Relativistic Langevin dynamics in expanding media

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We study the consequences of different realizations of diffusion processes in relativistic Langevin simulations. We elaborate on the Ito-Stratonovich dilemma by showing how microscopically calculated transport coefficients as obtained from a Boltzmann–Fokker-Planck equation can be implemented to lead to an unambiguous realization of the Langevin process. Pertinent examples within the prepoint (Ito) and postpoint (Hänggi-Klimontovich) Langevin prescriptions are worked out explicitly. Deviations from this implementation are shown to generate variants of the Boltzmann distribution as the stationary (equilibrium) solutions. Finally, we explicitly verify how the Lorentz invariance of the Langevin process is maintained in the presence of an expanding medium, including the case of an "elliptic flow" transmitted to a Brownian test particle. This is particularly relevant for using heavy-flavor diffusion as a quantitative tool to diagnose transport properties of QCD matter as created in ultrarelativistic heavy-ion collisions.

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I. INTRODUCTION

Since its introduction more than 100 years ago, Brownian motion has remained a valuable and versatile tool to study a wide variety of physical systems. In recent years considerable efforts have been devoted to its extension and reliable implementation for relativistic systems [1–5]. In nuclear physics it has been applied to describe transport processes in the fireball created in high-energy collisions of nuclei, e.g., the relativistic diffusion of charged-particle sources [6] and, most prominently, the diffusion of heavy quarks as "Brownian markers" in quark-gluon plasma (QGP) [7–11], to deduce its transport properties (see, e.g., Ref. [12] for a recent review). Since charm- and bottom-quark masses are much larger than the typical temperatures, as well as the constituent masses of the equilibrated medium, a separation of the heavy-quark (HQ) relaxation time and collision time emerges [9,12], thus justifying a soft-collision approximation to be accommodated by Fokker-Planck dynamics [13]. In practice, the Fokker-Planck equation is routinely realized by stochastic Langevin processes [2,3,12,14]. However, it is known that the implementation of the Langevin equation is not unique but depends on the realization of the stochastic integral, resulting in (seemingly) different Fokker-Planck equations, known as the "Ito-Stratonovich dilemma" [2,3,14]. Moreover, the ambiguities in the Langevin discretization scheme raise concerns regarding the asymptotic phase-space distribution of the relativistic Brownian particles under consideration. The latter has been an issue of debate (see Ref. [15] and references therein) but should be constrained by the long-time limit of equilibrium [3,13,16,17], i.e., by a "detailed balancing" of the drag and diffusion terms of the underlying Fokker-Planck equation.

The large collective flow of the medium created in ultrarelativistic heavy-ion collisions (URHICs), reaching collective velocities in excess of half the speed of light, and, in particular, angular modulations thereof (such as elliptic flow), call for a thorough understanding of differences in the realization of *relativistic* Langevin simulations. Therefore, the description of the phase-space distribution of a Brownian particle (the heavy quark), which is usually formulated in laboratory frame coordinates, needs to manifestly recover the equilibrium limit given by the Lorentz-invariant Boltzmann-Jüttner distribution [18,19]. This is evident as the underlying Fokker-Planck equation is to yield a good approximation of the Lorentz-covariant Boltzmann equation [1,13,14]. This problem has been addressed, e.g., in Refs. [16] and [20] within the so-called Ito realization, while pertinent Fokker-Planck equations following from different Langevin prescriptions have been given in Ref. [3]. A Lorentz-covariant interpretation of the Langevin process has been given in Ref. [21], where the relativistic fluctuation-dissipation theorem has been derived from the equilbrium condition.

In the present work we approach these issues from a different angle. Rather than considering a phenomenologically motivated statistical process, our starting point is a Fokker-Planck equation with transport coefficients obtained from an underlying microscopic theory, in the sense of an approximate treatment of the collision integral in the transport equation. Specifically for the case of HQ diffusion in the QGP, where one aims at understanding transport properties from the underlying in-medium QCD force, this is a more natural line of approach which we would like to illuminate here. After recovering analytic results for the generalized relativistic Einstein relation for these coefficients, we discuss their implementation in different Langevin realizations. We verify their uniqueness in explicit numerical examples, in particular, including the case of (anisotropically) expanding media. We also show how variations in the Langevin coefficients induce modifications to the long-time (equilibrium) limit of the distribution of the Brownian particle. We explicitly discuss the algorithm suitable for a correct implementation of the postpoint Langevin process. For definiteness, our numerical applications are illustrated in the context of HQ diffusion in an expanding QGP as formed in URHICs.

Our article is organized as follows. In Sec. II we introduce the Fokker-Planck equation as an approximate description of the Boltzmann equation and recall the general equilibrium condition constraining its drag and diffusion coefficients. In Sec. III we elaborate how Langevin prescriptions emerge from the pertinent equilibrium conditions to ensure a uniform outcome of the Fokker-Planck framework, i.e., how Fokker-Planck equations resulting from different Langevin prescriptions take the same form in terms of universal drag and diffusion coefficients of an underlying microscopic theory. In Sec. IV Langevin prescriptions are illustrated with numerical calculations for different model systems for flowing media. We demonstrate that both pre- and postpoint Langevin schemes lead to the Lorentz-invariant Boltzmann-Jüttner distribution for test particles in the presence of collective flow as the long-time limit of the Langevin process, if and only if the proper equilibrium condition is imposed. Some variants of the realization of the stochastic Langevin process and their consequences on the long-time limit are also discussed in this section. We summarize and conclude in Sec. V.

II. FOKKER-PLANCK EQUATION AND GENERAL EQUILIBRIUM CONDITION

When a heavy particle is immersed in a medium of light constituents at a low to moderate temperature, $T \lesssim m$, its momentum change due to collisions is relatively small. Employing this soft-scattering approximation [13], the Boltzmann integrodifferential equation describing the motion of the heavy particles in an equilibrated background medium reduces to the Fokker-Planck equation for the phase-space distribution function, f, of the "Brownian" particle [13]

$$\frac{\partial f(t,\boldsymbol{p})}{\partial t} = \frac{\partial}{\partial p_i}\left\{A_i(\boldsymbol{p}) f(t,\boldsymbol{p}) + \frac{\partial}{\partial p_j}[B_{ij}(\boldsymbol{p}) f(t,\boldsymbol{p})]\right\}, \quad (1)$$

with $i,j \in \{1,2,3\}$. We focus on a spatially homogeneous static medium without external force, and thus the phase-space density is independent of $\boldsymbol{x}$. The drag and diffusion coefficients in Eq. (1), $A_i(\boldsymbol{p})$ and $B_{ij}(\boldsymbol{p})$, respectively, are obtained from an average of the moments of momentum transfer in heavy-light collisions, weighted by a transition probability given by the pertinent scattering matrix elements, $\mathcal{M}$, and the medium particle distribution, f^p:

$$\begin{aligned} A_i(\boldsymbol{p}) = &\frac{1}{2E(\boldsymbol{p})}\int \frac{d^3\boldsymbol{q}}{(2\pi)^3 2E(\boldsymbol{q})}\int \frac{d^3\boldsymbol{q}'}{(2\pi)^3 2E(\boldsymbol{q}')} \\ &\times \int \frac{d^3\boldsymbol{p}'}{(2\pi)^3 2E(\boldsymbol{p}')}\frac{1}{\gamma}\sum |\mathcal{M}|^2 \hat{f}(\boldsymbol{q}) \\ &(2\pi)^4\delta^4(p+q-p'-q')\,[(\boldsymbol{p}'-\boldsymbol{p})_i] \\ &\equiv \langle\langle(\boldsymbol{p}'-\boldsymbol{p})_i\rangle\rangle; \end{aligned} \quad (2)$$

$$B_{ij}(\boldsymbol{p}) = \frac{1}{2}\langle\langle(\boldsymbol{p}'-\boldsymbol{p})_i(\boldsymbol{p}'-\boldsymbol{p})_j\rangle\rangle. \quad (3)$$

Here, $\boldsymbol{p}$ and $\boldsymbol{p}'$ ($\boldsymbol{q}$ and $\boldsymbol{q}'$) are the heavy (light) particle's momentum before and after the collision, respectively, and $\hat{f} = f^p(1 \pm f^p)$ for bosons or fermions in the medium.

Defining a current

$$S_i(t,\boldsymbol{p}) = -\left\{A_i(\boldsymbol{p}) f(t,\boldsymbol{p}) + \frac{\partial}{\partial p_j}[B_{ij}(\boldsymbol{p}) f(t,\boldsymbol{p})]\right\}, \quad (4)$$

the Fokker-Planck equation can be cast as a continuity equation in momentum space [13]:

$$\frac{\partial f_Q(t,\boldsymbol{p})}{\partial t} + \frac{\partial}{\partial p_i}S_i(t,\boldsymbol{p}) = 0. \quad (5)$$

This identifies S_i as a particle-number current (flux), so that the number of heavy particles is conserved in the diffusion process. After sufficiently many collisions with the light partons, i.e., in the long-time limit, we expect the heavy particle to approach the same equilibrium distribution as for the medium constituents given by the relativistic Boltzmann-Jüttner distribution [22],

$$f_{\rm eq}(p,T) = N\exp[-E(p)/T], \quad (6)$$

where $E(p) = \sqrt{\boldsymbol{p}^2 + m^2}$ is the relativistic on-shell energy of the Brownian particle and T the temperature of the equilibrated medium. In addition, in statistical equilibrium, the particle flux has to vanish [13]: $S_i(\boldsymbol{p}) = 0$. Together with the Boltzmann-Jüttner distribution, (6), this yields a dissipation-fluctuation relation between drag and diffusion coefficient,

$$A_i(\boldsymbol{p},T) = B_{ij}(\boldsymbol{p},T)\frac{1}{T}\frac{\partial E(p)}{\partial p_j} - \frac{\partial B_{ij}(\boldsymbol{p},T)}{\partial p_j}. \quad (7)$$

In Eq. (7) and in the following, a summation over repeated indices is implied. This is the manifestation of the detailed-balance property of the collision-transition probabilities, which is due to the unitarity of the S matrix of quantum-field theory and thus embodied in the collision integral of the underlying full Boltzmann equation [13]. This relation is not *a priori* fulfilled by Eqs. (2) and (3) and may suffer in accuracy if the assumption of a forward-peaked transition-matrix element is not well satisfied. In order for the heavy particle to approach the same distribution as for the medium particles, the drag and diffusion coefficients are not independent but have to be related to each other precisely as specified by the dissipation-fluctuation relation, (7). This general equilibrium condition plays a central role in the following discussion.

III. STOCHASTIC LANGEVIN REALIZATION OF FOKKER-PLANCK DIFFUSION

A. Langevin simulation

The Fokker-Planck description of diffusion can be realized by Langevin's stochastic differential equation(s) [3,12,14]. Employing a spatially homogeneous static medium, we follow the notation in Ref. [12] to write the Langevin equations as

$$dx_j = \frac{p_j}{E}dt, \quad (8)$$

$$dp_j = -\Gamma(p,T)p_j dt + \sqrt{dt}\,C_{jk}(\boldsymbol{p} + \xi d\boldsymbol{p},T)\rho_k, \quad (9)$$

which specify the rules for updating the coordinate and momentum of the heavy particle in time steps, dt. In Eq. (9), $\Gamma(p,T)\boldsymbol{p}$ is the deterministic friction force, whereas the matrix of coefficients C_{jk} describes the stochastically fluctuating force with independent Gaussian noises ρ_k following a normal distribution, $P(\boldsymbol{\rho}) = (2\pi)^{-3/2}e^{-\boldsymbol{\rho}^2/2}$. Thus, there is no correlation in the stochastic forces at different times, $\langle F_j(t)F_k(t')\rangle = C_{jl}C_{kl}\delta(t-t')$, consistent with the assumption of uncorrelated momentum kicks underlying the

Fokker-Planck equation ("white noise"). However, it is not specified at what momentum argument the covariance matrix should be evaluated: $C_{jk} = C_{jk}(t,\boldsymbol{p}+\xi d\boldsymbol{p})$, with $\xi \in [0,1]$, e.g., $\xi = 0$ for prepoint (Ito) [23], $\xi = 1/2$ for midpoint (Stratonovich), or $\xi = 1$ for postpoint (Hänggi-Klimontovich) [2] realizations of the stochastic integral. We return to this point below.

The phase-space distribution determined by the Langevin equations, (8) and (9), satisfies a Fokker-Planck equation, which can be found by calculating the average change in an arbitrary phase-space function with time [12]. The resulting equation reads

$$\frac{\partial f(t,\boldsymbol{p})}{\partial t} = \frac{\partial}{\partial p_j}\left[\left(\Gamma(p)p_j - \xi C_{lk}(\boldsymbol{p})\frac{\partial C_{jk}(\boldsymbol{p})}{\partial p_l}\right)f(t,\boldsymbol{p})\right] + \frac{1}{2}\frac{\partial^2}{\partial p_j \partial p_k}[C_{jl}(\boldsymbol{p})C_{kl}(\boldsymbol{p})f(t,\boldsymbol{p})]. \tag{10}$$

Comparing Eqs. (10) and (1) leads to

$$A_j(\boldsymbol{p}) = A(p)p_j = \Gamma(p)p_j - \xi C_{lk}(\boldsymbol{p})\frac{\partial C_{jk}(\boldsymbol{p})}{\partial p_l}, \tag{11}$$

$$B_{jk}(\boldsymbol{p}) = B_0(p)P^{\perp}_{jk}(\boldsymbol{p}) + B_1(p)P^{\parallel}_{jk}(\boldsymbol{p}) = \frac{1}{2}C_{jl}(\boldsymbol{p})C_{kl}(\boldsymbol{p}), \tag{12}$$

where $P^{\perp}_{jk}(\boldsymbol{p}) = \delta_{jk} - p_j p_k/p^2$ and $P^{\parallel}_{jk}(\boldsymbol{p}) = p_j p_k/p^2$ are the corresponding projection operators, so that

$$C_{jk}(\boldsymbol{p}) = \sqrt{2B_0(p)}P^{\perp}_{jk}(\boldsymbol{p}) + \sqrt{2B_1(p)}P^{\parallel}_{jk}(\boldsymbol{p}). \tag{13}$$

Two comments are in order here. First, note that the friction coefficient, $\Gamma(p,T)$, appearing in the Langevin equation, (9), is a derived quantity, given in terms of the drag and diffusion coefficients, $A(p,T)$, $B_0(p,T)$, and $B_1(p,T)$, as determined by microscopic scattering-transition matrix elements (e.g., they relate to HQ energy loss due to elastic heavy-light collisions [24]). Second, the Fokker-Planck equation and the Langevin equation are specified for a spatially homogeneous static medium; neither of them is manifestly Lorentz covariant. Thus, in the case of a flowing medium, momentum updates in the Langevin equation, (9), have to be calculated in the local fluid rest frame and then boosted back to the moving frame when performing the diffusion simulations. It is readily proved that the coordinate updates, (8), can be equivalently done in the moving frame; hereafter, we refer to the latter as the laboratory frame.

B. Evaluation of equilibrium condition

We now proceed to analyze the equilibrium condition for two implementations of the Langevin process, the prepoint and postpoint prescriptions, and work out their manifestations in the Fokker-Planck framework. For the sake of brevity, but without loss of generality, we work with a diagonal approximation of the diffusion coefficient from here on. Putting $B_0(p) = B_1(p) = D(p)$, the covariance matrix, (13), reduces to $C_{jk}(\boldsymbol{p}) = \sqrt{2D(p)}\delta_{jk}$. Utilizing Eq. (11), the general equilibrium condition, (7), simplifies to

$$A(p) = \frac{1}{E(p)}\left(\frac{D[E(p)]}{T} - \frac{\partial D[E(p)]}{\partial E}\right) \tag{14}$$

with

$$\Gamma(p) = \frac{1}{E(p)}\left(\frac{D[E(p)]}{T} - (1-\xi)\frac{\partial D[E(p)]}{\partial E}\right). \tag{15}$$

Thus, for a given drag coefficient A, Eq. (14) should be solved to obtain the diffusion coefficient D, which can then be used to deduce the friction force Γ from Eq. (15). Alternative procedures have been adopted in the literature by, e.g., calculating D and adjusting A [9,25]. Condition (15) has also been derived as the generalization of the fluctuation-dissipation theorem with Boltzmann-Jüttner distributions as the equilibrium solution in Ref. [21].

In the nonrelativistic limit, both $D(p) = D$ and $\Gamma(p) = \gamma$ become independent of p, and $E(p) \to m$; the equilibrium condition reduces to

$$D = m\gamma T, \tag{16}$$

which is Einstein's classical fluctuation-dissipation relation [13].

In terms of the diagonal diffusion coefficient, the Langevin updating rules now read

$$dx_j = \frac{p_j}{E}dt, \tag{17}$$

$$dp_j = -\Gamma(p)p_j dt + \sqrt{2dt\, D(|\boldsymbol{p}+\xi d\boldsymbol{p}|)}\rho_j. \tag{18}$$

In the following, we discuss their explicit forms in the prepoint and postpoint Langevin prescriptions as following from the corresponding equilibrium condition and show that they can both be rendered compatible for a given microscopic model.

1. Prepoint scheme: $\xi = 0$

In this scheme, the equilibrium conditions, (14) and (15), read

$$\Gamma(p) = \frac{1}{E(p)}\left(\frac{D[E(p)]}{T} - \frac{\partial D[E(p)]}{\partial E}\right) = A(p). \tag{19}$$

Note that the friction force entering the Langevin equation is equal to the drag coefficient defined by Eq. (2).

Inserting $C_{jk}(\boldsymbol{p}) = \sqrt{2D(p)}\delta_{jk}$ into Eq. (10), the Fokker-Planck equation realized in the prepoint Langevin scheme takes the form

$$\frac{\partial}{\partial t}f(t,\boldsymbol{p}) = \frac{\partial}{\partial p_i}\left\{\Gamma(p)p_i f(t,\boldsymbol{p}) + \frac{\partial}{\partial p_i}[D(p)f(t,\boldsymbol{p})]\right\}. \tag{20}$$

The corresponding Langevin updating rules now read

$$dx_j = \frac{p_j}{E}dt, \tag{21}$$

$$dp_j = -\Gamma(p)p_j dt + \sqrt{2dt\, D(p)}\rho_j, \tag{22}$$

where carrying out the Langevin time steps is straightforward: starting with initial coordinate $\boldsymbol{x}$ and momentum $\boldsymbol{p}$ of a test particle, calculate the coordinate increment dx_j within the time step dt using Eq. (21); at the same time substitute the drag coefficient $A(p)$ $[= \Gamma(p)]$ evaluated at $p = |\boldsymbol{p}|$ and the corresponding $D(p)$ calculated from Eq. (14) into Eq. (22) to calculate the momentum increment. Then go to the next time step with (new) initial coordinate $\boldsymbol{x} + d\boldsymbol{x}$ and momentum $\boldsymbol{p} + d\boldsymbol{p}$.

2. Postpoint scheme: $\xi = 1$

In this scheme, the equilibrium conditions read

$$D[E(p)] = \Gamma(p)E(p)T, \tag{23}$$

$$\Gamma(p) = A(p) + \frac{1}{E(p)}\frac{\partial D[E(p)]}{\partial E}. \tag{24}$$

Here, the scheme-dependent relation takes a simple form, but the "price" to pay is that the friction force $\Gamma(p)$ figuring into the Langevin equation is different from the drag coefficient $A(p)$. In this sense, starting from a microscopic model for $A(p)$, there is no difference in the choice of the prepoint or the postpoint scheme.

The corresponding Fokker-Planck equation in the postpoint scheme takes the form

$$\frac{\partial}{\partial t}f(t,\boldsymbol{p}) = \frac{\partial}{\partial p_i}\left\{\Gamma(p)p_i f(t,\boldsymbol{p}) + D(p)\frac{\partial}{\partial p_i}f(t,\boldsymbol{p})\right\}. \tag{25}$$

This Fokker-Planck equation appears to be different from its counterpart realized in the prepoint realization, Eq. (20). However, upon substituting the different expressions for Γ, Eqs. (19) and (24), for the prepoint and the postpost Langevin scheme into Eqs. (20) and (25), respectively, one immediately sees that the Fokker-Planck equations realized in the pre- and postpoint Langevin schemes are actually the same in terms of $A(p)$ and $D(p)$. This is a desired result since the (approximate) realization of the underlying full Boltzmann equation (including the asymptotic solution for the distribution of test particles) within a Fokker-Planck equation should be independent of the implementation of the stochastic process (i.e., Langevin scheme). Thus, the "Ito-Stratonovich dilemma," which suggests that different Langevin prescriptions are not sufficient in order to uniquely determine the Fokker-Planck equation, does not appear here, as a benefit of the well-defined microscopic process.

The Langevin updating rules in the postpoint scheme read

$$dx_j = \frac{p_j}{E}dt, \tag{26}$$

$$dp_j = -\Gamma(p)p_j dt + \sqrt{2dt\,D(|\boldsymbol{p}+d\boldsymbol{p}|)}\rho_j. \tag{27}$$

Starting with initial coordinate $\boldsymbol{x}$ and momentum $\boldsymbol{p}$, the coordinate update is trivial at given time step dt, but the momentum update involves a two-step computation: first, use the prepoint scheme, Eq. (22), to calculate the momentum increment $d\boldsymbol{p}$ with $\Gamma(p)$ and $D(p)$; then evaluate the diffusion coefficient D at the argument $|\boldsymbol{p}+d\boldsymbol{p}|$ and calculate $dp_j^{\text{diffusion}} \equiv \sqrt{2dt\,D(|\boldsymbol{p}+d\boldsymbol{p}|)}\rho_j$, while $dp_j^{\text{drag}} = -\Gamma(p)p_j dt$ has already been calculated in the first step; finally, add up $dp_j^{\text{diffusion}}$ and dp_j^{drag} to obtain the total momentum increment for the present time step. Note that in the two-step momentum update procedure, the same dt and ρ_j should be used. A variant where different dt values are used is discussed in the case of a flowing medium in Secs. IV B and IV C.

Our main results in this section—Eqs. (19), (23), and (24)—show the correct relation between the microscopic transport coefficients, well defined in a relativistic Boltzmann dynamics, and the two stochastic processes considered here. They also confirm the results for the relativistic dissipation-fluctuation theorem obtained in Ref. [21].

IV. NUMERICAL CALCULATIONS WITH DIFFERENT BACKGROUND MEDIA

In this section we perform numerical simulations of the two Langevin prescriptions discussed above (and some variants thereof previously employed in the literature) to explicitly examine their consequences for the long-time limits, in particular, in the case of flowing media. For definiteness we adopt parameter values for masses, temperatures, and flow profiles representing the problem of HQ diffusion in a QGP. We start with a homogeneous static medium (Sec. IV A), followed by a simple one-dimensional (1D) flow scenario (Sec. IV B), and, finally, study a more realistic elliptically expanding fireball (Sec. IV C). In all cases we use large drag and diffusion coefficients and perform the simulations until the stationary state has been reached, demonstrating their universal convergence to the analytical solutions for the corresponding Fokker-Planck equations.

A. Homogeneous static medium

Let us assume a homogeneous static medium with temperature $T = 0.18$ GeV with a Brownian particle of mass $m = 1.5$ GeV immersed (we work in natural units where the velocity of light, Planck constant, and Boltzmann constant are equal to unity: $c = \hbar = k_{\mathrm{B}} = 1$). The preceding Fokker-Planck and Langevin equations can be readily applied; we focus on the projection on the z component of the momentum distribution dN/dp_z of the test particle. It has been checked that the equilibrium conditions are reached independent of arbitrarily chosen initial conditions, as expected.

We first adopt the prepoint scenario in a simplistic scenario where a large constant friction coefficient ($\Gamma = 20$ fm^{-1}) is complemented by a diffusion coefficient $D = \Gamma E T$. This leads to a stationary distribution,

$$\frac{dN}{d^3x\,d^3p} = \frac{m}{E}\exp\left[-\frac{E(p)}{T}\right], \tag{28}$$

as shown in Fig. 1(a). It can be easily verified analytically by plugging the drag and diffusion coefficients into the Fokker-Planck equation, (20), and performing the momentum derivatives, as also discussed in Ref. [2]. However, this form of drag and diffusion coefficient does *not* comply with the prepoint equilibrium condition, (19), and thus the simulation fails to converge to the Boltzmann-Jüttner distribution.

To illustrate the importance of implementing the proper equilibrium condition, we have performed Langevin simulations within the prepoint scheme using two types of momentum dependencies of the diffusion coefficient:

$$\text{(i)}\quad \Gamma = 20/E\ \text{GeV/fm}, \quad D = \Gamma E T = 20T\ \text{GeV/fm}; \tag{29}$$

$$\text{(ii)}\quad \Gamma = 300(1+T/E)/E^2\ \text{GeV}^2\text{/fm}, \quad D = 300\,T/E\ \text{GeV}^2\text{/fm}. \tag{30}$$

The lifetime of the system in these simulations has been set to 10 fm, and it has been checked that the stationary distribution has been reached.

The simulated results are also shown in Fig. 1(a). Again, their agreement with the Boltzmann-Jüttner distribution can be analytically verified by substituting the coefficients into the

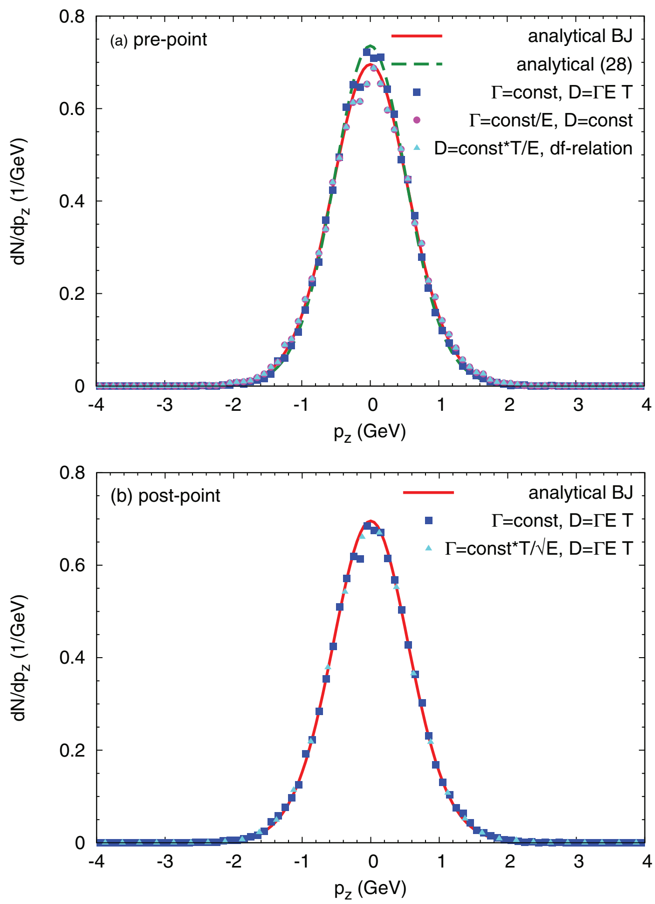

FIG. 1. (Color online) Distribution dN/dp_z from Langevin simulations for heavy quarks with mass $m = 1.5$ GeV, diffusing in a static medium at temperature $T = 0.18$ GeV, compared to calculations with the corresponding analytical phase-space distributions: (a) prepoint Langevin scheme; (b) postpoint Langevin scheme. See text for more details.

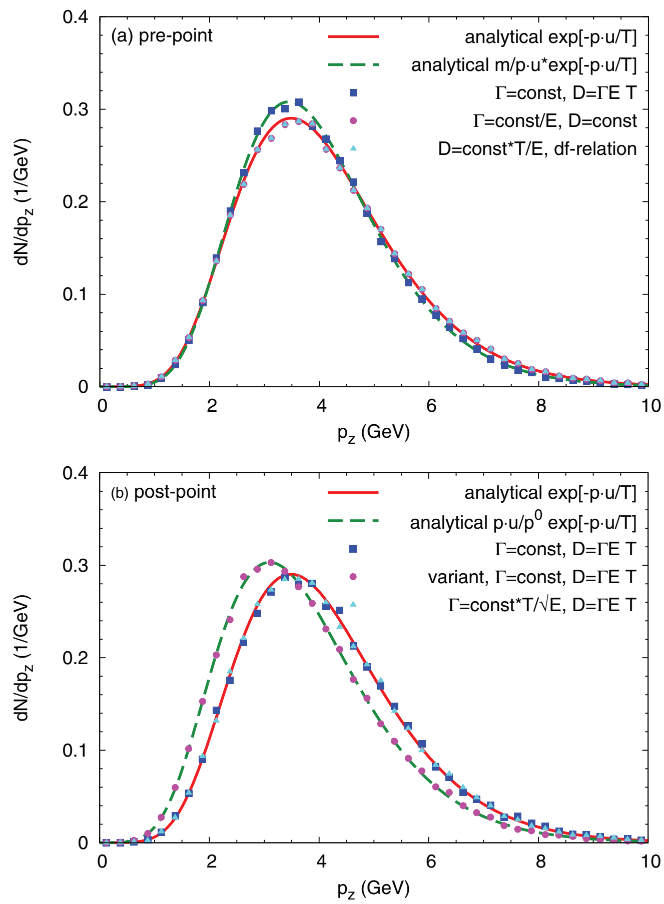

FIG. 2. (Color online) Langevin simulation results for heavy quarks ($m = 1.5$ GeV) diffusing in a flowing medium ($T = 0.18$ GeV, $v_z = 0.9$) compared to calculations with analytical phase-space distributions: (a) prepoint Langevin scheme; (b) postpoint Langevin scheme. The distribution obtained with a variant of the postpoint scheme and the corresponding blast-wave distribution are also shown. See text for more details.

Fokker-Planck equation, (20), and carrying out the momentum derivatives.

Next, we employ the postpoint scenario. The simulated results are shown in Fig. 1(b). Here, the Langevin simulations with large drag reproduce well the Boltzmann-Jüttner distribution, whether the friction is constant ($\Gamma = 20/\text{fm}$, $D = \Gamma ET$) or not ($\Gamma = 40\sqrt{\text{GeV}}\ \text{fm}^{-1}/\sqrt{E(p)}$, $D = \Gamma ET$), since the postpoint equilibrium condition, (23), is always fulfilled. This is easily verified by plugging the coefficients into the corresponding Fokker-Planck equation, (25).

To summarize this part, we have confirmed through numerical simulations that in order for the stationary Langevin limit to converge to the Boltzmann-Jüttner distribution, the equilibrium condition must be *exactly* fulfilled.

B. Constant 1D flow

We now introduce a constant 1D medium flow with velocity field $v_x = 0$, $v_y = 0$, and $v_z = 0.9$. The medium temperature, $T = 0.18$ GeV, and HQ mass, $m = 1.5$ GeV, are as before.

The numerical simulations in the prepoint scheme directly translate the result for the static medium into the corresponding "blast-wave" distribution, obtained by replacing E with $p \cdot u$. Specifically, a momentum-independent drag complemented by the naive $D = \Gamma ET$ leads to a single-particle phase-space distribution $dN/d^3x d^3p = m/(p \cdot u)\exp(-p \cdot u/T)$, while general momentum-dependent coefficients that fulfill the prepoint equilibrium condition, (19), give the Boltzmann-Jüttner distribution, $dN/d^3x\, d^3p = \exp(-p \cdot u/T)$ [see Fig. 2(b)].

For the postpoint scenario, where the equilibrium condition takes the simple form, (23), the momentum update involves two steps in the fluid rest frame. There seems to be an ambiguity in the time increment dt^* used in the two-step computation [here and in the following, variables with (without) a superscript asterisk refer to the fluid rest (laboratory) frame]. For the first step, it is clear that $dt^*_{(1)} = dt\frac{E^*}{E} = dt\frac{p \cdot u}{p^0}$, with $E = p^0$ being the laboratory-frame energy prior to the momentum update and $E^* = p \cdot u$ the corresponding energy measured in the fluid rest frame. One then updates the momentum and obtains $p^{*\mu}_{(1)} = (E^*_{(1)}, \boldsymbol{p}^*_{(1)})$ in the fluid rest frame; the corresponding laboratory-frame four-momentum, $p^{\mu}_{(1)} = (E_{(1)}, \boldsymbol{p}_{(1)})$, follows from a boost using the fluid velocity u^μ. In the subsequent second-step momentum update, one finds a particle phase-space distribution, $dN/d^3xd^3p = (p \cdot u/p^0)\exp(-p \cdot u/T)$, in the laboratory frame if one uses $dt^*_{(2)} = dt\frac{E^*_{(1)}}{E_{(1)}} = dt\frac{p_{(1)}\cdot u}{E_{(1)}} \neq dt^*_{(1)}$. This is different from the Boltzmann-Jüttner distribution (we denote it a "variant"), as illustrated in Fig. 2(b). One finds both analytically and numerically that the Boltzmann-Jüttner distribution is recovered when using $dt^*_{(2)} = dt^*_{(1)}$ in the second-step momentum update. Recalling that in the general derivation of the Fokker-Planck equation from the Langevin equations [12] (for a static thermal medium), a fixed $dt^* = dt^*_{(1)}$ is adopted, we conclude that in the postpoint scheme, one should use the same $dt^* = dt^*_{(1)}$ for both momentum-update steps in order to obtain the Lorentz-invariant Boltzmann-Jüttner distribution in the presence of flow.

C. Elliptic fireball

In noncentral heavy-ion collisions (i.e., at a nonzero impact parameter), the initial shape of the fireball is nonspherical in the x-y plane transverse to the beam axis. The dominant deformation of the shape is elliptic ("almond shaped"). Interactions among particles, creating pressure gradients in the fireball, convert this initial spatial asymmetry into a particle momentum anisotropy between p_x and p_y. The prevalent deformation is again elliptic, leading to the notion of an "elliptic flow," quantified by the coefficient of the second harmonic, $v_2(p_T)$, in the azimuthal-angle distribution of the particle spectrum [26,27],

$$\frac{dN}{p_T dp_T d\phi_p} = \frac{dN}{2\pi p_T dp_T}[1 + 2v_2(p_T)\cos(2\phi_p) + \cdots], \tag{31}$$

where $p_T = \sqrt{p_x^2 + p_y^2}$ is the transverse momentum of the emitted particles. This phenomenon is also observed in the expansion of strongly interacting clouds of cold atoms [28]. HQs (or hadrons containing HQs) are believed to acquire a v_2 through the coupling to the collective motion of the light particles in the QGP [9,12]. In the following, we employ an elliptically expanding fireball, introduced in Ref. [29] (see also the discussion in Ref. [30] for more details) to model the QGP medium evolution, in order to scrutinize the Langevin simulation of HQ diffusion in the QGP background. We again take the HQ mass to be $m = 1.5$ GeV and employ the same two sets of coefficients Γ and D as specified in Eqs. (29) and (30), satisfying the equilibrium conditions. This time the Langevin simulation runs in parallel to an isentropically expanding fireball which stops at the decoupling temperature $T_f = 0.18$ GeV. We compute the spectrum and elliptic flow and compare them to the results of a direct blast-wave calculation which corresponds to the equilibrium limit of the fireball.

Let us first discuss the HQ p_T spectrum, shown in Fig. 3. For the prepoint scenario [Fig. 3(a)], Langevin simulation results translate again directly into the corresponding blast-wave distributions (obtained by replacing E with $p\cdot u$). For a momentum-independent drag coefficient complemented by the naive $D = \Gamma ET$ (at variance with the equilibrium condition), the HQ phase-space distribution assumes the form $dN/d^3xd^3p = m/(p\cdot u)\exp(-p\cdot u/T)$, while general momentum dependent coefficients that fulfill the prepoint equilibrium condition, (19), accurately recover the Boltzmann-Jüttner distribution $dN/d^3xd^3p = \exp(-p\cdot u/T)$. For the postpoint scenario [Fig. 3(b)], again, once the corresponding equilibrium condition, (23), is satisfied, the Langevin simulation also yields the correct Lorentz-invariant Boltzmann distribution, while the "variant" scheme leads to an explicitly frame-dependent distribution $dN/d^3xd^3p = (p\cdot u/p^0)\exp(-p\cdot u/T)$. This results from using a different $dt^*_{(2)} \neq dt^*_{(1)}$ in the two-step momentum update, as discussed in Sec. IV B.

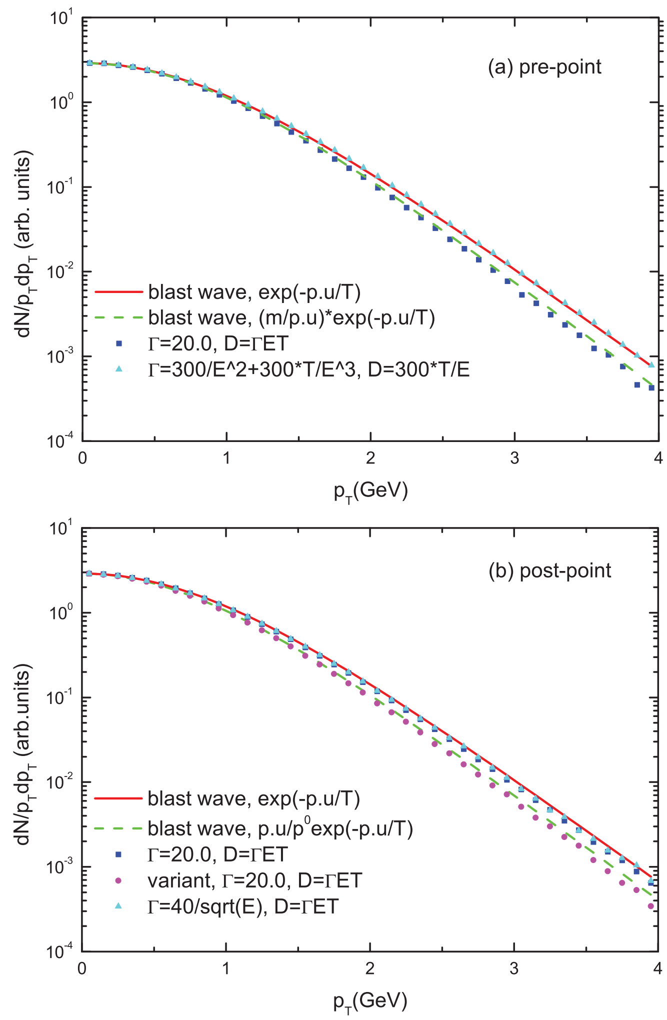

FIG. 3. (Color online) Langevin simulation of the p_T spectrum of a heavy quark ($m = 1.5$ GeV) diffusing in a fireball ($T_i = 0.33$ GeV, $T_f = 0.18$ GeV), compared to the direct blast-wave calculations. (a) Prepoint Langevin scheme; (b) postpoint Langevin scheme. See text for more details.

The HQ $v_2(p_T)$ obtained from the equilibrium limit of the Langevin simulations and its comparison with the direct blast-wave calculations are shown in Fig. 4. The agreement between different implementations (prepoint, postpoint, and variants) of Langevin simulations and the corresponding blast-wave distributions confirm the conclusions for the p_T spectra, reproducing accurately even rather subtle angular modulations in relativistic flow fields.

V. SUMMARY AND CONCLUSIONS

In this work we have explored aspects of relativistic Langevin dynamics, in particular, their uniqueness relative

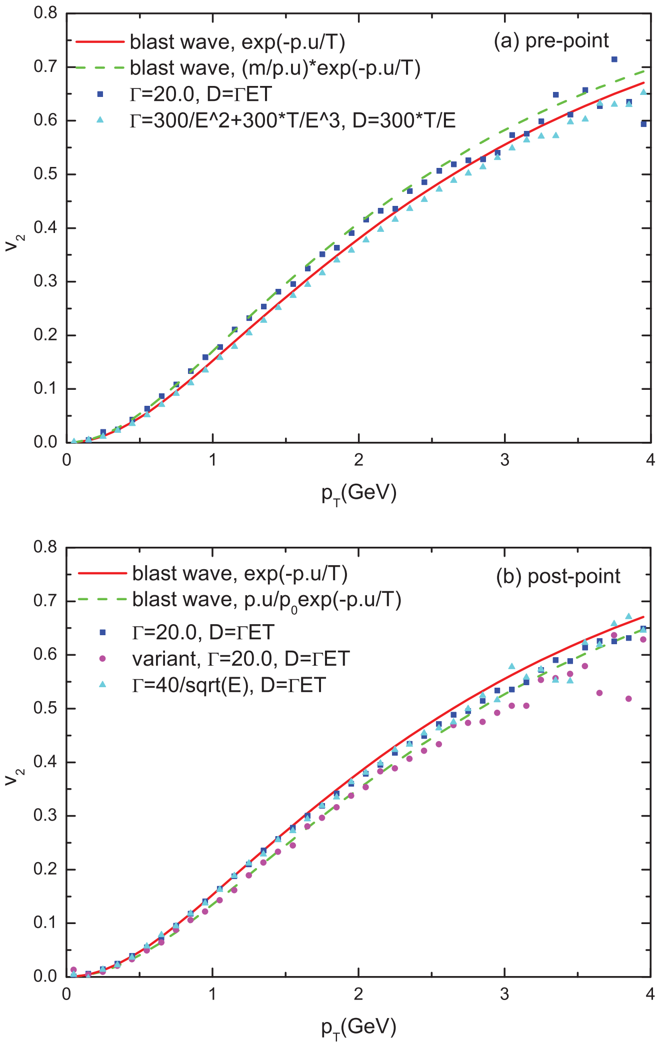

FIG. 4. (Color online) Langevin simulation results for $v_2(p_T)$ for a heavy quark ($m = 1.5$ GeV) diffusing in a QGP ($T_f = 0.18$ GeV) compared to direct blast-wave calculations with the flow field and temperature of the background medium (fireball). (a) Prepoint Langevin scheme; (b) postpoint Langevin scheme.

to a Fokker-Planck description and their manifestation in the presence of non-trivially-flowing media. Compared to previous studies, which started with a phenomenologically defined stochastic process, our considerations commenced from a microscopic theory for the interactions of a Brownian particle in a fluid of light particles, where the Fokker-Planck equation emerges from the Boltzmann equation with well-defined transport coefficients. We thus started by re-establishing the general constraint between the drag and the diffusion coefficients in order for the asymptotic solution of the Fokker-Planck equation to converge to the Boltzmann-Jüttner distribution in the equilibrium limit. Based on this "master equation" we investigated two widely used Langevin realizations of the Fokker-Planck equation and explicitly obtained the equilibrium conditions for the coefficients in these schemes. It followed that both prepoint and postpoint Langevin equations obey an equivalent Fokker-Planck equation in terms of the original drag and diffusion coefficients, thus illuminating the "Ito-Stratonovich dilemma," i.e., the prepoint and the postpoint Langevin algorithms turn out to be equally adequate to describe the same microphysics. We verified these results by explicit numerical simulations, recovering the Boltzmann-Jüttner distribution as the equilibrium limit of heavy test particles, if and only if the corresponding equilibrium condition is implemented exactly. We furthermore confirmed that the Langevin dynamics preserves the Lorentz invariance of the particle phase-space distribution in the presence of collective-flow fields of the background medium: the particle energy in the fluid rest frame, E^*, simply converts to $p \cdot u$, where p is the particle's four-momentum in the laboratory frame, and u is the fluid four-velocity. This, in particular, showed the fulfillment of Lorentz covariance through the two levels of approximation from full Boltzmann transport to the Langevin process. We believe that these insights are, in particular, useful for reliable simulations of HQ diffusion in heavy-ion collisions, where the coupling of the Brownian particle to the rather subtle relativistic flow fields has become a quantitative tool to extract transport properties of the background medium.

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