2} \text{sign}_C(x^0 - y^0)\Pi_\varrho(x, y) \end{aligned}$$

and

$$\Sigma(x, y) = \Sigma_F(x, y) - \frac{i}{2} \text{sign}_C(x^0 - y^0)\Sigma_\varrho(x, y).$$

The local part of the Higgs self-energy causes a mass shift only, wherefore we define the effective mass by

$$\begin{aligned} M_{ab}^2(x) &= m_B^2 \delta_{ab} + \Pi_{ab}^{\text{(local)}}(x) \\ &= m_B^2 \delta_{ab} + 4\lambda(G_{dd}(x, x)\delta_{ab} + 2G_{ab}(x, x)). \end{aligned} \quad (15)$$

After convolving Eqs. (7) and (8) from the right with the corresponding complete propagators, we observe that both equations split into two complementary evolution equations for the statistical propagators and the spectral functions, respectively [36]:

$$\begin{aligned} &(-\partial_{x^\mu} \partial_{x_\mu} \delta_{ac} + M_{ac}^2(x))G_{F,cb}(x, y) \\ &= \int_0^{y^0} d^4z \Pi_{F,ac}(x, z)G_{\varrho,cb}(z, y) \\ &\quad - \int_0^{x^0} d^4z \Pi_{\varrho,ac}(x, z)G_{F,cb}(z, y), \end{aligned} \quad (16)$$

$$\begin{aligned} &(-\partial_{x^\mu} \partial_{x_\mu} \delta_{ac} + M_{ac}^2(x))G_{\varrho,cb}(x, y) \\ &= - \int_0^{x^0} d^4z \Pi_{\varrho,ac}(x, z)G_{\varrho,cb}(z, y), \end{aligned} \quad (17)$$

$$\begin{aligned} \not{\partial}_x S_{F,lm}(x, y) &= \int_0^{y^0} d^4z \Sigma_{F,lk}(x, z)S_{\varrho,km}(z, y) \\ &\quad - \int_0^{x^0} d^4z \Sigma_{\varrho,lk}(x, z)S_{F,km}(z, y) \end{aligned} \quad (18)$$

and

$$\not{\partial}_x S_{\varrho,lm}(x, y) = - \int_0^{x^0} d^4z \Sigma_{\varrho,lk}(x, z)S_{\varrho,km}(z, y). \quad (19)$$

Nowadays, it is practically impossible to solve the Kadanoff-Baym equations numerically in this general form. However, for initial conditions which are invariant under spatial translations, spatial rotations, parity, charge conjugation, and chiral transformations, the propagators

take the form [36]

$$G_{ab}(x, y) = \int \frac{d^3k}{(2\pi)^3} \exp(i\mathbf{k}(x - \mathbf{y}))G(x^0, y^0, k)\delta_{ab} \quad (20)$$

and

$$\begin{aligned} S_{lm}(x, y) &= \int \frac{d^3k}{(2\pi)^3} \exp(i\mathbf{k}(x - \mathbf{y})) \left(S_V^0(x^0, y^0, k)\gamma_0 \right. \\ &\quad \left. - i \frac{k^j}{k} S_V(x^0, y^0, k)\gamma_j \right) \delta_{lm}, \end{aligned} \quad (21)$$

where $k = |\mathbf{k}|$. The index V indicates that S_V^μ would transform as a vector under a Lorentz transformation. Due to CP invariance, the statistical and spectral vector components of the lepton propagator satisfy

$$\begin{aligned} S_{V,F}^0(x^0, y^0, k) &= -S_{V,F}^0(y^0, x^0, k) \\ &= S_{V,F}^{*0}(x^0, y^0, k) \\ S_{V,F}(x^0, y^0, k) &= S_{V,F}(y^0, x^0, k) \\ &= S_{V,F}^{*}(x^0, y^0, k) \\ S_{V,\varrho}^0(x^0, y^0, k) &= S_{V,\varrho}^0(y^0, x^0, k) \\ &= S_{V,\varrho}^{*0}(x^0, y^0, k) \\ S_{V,\varrho}(x^0, y^0, k) &= -S_{V,\varrho}(y^0, x^0, k) \\ &= S_{V,\varrho}^{*}(x^0, y^0, k) \end{aligned} \quad (22)$$

Thus, the explicit factor of i makes $S_{V,F}^0$, $S_{V,F}$, $S_{V,\varrho}^0$ and $S_{V,\varrho}$ real-valued quantities:

$$\text{Im}(S_{V,F}^0) = \text{Im}(S_{V,F}) = \text{Im}(S_{V,\varrho}^0) = \text{Im}(S_{V,\varrho}) = 0. \quad (23)$$

Furthermore, the canonical equal-time anticommutation relations for fermion fields imply

$$S_{V,\varrho}^0(t, t, k) = 1 \quad \text{and} \quad S_{V,\varrho}(t, t, k) = 0, \quad (24)$$

the second equality being consistent with the antisymmetry of the spacelike vector-component of the lepton spectral function, cf. Eq. (22). Of course, the relations (20)–(23) also hold for the corresponding self-energies, so that the Kadanoff-Baym equations can be simplified drastically. The simplified Kadanoff-Baym equations for the Higgs propagator read [36]

$$\begin{aligned} &[\partial_{x^0}^2 + k^2 + M^2(x^0)]G_F(x^0, y^0, k) \\ &= \int_0^{y^0} dz^0 \Pi_F(x^0, z^0, k)G_\varrho(z^0, y^0, k) \\ &\quad - \int_0^{x^0} dz^0 \Pi_\varrho(x^0, z^0, k)G_F(z^0, y^0, k) \end{aligned} \quad (25)$$

and

$$\begin{aligned} &[\partial_{x^0}^2 + k^2 + M^2(x^0)]G_\varrho(x^0, y^0, k) \\ &= - \int_0^{x^0} dz^0 \Pi_\varrho(x^0, z^0, k)G_\varrho(z^0, y^0, k). \end{aligned} \quad (26)$$

In the same way, the 128 complex-valued Kadanoff-Baym equations (18) and (19) for the lepton propagator can be reduced to the following 4 real-valued equations [36]:

$$\begin{aligned} \partial_{x^0} S_{V,F}^0(x^0, y^0, k) + k S_{V,F}(x^0, y^0, k) = & - \int_0^{y^0} dz^0 [\Sigma_{V,F}^0(x^0, z^0, k) S_{V,\varrho}^0(z^0, y^0, k) + \Sigma_{V,F}(x^0, z^0, k) S_{V,\varrho}(z^0, y^0, k)] \\ & + \int_0^{x^0} dz^0 [\Sigma_{V,\varrho}^0(x^0, z^0, k) S_{V,F}^0(z^0, y^0, k) + \Sigma_{V,\varrho}(x^0, z^0, k) S_{V,F}(z^0, y^0, k)], \end{aligned} \quad (27)$$

$$\begin{aligned} \partial_{x^0} S_{V,F}(x^0, y^0, k) - k S_{V,F}^0(x^0, y^0, k) = & \int_0^{y^0} dz^0 [\Sigma_{V,F}(x^0, z^0, k) S_{V,\varrho}^0(z^0, y^0, k) - \Sigma_{V,F}^0(x^0, z^0, k) S_{V,\varrho}(z^0, y^0, k)] \\ & - \int_0^{x^0} dz^0 [\Sigma_{V,\varrho}(x^0, z^0, k) S_{V,F}^0(z^0, y^0, k) - \Sigma_{V,\varrho}^0(x^0, z^0, k) S_{V,F}(z^0, y^0, k)], \end{aligned} \quad (28)$$

$$\partial_{x^0} S_{V,\varrho}^0(x^0, y^0, k) + k S_{V,\varrho}(x^0, y^0, k) = \int_{y^0}^{x^0} dz^0 [\Sigma_{V,\varrho}^0(x^0, z^0, k) S_{V,\varrho}^0(z^0, y^0, k) + \Sigma_{V,\varrho}(x^0, z^0, k) S_{V,\varrho}(z^0, y^0, k)] \quad (29)$$

and

$$\partial_{x^0} S_{V,\varrho}(x^0, y^0, k) - k S_{V,\varrho}^0(x^0, y^0, k) = - \int_{y^0}^{x^0} dz^0 [\Sigma_{V,\varrho}(x^0, z^0, k) S_{V,\varrho}^0(z^0, y^0, k) - \Sigma_{V,\varrho}^0(x^0, z^0, k) S_{V,\varrho}(z^0, y^0, k)]. \quad (30)$$

The expressions for the Higgs and lepton self-energies are given in Appendix A. As explained in more detail in Ref. [36], one can define an effective kinetic energy distribution $\omega(t, k)$, as well as effective scalar and fermion particle number distributions $n_s(t, k)$ and $n_f(t, k)$, which can be obtained from the statistical propagators according to

$$\omega^2(t, k) = \left(\frac{\partial_{x^0} \partial_{y^0} G_F(x^0, y^0, k)}{G_F(x^0, y^0, k)} \right)_{x^0=y^0=t}, \quad (31)$$

$$n_s(t, k) = \omega(t, k) G_F(t, t, k) - \frac{1}{2}, \quad (32)$$

and

$$n_f(t, k) = \frac{1}{2} - S_{V,F}(t, t, k). \quad (33)$$

The definition of such particle numbers is necessary in order to make contact to Boltzmann equations, e. g. when comparing numerical solutions of Boltzmann and Kadanoff-Baym equations, which we will do in Sec. V. We emphasize, however, that the Kadanoff-Baym equations are self-consistent evolution equations for the complete propagators of our system, and that one has to follow the evolution of the two-point functions throughout the complete 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 densities along the bisecting line of this plane.

IV. BOLTZMANN EQUATIONS

In this section we briefly sketch the standard way of deriving Boltzmann equations from Kadanoff-Baym equations [14, 15, 18, 44–46]. One has to employ a Wigner trans-

formation, a first-order gradient expansion, the Kadanoff-Baym ansatz and the quasiparticle approximation.

First, we subtract Eq. (25) [Eq. (27)] with x^0 and y^0 interchanged from Eq. (25) [Eq. (27)]. Then we reparametrize the propagators and the self-energies by center and relative times, e. g.

$$G(u^0, v^0, k) = G\left(\frac{u^0 + v^0}{2}, u^0 - v^0, k\right).$$

Next, we define the center time $t = \frac{x^0 + y^0}{2}$ and the relative time $s^0 = x^0 - y^0$, and observe on the left-hand side of the difference equations that

$$\partial_{x^0} \partial_{x^0} - \partial_{y^0} \partial_{y^0} = 2\partial_t \partial_{s^0}$$

and

$$\partial_{x^0} + \partial_{y^0} = \partial_t$$

are automatically of first order in ∂_t . Furthermore, we Taylor expand the effective masses on the left-hand side of the difference equation for the scalars as well as the propagators and self-energies on the right-hand sides of both difference equations to first order in ∂_t around t . After that, we Fourier transform the difference equations with respect to the relative time s^0 . The Wigner transformed scalar statistical propagator and scalar spectral function are given by

$$G_F(t, \omega, k) = \int ds^0 \exp(i\omega s^0) G_F(t, s^0, k),$$

$$G_\varrho(t, \omega, k) = -i \int ds^0 \exp(i\omega s^0) G_\varrho(t, s^0, k).$$

As $G_\varrho(t, s^0, k)$ is a real-valued odd function of the relative time s^0 , we introduced an explicit factor of $-i$ in order to

make its Wigner transform again a real-valued function. For similar reasons we also introduce a factor of $-i$ for the Wigner transforms of $S_{V,\varrho}(t, s^0, k)$, $S_{V,F}^0(t, s^0, k)$, $S_{V,R}^0(t, s^0, k)$, and $S_{V,A}^0(t, s^0, k)$,⁶ as well as the corresponding self-energies. In order to be able to really perform the Fourier transformation, we have to send the initial time to $-\infty$. At least for large x^0 and y^0 this can be justified by taking into account that correlations between earlier and later times are suppressed exponentially [1,40]. For early times, however, this is certainly not the case. The result of all these transformations are quantum-kinetic equations for the statistical propagators G_F and $S_{V,F}^0$ [16–18,47–50]⁷:

$$-\{ \Omega; G_F \}_{PB} = \Pi_{\varrho} G_F - \Pi_F G_{\varrho} + \{ \Pi_F; \text{Re}(G_R) \}_{PB} \quad (34)$$

and

$$\begin{aligned} \{ W; S_{V,F}^0 \}_{PB} &= \Sigma_{V,\varrho}^0 S_{V,F}^0 - \Sigma_{V,F}^0 S_{V,\varrho}^0 + \Sigma_{V,\varrho} S_{V,F} \\ &\quad - \Sigma_{V,F} S_{V,\varrho} - \{ \Sigma_{V,F}^0; \text{Re}(S_{V,R}^0) \}_{PB} \\ &\quad + \{ \text{Re}(\Sigma_{V,R}); S_{V,F} \}_{PB} \\ &\quad + \{ \Sigma_{V,F}; \text{Re}(S_{V,R}) \}_{PB}, \end{aligned} \quad (35)$$

where the Poisson brackets are defined by

$$\{ f; g \}_{PB} = -[\partial_t f][\partial_{\omega} g] + [\partial_{\omega} f][\partial_t g].$$

The auxiliary functions

$$\Omega(t, \omega, k) = -\omega^2 + k^2 + M^2(t) + \text{Re}(\Pi_R(t, \omega, k))$$

and

$$W(t, \omega, k) = \omega + \text{Re}(\Sigma_{V,R}^0(t, \omega, k))$$

have been introduced to simplify the notation. Employing the first-order Taylor expansion is clearly not justifiable for early times when the equal-time propagator is rapidly oscillating [1,23]. Consequently, one might expect that the above quantum-kinetic equations and also the Boltzmann equations, which we derive subsequently, fail to describe the early-time evolution and that errors accumulated for early times cannot be remedied at late times. In fact, the first-order gradient expansion is motivated by equilibrium considerations: In equilibrium the propagator depends on the relative coordinates only. There is no dependence on the center coordinates, and one may hope that there are situations out of equilibrium where the propagator depends only moderately on the center coordinates. This is clearly the case for late times when our

system is sufficiently close to equilibrium. However, already after moderate times the rapid oscillations mentioned above, have died out and are followed by a monotonous drifting regime [1,40]. In this drifting regime the second derivative with respect to t should be negligible as compared to the first-order derivative, and a consistent Taylor expansion can be justified even though the system may still be far from equilibrium. Here, it is crucial that the Taylor expansion is performed consistently for two reasons: First, this guarantees that the quantum-kinetic equations satisfy exactly the same conservation laws as the full Kadanoff-Baym equations do [17]. Second, it has been shown that neglecting the Poisson brackets severely restricts the range of validity of the quantum-kinetic transport equations [50,51].

In order to derive Boltzmann equations from the quantum-kinetic equations for the statistical propagators (34) and (35), first we have to discard the Poisson brackets on the right-hand sides, thereby sacrificing the consistency of the gradient expansion. On the left-hand sides we remove the time dependence of the auxiliary quantities Ω and W . We take

$$W(t, \omega, k) = \omega$$

and

$$\Omega(t, \omega, k) = -\omega^2 + k^2 + m^2,$$

where m is the thermal mass of the scalars. After that, we employ the Kadanoff-Baym ansatz

$$G_F(t, \omega, k) = G_{\varrho}(\omega, k)(\frac{1}{2} + n_s(t, \omega, k)) \quad (36)$$

and

$$S_F(t, \omega, k) = S_{\varrho}(\omega, k)(\frac{1}{2} - n_f(t, \omega, k)) \quad (37)$$

which also can be motivated by equilibrium considerations. In fact, this is a generalization of the fluctuation-dissipation theorem, which states that, for a system in thermal equilibrium, the statistical propagator is proportional to the spectral function. The fluctuation dissipation theorem can be recovered from Eqs. (36) and (37) by discarding the dependence on the center time t and fixing n_s and n_f to be the Bose-Einstein and Fermi-Dirac distribution function, respectively. The last approximation, which is necessary to arrive at the Boltzmann equations, is the so-called quasiparticle (or on-shell) approximation. For the scalars this means that the spectral function takes the form

$$G_{\varrho}(\omega, k) = \frac{\pi}{E(k)} (\delta(\omega - E(k)) - \delta(\omega + E(k))),$$

where the quasiparticle energy is given by

$$E(k) = \sqrt{m^2 + k^2}.$$

For the lepton spectral function we assume

⁶The retarded and advanced propagators, e. g. $G_R(x^0, y^0, k) = \theta(x^0 - y^0)G_{\varrho}(x^0, y^0, k)$ and $G_A(x^0, y^0, k) = -\theta(y^0 - x^0) \times G_{\varrho}(x^0, y^0, k)$, and self-energies have to be introduced in order to remove the upper boundaries of the memory integrals in the Kadanoff-Baym equations.

⁷The complete and closed set of these quantum-kinetic equations comprehends 9 equations and self-energies, which, for completeness, are shown in Appendix B.

$$S_{V,\varrho}^0(\omega, k) = \pi(\delta(\omega - k) + \delta(\omega + k)),$$

$$S_{V,\varrho}(\omega, k) = \pi(\delta(\omega - k) - \delta(\omega + k)).$$

Once more, we would like to stress that the exact time evolution of the spectral functions is determined by the Kadanoff-Baym equations. It has been shown that the spectral function can be parameterized by a Breit-Wigner function with a nonvanishing width [26,29]. To reduce the width of this Breit-Wigner curve to zero is certainly not a controllable approximation and leads to very large qualitative discrepancies between the results produced by the Kadanoff-Baym and Boltzmann equations. In fact this approximation can only be justified if our system consists of stable, or at least very long-lived, quasiparticles, whose mass is much larger than their decay width. We also would like to note that a completely self-consistent determination of the thermal mass in the framework of the Boltzmann equation requires the solution of an integral equation for $E(k)$, which would drastically increase the complexity of our numerics. As none of our physical results depend on the exact value of the thermal mass, for convenience, we use the equilibrium value of the thermal scalar mass as determined by the Kadanoff-Baym equations. Eventually, we define the quasiparticle number densities by

$$n_s(t, k) = n_s(t, E(k), k)$$

and

$$n_f(t, k) = n_f(t, k, k).$$

After equating the positive energy components in Eqs. (34) and (35) we arrive at the following Boltzmann equations:

$$\begin{aligned} \partial_t n_s(t, k) &= 2\pi\eta^2 \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta^3(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ &\times \delta(E(k) - p - q) \frac{1}{E(k)} \left(1 - \frac{\mathbf{p}\mathbf{q}}{pq}\right) \\ &\times [(n_s(t, k) + 1)n_f(t, p)n_f(t, q) \\ &- n_s(t, k)(n_f(t, p) - 1)(n_f(t, q) - 1)] \end{aligned} \quad (38)$$

and

$$\begin{aligned} \partial_t n_f(t, k) &= 2\pi\eta^2 \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta^3(\mathbf{k} + \mathbf{p} - \mathbf{q}) \\ &\times \delta(k + p - E(q)) \frac{1}{E(q)} \left(1 - \frac{\mathbf{k}\mathbf{p}}{kp}\right) \\ &\times [(n_f(t, k) - 1)(n_f(t, p) - 1)n_s(t, q) \\ &- n_f(t, k)n_f(t, p)(n_s(t, q) + 1)]. \end{aligned} \quad (39)$$

Exploiting isotropy the above 6-dimensional Boltzmann collision integrals can be reduced to 1-dimensional integrals:

$$\begin{aligned} \partial_t n_s(t, k) &= \frac{2\eta^2}{\pi^2 E(k)} \int_0^\infty dp \theta(q_0) J_s(k, p, q_0) \\ &\times [(n_s(t, k) + 1)n_f(t, p)n_f(t, q_0) \\ &- n_s(t, k)(n_f(t, p) - 1)(n_f(t, q_0) - 1)], \end{aligned} \quad (40)$$

$$\begin{aligned} \partial_t n_f(t, k) &= \frac{2\eta^2}{\pi^2} \int_0^\infty dq \theta(p_0) \frac{q}{E(q)} J_f(k, p_0, q) \\ &\times [(n_f(t, k) - 1)(n_f(t, p_0) - 1)n_s(t, q) \\ &- n_f(t, k)n_f(t, p_0)(n_s(t, q) + 1)]. \end{aligned} \quad (41)$$

The details of these calculations and the definitions of all of the auxiliary quantities are given in Appendix C. This simplification of the collision integrals is crucial in order to implement efficient computer programs for the numerical solution of the Boltzmann equations.

In this section we showed that the derivation of Boltzmann equations from Kadanoff-Baym equations requires a number of nontrivial approximations and assumptions. One has to employ a first-order gradient expansion, a Wigner transformation, and a quasiparticle approximation. In this sense, one can consider the Kadanoff-Baym equations as quantum Boltzmann equations resumming the gradient expansion up to infinite order and including memory and off-shell effects.

V. COMPARING BOLTZMANN VS. KADANOFF-BAYM

A. Initial conditions and numerical settings

In order to solve the Kadanoff-Baym equations numerically, we follow exactly the lines of Refs. [1,36] on a lattice with $2000^2 \times 32^3$ lattice sites. The values for the coupling constants are $\eta = 1$ and $\lambda = 0.25$. The initial conditions for the statistical propagators are determined by scalar and fermionic particle number distributions $n_s(t = 0, p)$ and $n_f(t = 0, p)$ according to

$$\begin{aligned} G_F(x^0, y^0, p)_{x^0=y^0=0} &= \frac{n_s(t = 0, p) + \frac{1}{2}}{\omega_0(p)}, \\ [\partial_{x^0} G_F(x^0, y^0, p)]_{x^0=y^0=0} &= 0, \\ [\partial_{x^0} \partial_{y^0} G_F(x^0, y^0, p)]_{x^0=y^0=0} &= \omega_0(p) \left(n_s(t = 0, p) + \frac{1}{2} \right), \\ S_{V,F}^0(x^0, y^0, p)_{x^0=y^0=0} &= 0, \\ S_{V,F}(x^0, y^0, p)_{x^0=y^0=0} &= \frac{1}{2} - n_f(t = 0, p), \end{aligned}$$

where $\omega_0(p)$ is the initial scalar kinetic energy distribution. On the other hand, the initial conditions for the spectral functions are determined by equal-time (anti-) commutation relations. We solve the Boltzmann and Kadanoff-Baym equations for three different sets of initial particle number distributions, which are shown in Fig. 5. All initial conditions correspond to the same (conserved) average

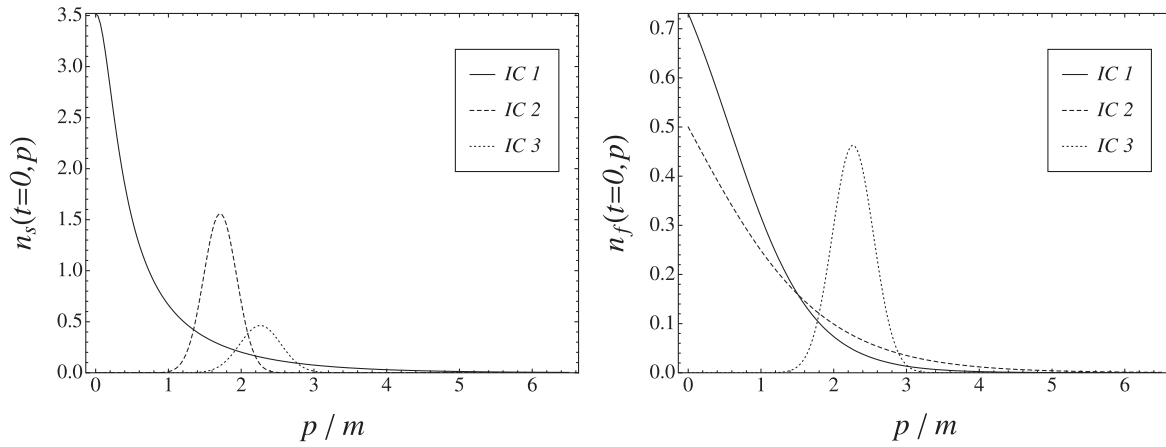


FIG. 5. These figures show the qualitative shape of the initial particle number distributions for scalars (left) and fermions (right). These distributions define the initial conditions (IC) for which we solved the Boltzmann and Kadanoff-Baym equations numerically. Because of computational limitations we could not solve the Boltzmann and Kadanoff-Baym equations for exactly the same initial conditions. The numerical solution of the Kadanoff-Baym equations called for systems with larger average energy and particle number densities. However, it is important to note, that our results are not in any way affected by these differences. For both types of equations, all initial conditions correspond to the same (conserved) average energy density. Above that, for the initial conditions IC1 and IC2 also the sum of the initial average number densities agree.

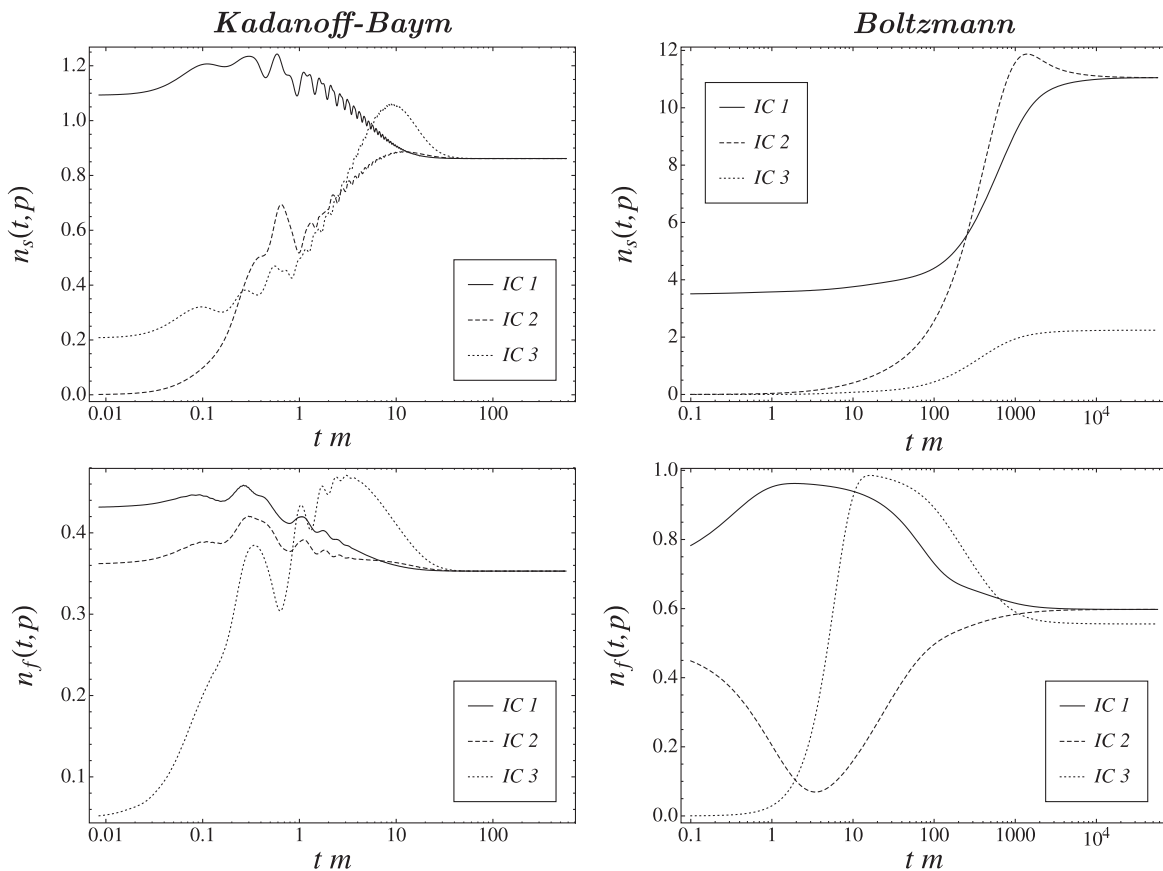


FIG. 6. These plots show the time evolution of the particle number distributions for fixed momentum modes and all initial conditions as determined by the Boltzmann and the Kadanoff-Baym equations. We see that the Kadanoff-Baym equations respect full universality, whereas the Boltzmann equations maintain only a restricted universality, cf. Fig. 7. The qualitative features of these plots do not depend on the momentum modes. Therefore, in order to get clear plots, we could choose a different momentum mode for each plot, which accounts for the different initial conditions on the Boltzmann and the Kadanoff-Baym side.

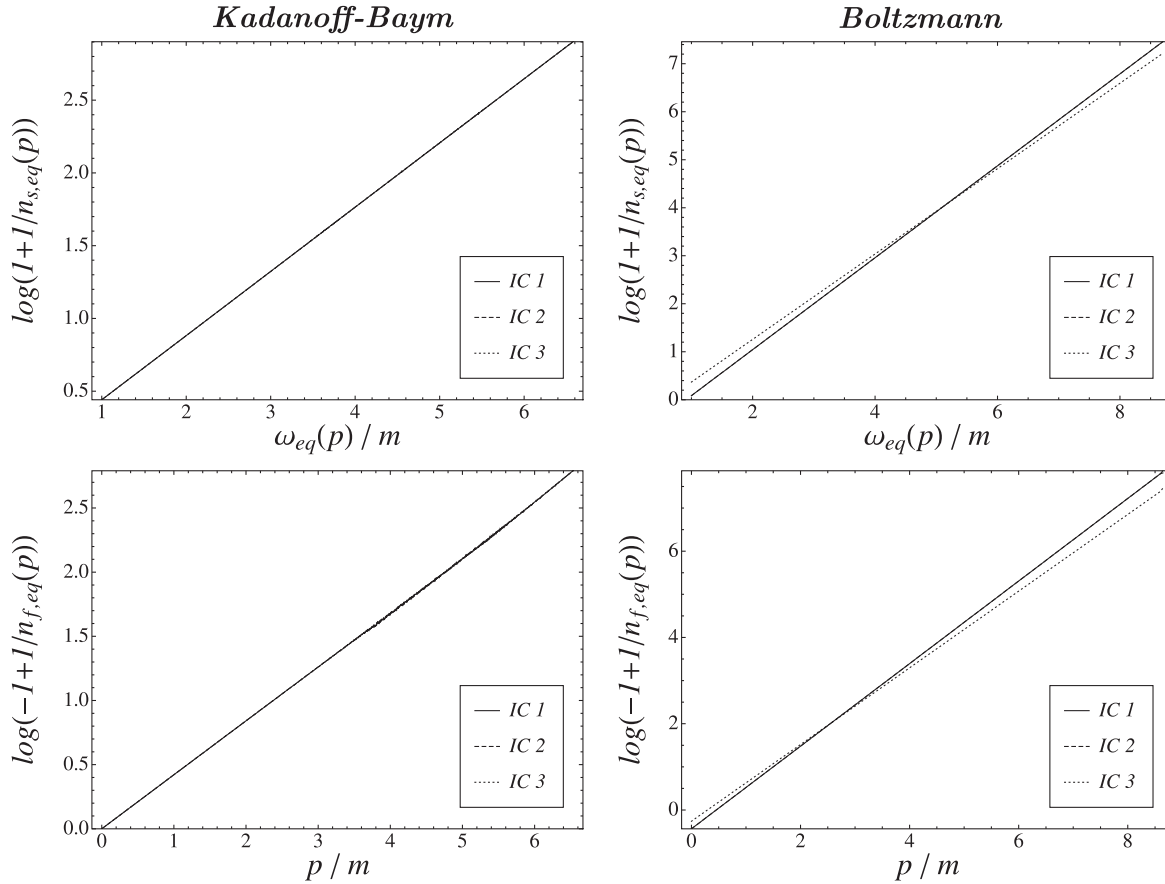


FIG. 7. Equilibrium particle number distributions. The straight lines in these plots prove that in equilibrium the particle number distributions indeed take the form of Bose-Einstein or Fermi-Dirac distribution functions, where the temperature is given by the inverse slope and the chemical potential is proportional to the y-axis intercept. The Kadanoff-Baym equations lead to a universal temperature $T = 2.3m$ and universally vanishing chemical potentials. The temperatures and chemical potentials predicted by the Boltzmann equations are given in Table I.

energy density. Above that, for the initial conditions IC1 and IC2 also the sum of the initial scalar and fermionic average particle number densities agree. The numerical solution of the Boltzmann equations proceeds along the lines of Ref. [1]. The scale in our plots is set by the scalar thermal mass $m = \omega_{\text{eq}}(p = 0)$, where $\omega_{\text{eq}}(p)$ is the effective kinetic energy distribution (31) for sufficiently late time t .

B. Universality

Figures 6 and 7 exhibit that the Kadanoff-Baym equations respect full universality: Fig. 6 shows the time evolution of the particle number distributions for a fixed momentum mode. The particle number distributions start from different initial values and go through very different early-time evolutions. Nevertheless, in the case of the Kadanoff-Baym equations they all approach the same universal late-time value. Figure 7 shows the particle number distributions for times when equilibrium has effectively been reached. In the case of Kadanoff-Baym equations, we observe that the equilibrium number distributions agree exactly independent of the initial conditions, which proves

that we could have shown the plots of Fig. 6 for any momentum mode. In particular, the straight lines in Fig. 7 prove that the equilibrium number distributions take the form of Bose-Einstein or Fermi-Dirac distribution functions with a universal temperature $T = 2.3m$ and universally vanishing chemical potentials.

In contrast to this, Boltzmann equations maintain only a restricted universality. Figures 6 and 7 reveal that only the initial conditions IC1 and IC2 lead to the same late-time behavior, which deviates significantly from the one approached by the third initial condition IC3. Again, the

TABLE I. Temperatures and chemical potentials as predicted by the Boltzmann equations. The values in this table have been obtained by fitting the equilibrium particle number distributions shown in Fig. 7 against Bose-Einstein and Fermi-Dirac distribution functions, respectively.

	T_s/m	T_f/m	μ_s/m	μ_f/m	μ_s/μ_f
IC1	1.044	1.044	0.910	0.455	1.999
IC2	1.044	1.044	0.910	0.455	2.001
IC3	1.125	1.124	0.586	0.293	1.997

straightness of the lines in Fig. 7 proves that the equilibrium number distributions take the form of Bose-Einstein or Fermi-Dirac distribution functions. However, the different slopes of the lines indicate that the temperature is not the same for all initial conditions, and the nonvanishing y-axis intercepts indicate that Boltzmann equations may predict different nonvanishing chemical potentials. Fitted values for these quantities are given in Table I.

The reason for the observed restriction of universality can be extracted from Fig. 8 where we plotted the time

evolution of the average particle number densities per degree of freedom

$$N_s(t) = \int \frac{d^3 p}{(2\pi)^3} n_s(t, p) \quad (42)$$

and

$$N_f(t) = \int \frac{d^3 p}{(2\pi)^3} n_f(t, p) \quad (43)$$

and their sum. Provided Φ -derivable approximations are employed, the Kadanoff-Baym equations conserve the av-

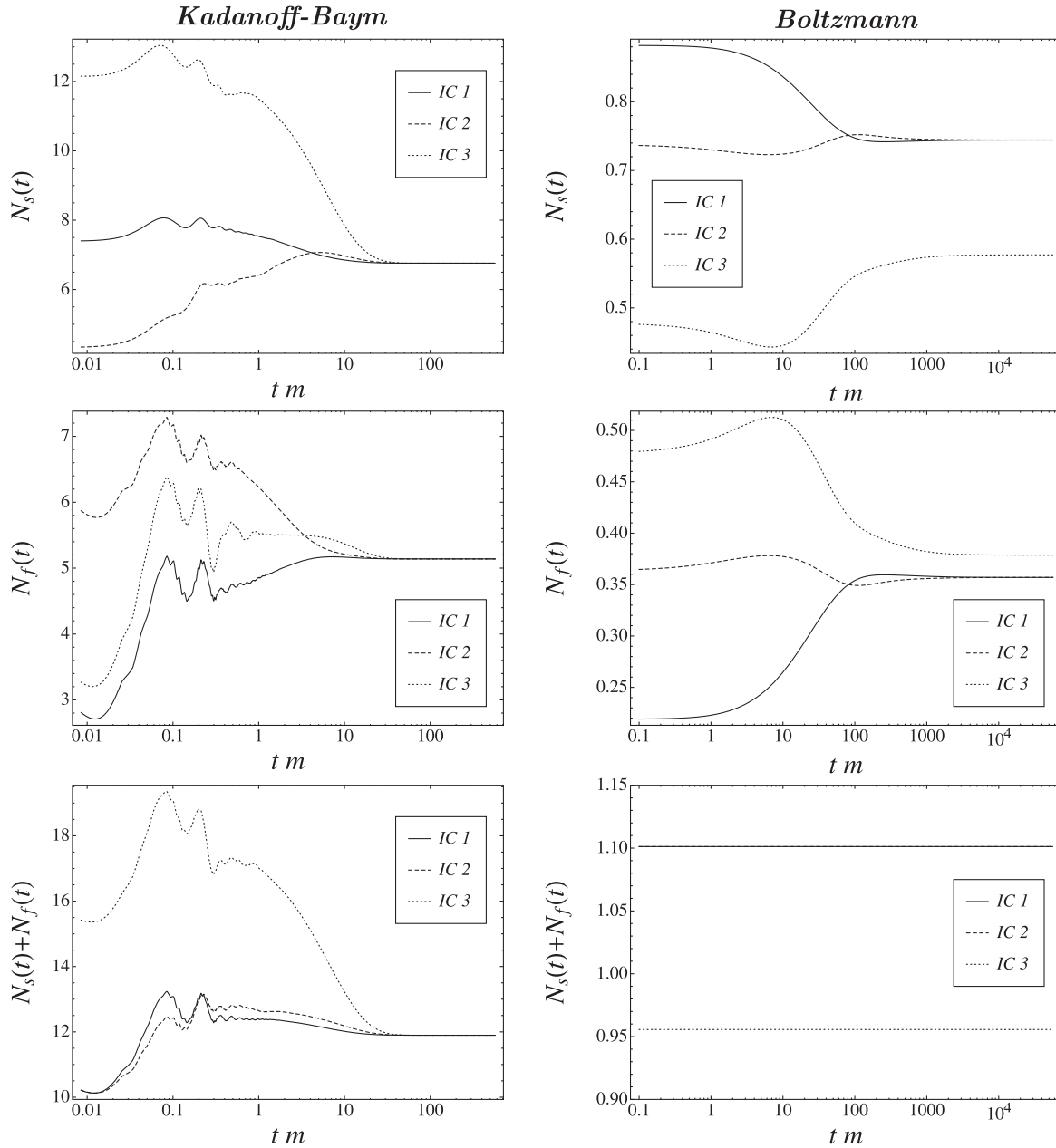


FIG. 8. Time evolution of the average particle number densities and their sum. The Kadanoff-Baym equations allow for a change of the latter quantity, whereas it is spuriously conserved by the Boltzmann equations. The quantitative disagreement of the average particle number densities can be attributed to different initial conditions and discretization schemes for the Boltzmann and the Kadanoff-Baym equations, and is of no relevance for the purpose of the present work.

erage energy density as well as global charges [37–39]. However, as we consider systems with vanishing net charge density neither of the above average particle number densities has to be conserved, nor their sum. Indeed, the Kadanoff-Baym equations include off-shell particle creation and annihilation [1,26], so that all of the quantities plotted in Fig. 8 may change as time goes on and approach a universal equilibrium value.

In contrast to this, due to the quasiparticle (or on-shell) approximation the Boltzmann equations (40) and (41) only include decay and recombination processes of the form

$$1 \text{ scalar} \leftrightarrow 2 \text{ fermions.} \quad (44)$$

More precisely, one of four scalars may decay into or be recombined from one of two fermion pairs. As a consequence the sum of the average particle number densities (42) and (43) is strictly conserved, as can be seen in Fig. 8. Of course, this spurious constant of motion severely restricts the evolution of the particle number distributions. As a result, the Boltzmann equations maintain only a restricted universality and, as will be discussed in the next subsection, fail to describe the process of quantum-chemical equilibration.

C. Chemical equilibration

In a system allowing for the creation and annihilation of particles, the chemical potential of particles, whose total number is not restricted by any conserved quantity, must vanish in thermodynamic equilibrium. Accordingly, as we consider systems with vanishing net charge density the chemical potentials for scalars and fermions should vanish once equilibrium has been reached. Indeed, Kadanoff-Baym equations lead to universally vanishing chemical potentials. In contrast to this, as one can see in Table I, the Boltzmann equations in general will give nonvanishing chemical potentials. For a system which includes only interactions of the form (44), in equilibrium the chemical potentials are expected to satisfy the relation

$$\mu_s = 2\mu_f.$$

As one can see in the right-most column of Table I, this relation is indeed fulfilled up to numerical errors $<0.3\%$. Thus, the Boltzmann equations (40) and (41) lead to a classical chemical equilibrium. As mentioned above, however, quantum-chemical equilibrium requires that the chemical potentials vanish for systems with vanishing net charge density. In this sense, the nonvanishing chemical potentials in Table I indicate that the description of quantum-chemical equilibration is out of reach of the Boltzmann equations (40) and (41).

D. Separation of time scales

As has been discussed in Ref. [1] in the framework of a purely scalar theory and in Ref. [32] in the framework of

the linear sigma model underlying our studies in this work, the Kadanoff-Baym equations strongly separate the time scales between the kinetic and the complete thermodynamic (including chemical) equilibration. This phenomenon has been called prethermalization [32], and implies that certain quantities approach their equilibrium values on time scales which are dramatically shorter than the thermodynamic equilibration time.

As we have seen in this work and in Ref. [1], standard Boltzmann equations cannot describe the phenomenon of quantum-chemical equilibration, and thus they also cannot describe the approach to the quantum-thermodynamic equilibrium. Consequently, standard Boltzmann equations cannot separate the time scales between the kinetic and the full thermodynamic equilibration and hence a description of prethermalization is out of reach of standard Boltzmann equations.

In the context of time scales, of course, it is also important to compare the thermalization times themselves. Here, it is interesting to note that for nonrelativistic systems Boltzmann equations yield smaller thermalization times than Kadanoff-Baym equations [24,25,27]. In contrast to this, however, in the framework of relativistic quantum fields far from equilibrium, Boltzmann equations give significantly larger thermalization times, as can be seen in Figs. 6 and 8, and in Ref. [1].

VI. CONCLUSIONS

In this article we addressed the question how reliable Boltzmann equations are as approximations to Kadanoff-Baym equations in the framework of a chirally invariant Yukawa-type quantum field theory coupling scalars with fermions. Starting from the 2PI effective action, we reviewed the derivation of the Kadanoff-Baym equations and the approximations which are necessary to eventually arrive at standard Boltzmann equations. We solved the Boltzmann and Kadanoff-Baym equations numerically for highly symmetric systems in $3 + 1$ space-time dimensions without any further approximations and compared their solutions for various nonequilibrium initial conditions.

We demonstrated that the Kadanoff-Baym equations respect universality: For systems with equal average energy density the late-time behavior coincides independent of the details of the initial conditions. In particular, independent of the initial conditions the particle number distributions, temperatures, chemical potentials and thermal masses predicted for times, when equilibrium has effectively been reached, coincide. Above that, Kadanoff-Baym equations incorporate the process of quantum-chemical equilibration: For systems with vanishing net charge density the chemical potentials vanish once equilibrium has effectively been reached. Last but not least, Kadanoff-Baym equations feature the phenomenon of prethermalization and separate the time scales between kinetic and full

thermodynamic (including quantum-chemical) equilibration.

The quasiparticle approximation introduces spurious constants of motion for standard Boltzmann equations (cf. Fig. 8), which severely restricts the evolution of the particle number distributions. As a result, Boltzmann equations cannot lead to a universal quantum-thermal equilibrium and maintain only a restricted universality: Only initial conditions for which the average energy density, all global charges and all spurious constants of motion agree from the very beginning, lead to the same equilibrium results. As shown in Table I, Boltzmann equations cannot describe the phenomenon of quantum-chemical equilibration and, in general, will lead to nonvanishing chemical potentials even for systems with vanishing net charge density. Because of the lack of quantum-chemical equilibration, the separation of time scales observed for the Kadanoff-Baym equations is absent in the case of the Boltzmann equations, which renders the description of prethermalization impossible.

Some of the approximations, which are required to derive Boltzmann equations from Kadanoff-Baym equations, are clearly motivated by equilibrium considerations. Taking the observed restriction of universality into account, we conclude that in the context of relativistic quantum fields one can safely apply standard Boltzmann equations only to systems which are sufficiently close to equilibrium, so that the spurious constants of motion emerging in Boltzmann equations already take their equilibrium values. However, for systems far from equilibrium standard Boltzmann equations work reliably neither for early times (no prethermalization) nor for late times (only restricted late-time universality, no quantum-chemical equilibration). Accordingly, for systems in the intermediate regime the results given by standard Boltzmann equations should be treated with care. For realistic scenarios, like leptogenesis or the quark-gluon plasma, non-negligible corrections to Boltzmann equations are expected, which should be evaluated.

Solving Kadanoff-Baym equations numerically is significantly more difficult than solving the corresponding standard Boltzmann equations. However, the considerable discrepancies found for numerical solutions of Kadanoff-Baym and Boltzmann equations revealed equally significant limitations for standard Boltzmann equations. Accordingly, the importance of numerical solutions of Kadanoff-Baym equations cannot be overestimated and it is certainly worth to face the arising difficulties.

In the present work we considered standard Boltzmann equations at lowest order in the particle number densities, and we employed the standard Kadanoff-Baym ansatz for their derivation. Further studies are needed in order to estimate whether and to what extent the situation for Boltzmann equations can be improved by including non-minimal collision terms or by employing a generalized Kadanoff-Baym ansatz.

In the future it will be important to perform a similar comparison of Boltzmann and Kadanoff-Baym equations also in the framework of gauge theories. Furthermore, a complete quantum mechanical description of leptogenesis would require a treatment of Kadanoff-Baym equations on an expanding space-time, which induces further nonequilibrium effects. Independent of the comparison of Boltzmann and Kadanoff-Baym equations we are looking forward to learning to which extent an entirely nonperturbative renormalization procedure affects the results quantitatively. Above all, such a nonperturbative renormalization procedure should have a stabilizing virtue for the computational algorithms.

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APPENDIX A: SELF-ENERGIES

In this appendix we give the expressions for the self-energies, which have to be inserted in the simplified Kadanoff-Baym equations (25)–(30). According to Eq. (20) the effective mass in Eqs. (25) and (26) is given by

$$M^2(x^0) = m_B^2 + 24\lambda \int \frac{d^3p}{(2\pi)^3} G_F(x^0, x^0, p).$$

Using the notation

$$S_V(x^0, y^0, \mathbf{k}) = \frac{\mathbf{k}}{k} S_V(x^0, y^0, k)$$

the statistical and spectral Higgs self-energies can be written in the form

$$\begin{aligned} \Pi_F(x^0, y^0, k) = & -8\eta^2 \int \frac{d^3p}{(2\pi)^3} \int d^3q \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ & \times \left[-S_{V,F}^0(x^0, y^0, q) S_{V,F}^0(x^0, y^0, p) \right. \\ & + \frac{1}{4} S_{V,e}^0(x^0, y^0, q) S_{V,e}^0(x^0, y^0, p) \\ & + S_{V,F}(x^0, y^0, \mathbf{q}) S_{V,F}(x^0, y^0, \mathbf{p}) \\ & \left. - \frac{1}{4} S_{V,e}(x^0, y^0, \mathbf{q}) S_{V,e}(x^0, y^0, \mathbf{p}) \right] \end{aligned}$$

and

$$\begin{aligned} \Pi_\varrho(x^0, y^0, k) &= -16\eta^2 \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ &\times [-S_{V,\varrho}^0(x^0, y^0, q) S_{V,F}^0(x^0, y^0, p) \\ &+ S_{V,\varrho}(x^0, y^0, \mathbf{q}) S_{V,F}(x^0, y^0, \mathbf{p})]. \end{aligned}$$

The simplified lepton self-energies are given by

$$\begin{aligned} \Sigma_{V,F}^0(x^0, y^0, k) &= -4\eta^2 \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ &\times \left[G_F(x^0, y^0, q) S_{V,F}^0(x^0, y^0, p) \right. \\ &\left. - \frac{1}{4} G_\varrho(x^0, y^0, q) S_{V,\varrho}^0(x^0, y^0, p) \right], \end{aligned}$$

$$\begin{aligned} \Sigma_{V,\varrho}^0(x^0, y^0, k) &= -4\eta^2 \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ &\times [G_\varrho(x^0, y^0, q) S_{V,F}^0(x^0, y^0, p) \\ &+ G_F(x^0, y^0, q) S_{V,\varrho}^0(x^0, y^0, p)], \end{aligned}$$

$$\begin{aligned} \Sigma_{V,F}(x^0, y^0, k) &= -4\eta^2 \frac{\mathbf{k}}{k} \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ &\times \left[G_F(x^0, y^0, q) S_{V,F}(x^0, y^0, \mathbf{p}) \right. \\ &\left. - \frac{1}{4} G_\varrho(x^0, y^0, q) S_{V,\varrho}(x^0, y^0, \mathbf{p}) \right], \end{aligned}$$

and

$$\begin{aligned} \Sigma_{V,\varrho}(x^0, y^0, k) &= -4\eta^2 \frac{\mathbf{k}}{k} \int \frac{d^3 p}{(2\pi)^3} \int d^3 q \delta(\mathbf{k} - \mathbf{p} - \mathbf{q}) \\ &\times [G_\varrho(x^0, y^0, q) S_{V,F}(x^0, y^0, \mathbf{p}) \\ &+ G_F(x^0, y^0, q) S_{V,\varrho}(x^0, y^0, \mathbf{p})]. \end{aligned}$$

APPENDIX B: QUANTUM-KINETIC EQUATIONS

Here we give the complete set of quantum-kinetic equations, which are obtained from the simplified Kadanoff-Baym equations (25)–(30) once one performs a Wigner transformation and a first-order gradient expansion. The quantum-kinetic equations for the scalars read:

$$-\{\Omega; G_F\}_{PB} = \Pi_\varrho G_F - \Pi_F G_\varrho + \{\Pi_F; \text{Re}(G_R)\}_{PB},$$

$$-\{\Omega; G_\varrho\}_{PB} = \{\Pi_\varrho; \text{Re}(G_R)\}_{PB},$$

$$G_R = \frac{1}{-\omega^2 + k^2 + M^2(t) + \Pi_R}. \quad (\text{B1})$$

It can be shown that [18]

$$G_\varrho = 2 \text{Im}(G_R) = \frac{-\Pi_\varrho}{\Omega^2 + \frac{1}{4} \Pi_\varrho^2}$$

indeed satisfies the kinetic equation for the scalar spectral function (B1). The quantum-kinetic equations for the fer-

mionic statistical propagators and spectral functions read:

$$\begin{aligned} \{W; S_{V,F}^0\}_{PB} &= \Sigma_{V,\varrho}^0 S_{V,F}^0 - \Sigma_{V,F}^0 S_{V,\varrho}^0 + \Sigma_{V,\varrho} S_{V,F} \\ &- \Sigma_{V,F} S_{V,\varrho} - \{\Sigma_{V,F}^0; \text{Re}(S_{V,R}^0)\}_{PB} \\ &+ \{\text{Re}(\Sigma_{V,R}); S_{V,F}\}_{PB} \\ &+ \{\Sigma_{V,F}; \text{Re}(S_{V,R})\}_{PB}, \end{aligned}$$

$$\begin{aligned} \{W; S_{V,F}\}_{PB} &= \Sigma_{V,\varrho}^0 S_{V,F} + \Sigma_{V,F}^0 S_{V,\varrho} + \Sigma_{V,\varrho} S_{V,F}^0 \\ &+ \Sigma_{V,F} S_{V,\varrho}^0 + \{\text{Re}(\Sigma_{V,R}); S_{V,F}^0\}_{PB} \\ &- \{\Sigma_{V,F}^0; \text{Re}(S_{V,R})\}_{PB} \\ &+ \{\Sigma_{V,F}; \text{Re}(S_{V,R}^0)\}_{PB}, \end{aligned}$$

$$\begin{aligned} \{W; S_{V,\varrho}^0\}_{PB} &= -\{\Sigma_{V,\varrho}^0; \text{Re}(S_{V,R}^0)\}_{PB} - \{\text{Re}(\Sigma_{V,R}); S_{V,\varrho}^0\}_{PB} \\ &- \{\Sigma_{V,\varrho}; \text{Re}(S_{V,R})\}_{PB}, \end{aligned}$$

and

$$\begin{aligned} \{W; S_{V,\varrho}\}_{PB} &= \{\Sigma_{V,\varrho}^0; \text{Re}(S_{V,R})\}_{PB} - \{\text{Re}(\Sigma_{V,R}); S_{V,\varrho}^0\}_{PB} \\ &+ \{\Sigma_{V,\varrho}; \text{Re}(S_{V,R}^0)\}_{PB}. \end{aligned}$$

The quantum-kinetic equations for the retarded lepton propagators read

$$S_{V,R}^0 = \frac{W - \frac{i}{2} \Sigma_{V,\varrho}^0}{(W - \frac{i}{2} \Sigma_{V,\varrho}^0)^2 - (k - \text{Re}(\Sigma_{V,R}) - \frac{i}{2} \Sigma_{V,\varrho})^2}$$

and

$$S_{V,R} = -\frac{k - \text{Re}(\Sigma_{V,R}) - \frac{i}{2} \Sigma_{V,\varrho}}{(W - \frac{i}{2} \Sigma_{V,\varrho}^0)^2 - (k - \text{Re}(\Sigma_{V,R}) - \frac{i}{2} \Sigma_{V,\varrho})^2}.$$

APPENDIX C: SIMPLIFYING THE BOLTZMANN COLLISION INTEGRALS

This appendix reveals the details of the calculation leading from the Boltzmann equations (38) and (39) to their simplified versions (40) and (41) [1,52]. For zero momentum the evaluation of the collision integral in Eq. (38) is literally trivial:

$$\begin{aligned} \partial_t n_s(t, k=0) &= -\frac{m\eta^2}{4\pi} [(n_s(t, k=0) + 1) \\ &\times n_f(t, p) n_f(t, q) - n_s(t, k=0) \\ &\times (n_f(t, p) - 1)(n_f(t, q) - 1)]_{p=q=m/2}. \end{aligned}$$

For $k > 0$ a little more work has to be done. We rewrite Eq. (38) using the Fourier representation of the momentum conservation δ function

$$\delta^3(\mathbf{k} - \mathbf{p} - \mathbf{q}) = \int \frac{d^3 \xi}{(2\pi)^3} \exp(-ik\xi + ip\xi + iq\xi)$$

and spherical coordinates. The scalar product of two vectors is then given by

$$p \cdot q = pq(\sin\vartheta_p \sin\vartheta_q \cos(\varphi_p - \varphi_q) + \cos\vartheta_p \cos\vartheta_q).$$

We perform the integrals over the solid angles in the order $\Omega_q, \Omega_p, \Omega_\xi$. Using the notation

$$j(x) = \frac{\sin(x)}{x} - \cos(x)$$

we find

$$\begin{aligned} & \int d\Omega_q \exp(iq\xi) \left(\frac{pq}{pq} - 1 \right) \\ &= \frac{4\pi}{q\xi} (i \cos(\vartheta_p) j(q\xi) - \sin(q\xi)), \\ & \int d\Omega_p \exp(ip\xi) (i \cos(\vartheta_p) j(q\xi) - \sin(q\xi)) \\ &= -\frac{4\pi}{p\xi} (j(p\xi)j(q\xi) + \sin(p\xi) \sin(q\xi)), \\ & \int d\Omega_\xi \exp(-ik\xi) \\ &= \frac{4\pi}{k\xi} \sin(k\xi). \end{aligned}$$

After defining the auxiliary function

$$\begin{aligned} J_s(k, p, q) &= -pq \int_0^\infty d\xi \frac{\sin(k\xi)}{k\xi} (j(p\xi)j(q\xi) + \sin(p\xi) \\ &\quad \times \sin(q\xi)) \\ &= -\frac{\pi}{16k} (k^2 - (p+q)^2) (\text{sign}(k-p-q) \\ &\quad - \text{sign}(k+p-q) - \text{sign}(k-p+q) \\ &\quad + \text{sign}(k+p+q)) \end{aligned}$$

and integrating over q , we eventually arrive at Eq. (40), where

$$q_0 = E(k) - p.$$

Next, we work out the collision integral for the fermions. First of all, we integrate Eq. (39) over Ω_k . On the left-hand side this gives a factor of 4π . On the right-hand side we evaluate the integrals over the solid angles in the order $\Omega_q, \Omega_p, \Omega_k, \Omega_\xi$:

$$\begin{aligned} & \int d\Omega_q \exp(iq\xi) \\ &= \frac{4\pi}{q\xi} \sin(q\xi), \\ & \int d\Omega_p \exp(-ip\xi) \left(\frac{kp}{kp} + 1 \right) \\ &= \frac{4\pi}{p\xi} (\sin(p\xi) - i \cos(\vartheta_k) j(p\xi)), \\ & \int d\Omega_k \exp(-ik\xi) (\sin(p\xi) - i \cos(\vartheta_k) j(p\xi)) \\ &= \frac{4\pi}{k\xi} (\sin(k\xi) \sin(p\xi) - j(k\xi)j(p\xi)), \\ & \int d\Omega_\xi = 4\pi. \end{aligned}$$

Defining the auxiliary function

$$\begin{aligned} J_f(k, p, q) &= p \int_0^\infty d\xi \frac{\sin(q\xi)}{k\xi} (\sin(k\xi) \sin(p\xi) \\ &\quad - j(k\xi)j(p\xi)) \\ &= \frac{\pi}{16k^2} ((k-p)^2 - q^2) (\text{sign}(k-p-q) \\ &\quad - \text{sign}(k+p-q) - \text{sign}(k-p+q) \\ &\quad + \text{sign}(k+p+q)) \end{aligned}$$

and integrating over p yields Eq. (41), where

$$p_0 = E(q) - k.$$

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