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Work, dissipation, and fluctuations in nonequilibrium physics

Relativistic fluctuation theorems

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Abstract

To reveal how nonequilibrium physics and relativity theory intertwine, this article studies relativistic Brownian motion under cosmic expansion. Two fluctuation theorems for the entropy Δs, which is locally produced in this extreme nonequilibrium situation, are presented and proven. The first, $\langle \mathrm{e}^{-\Delta s} \rangle = 1$, is a generalization of the second law of thermodynamics, that remains valid at relativistic particle energies and under high cosmic expansion rates. From this relation follows that the probability of observing a local reduction of entropy is exponentially small even if the universe was to recollapse. For the special case of the Einstein–de Sitter universe, an additional relation, $\langle \mathrm{e}^{-\Delta s-\Delta h} \rangle = 1$, is derived which holds simultaneously with the first relation and where Δh is proportional to the Hubble constant. Furthermore, the fluctuation theorems are shown to provide a physical criterion to resolve the known discretization dilemma arising in special-relativistic Brownian motion. Explicit examples and a general method for the computation of non-Gaussian entropy fluctuations are provided. ***To cite this article: A. Fingerle, C. R. Physique 8 (2007).***

Résumé

Théorèmes de fluctuations relativistes. Pour révéler comment la physique de non-équilibre et la théorie relativiste se combinent, cet article étudie le mouvement brownien relativiste sous l'effet de l'expansion cosmique. Deux théorèmes de fluctuations sont présentés et démontrés pour l'entropie Δs qui est localement produite dans cette situation de non-équilibre extrême. Le premier, $\langle \mathrm{e}^{-\Delta s} \rangle = 1$, est une généralisation du second principe de la thermodynamique qui reste valable aux énergies relativistes des particules et pour de hauts taux d'expansion cosmique. De cette relation, il suit que la probabilité d'observer une réduction locale de l'entropie est exponentiellement petite même si l'univers venait à se recomprimer. Dans le cas spécial de l'univers d'Einstein–de Sitter, une relation supplémentaire, $\langle \mathrm{e}^{-\Delta s-\Delta h} \rangle = 1$, est dérivée qui est valable conjointement avec la première relation et où Δh est proportionnel à la constante de Hubble. De plus, il est montré que les théorèmes de fluctuations fournissent un critère physique pour résoudre le dilemme connu de la discrétisation dans le mouvement brownien en relativité restreinte. Des exemples explicites et une méthode générale pour le calcul des fluctuations non-gaussiennes d'entropie sont donnés. ***Pour citer cet article : A. Fingerle, C. R. Physique 8 (2007).***

Keywords: Fluctuation theorems; Nonequilibrium physics

Mots-clés : Théorèmes de fluctuations ; Physique de non-équilibre

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1. Introduction

The physical basis of the direction of time has been discussed since Boltzmann's H-Theorem in 1872. A priori, the thermodynamic arrow of time has to be distinguished from the possibility of a prime direction of time defined by the expansion of the universe [1]. By now we know that due to the dominating dark energy component of about 72%, our universe is very likely to expand forever [2]. Yet, the fascinating cosmological arrow of time could not be based on a firm theoretical ground [3–7]. So one may still ask: Is it a mere coincidence that our memory strictly refers to times when the size of the universe was smaller? Put in physical terms, the guiding question of this article is: Does the cosmic expansion rate effect the production of entropy by nonequilibrium processes? While a general theory of nonequilibrium thermodynamics does not exist, fluctuation theorems (FTs) provide a unique starting point to develop the means to address such a fundamental question. First progress in the description of entropy production and giant fluctuations beyond linear-response was made in the 1970s [8], and a major advance was achieved in recent years with the derivation of FTs for various classes of systems [9–14]. FTs generalize the second law of thermodynamics. The second law states that the Gibbs entropy S of an ensemble may not decrease,

$$\Delta S \geqslant 0 \quad \text{at any time} \tag{1}$$

The FTs naturally extend the concept of entropy and allow statements about the probability of observing isolated 'violations' of (1). To this end the FTs assign a change Δs of entropy to an observation of a few or even single particles. When a nonequilibrium system of finite size is observed, the entropy Δs produced within a certain time interval is a fluctuating quantity. The founders of statistical mechanics, L. Boltzmann and J.W. Gibbs were well aware that the second law holds only for the entropy $\Delta S = \langle \Delta s \rangle$ of an infinite ensemble. The angle brackets denote the ensemble average over observations of equal systems. Boltzmann mentioned the possibility of 'violations', $\Delta s < 0$, in his famous reply to the Poincaré recurrence objection (in a written argument with E. Zermelo) and designated the second law as a theorem of probability ('Wahrscheinlichkeitssatz'), emphasizing that the second law cannot be expected to hold for few particles [15]. Loco citato, he referred to Gibbs [16] who had concluded: "*The impossibility of an incompensated decrease of entropy seems to be reduced to an improbability*". It is this improbability that is quantified by FTs.

For the steady state of strongly chaotic systems the detailed FT,

$$\frac{\text{Prob}(\Delta s = +ak_{\text{B}})}{\text{Prob}(\Delta s = -ak_{\text{B}})} = \text{e}^{a} \quad \text{for any } a \tag{2}$$

was proven in the limit of infinite observation time [10]. The detailed FT (2) was also derived in [11] for a non-relativistic particle in contact with a heat bath at temperature T. Initially, only the external change in the bath entropy, $\Delta s_{\text{e}} = \Delta Q/T$ with the energy ΔQ dissipated into the surrounding bath, was taken into account [11,12]. In [13] it was pointed out that when the particle is assigned an intrinsic entropy $s_{\text{s}} = -k_{\text{B}} \ln P$ (with the particle's phase space density P), the sum of intrinsic and external entropy, $\Delta s = \Delta s_{\text{s}} + \Delta s_{\text{e}}$, obeys the FT (2) even for a finite observation time.[1] This is the definition of entropy applied throughout the article. Furthermore, for non-stationary states in the presence of time-dependent driving forces, an integral FT of the form

$$\left\langle \text{e}^{-\Delta s/k_{\text{B}}} \right\rangle = 1 \tag{3}$$

was proven and linked to the Jarzynski relation [14]. Technically, the averaging over observations, $\langle \cdots \rangle$, is a path integral over trajectories, which is explained in the following section.

The detailed FT (2), the integral FT (3), and the second law of thermodynamics (1) form a consistent hierarchy of statements: from Eq. (2) follows (3) by integrating over a, and Eq. (3) implies (1) by virtue of the Jensen inequality.

We proceed as follows. In Section 2, FTs for general processes are derived. The recent unification [17–19] of Einstein's 1905 publications on Brownian motion [20] and special relativity [21] is briefly reviewed in Section 3. Based on these findings, the results of Section 4 are twofold. First, for the relativistic Brownian processes of [18] and [19], we reconcile the FTs (2) and (3), which have become a paradigm of nonequilibrium physics, with special

[1] In the earlier FT of Evans and Searles a similar term was added to the dissipation function (Eq. (2.6) in [22]), that is not present in the Gallavotti–Cohen FT [10], resulting in a FT for chaotic systems which holds for finite time. For the stochastic formulation of finite time FTs such a term was considered in [23], Eqs. (5.9) and (5.11).

relativity. For the similar process suggested in [17], FTs follow by analogous reasoning. In [18] and [19] it was pointed out that the relativistic time dilation leads to multiplicative coupling, necessitating a careful choice of the discretization rule. We show explicitly that there is one relativistic detailed FT (2) and one relativistic integral FT (3) valid for all choices. Second, we shall find the physically correct expression for the entropy production following from relativistic FTs when the Hänggi–Klimontovich discretization rule is applied. In Section 5 we go beyond special relativity with a set of two general-relativistic integral FTs for the cosmological standard model. These expose clearly the role of cosmic expansion in entropy production. We shall identify the entropy production which is solely due to the Hubble expansion of space. Such entropy producing processes dominate when the expansion rate of the universe exceeds the particle scattering rate, for instance in an early inflationary phase after the big bang. The Sections 4 and 5 each conclude with examples where we explicitly compute the non-Gaussian fluctuations $P(\Delta s)$, $P(\Delta s_\mathrm{s})$ and $P(\Delta s_\mathrm{e})$ of entropy production.

2. Stochastic formulation of the fluctuation theorem

This section gives a general derivation of the FT for stochastic processes and emphasizes that every broken symmetry implies a FT.

2.1. The integral fluctuation theorem

Let $\mathbf{\Gamma}(t)$ denote the state of the observed system, which performs a time continuous stochastic process under the influence of a thermal environment. Its stochastic dynamics are described completely by the probability distribution $P[\mathbf{\Gamma},\mathbf{C}]$, which gives the probability of observing a certain system trajectory $\mathbf{\Gamma}$. This probability depends on the environmental conditions: $\mathbf{C}$ describes a set of external parameters, such as the environmental temperature $T(t)$, external forces (for example, acting on a charged system by an electric field $\mathbf{E}(t)$), or—as we shall consider finally in the general-relativistic case—the curvature of spacetime. All these external parameters may vary during the process, so that $\mathbf{C}(t)$ is a deterministic protocol. The general idea underlying stochastic formulations of fluctuation theorems is as follows. Consider an arbitrary transformation $\mathcal{T}$, which does not leave the physical dynamics (represented by a Langevin or Fokker–Planck equation) invariant. While $P[\mathbf{\Gamma},\mathbf{C}]$ describes the dynamics of the original stochastic system, the transformed stochastic dynamics will be given by another probability distribution $\tilde{P}[\mathbf{\Gamma},\mathbf{C}]$. Assuming P and $\tilde{P}$ to have the same support, we define

$$\Delta s[\mathbf{\Gamma},\mathbf{C}] \equiv k_\mathrm{B}\ln P[\mathbf{\Gamma},\mathbf{C}] - k_\mathrm{B}\ln \tilde{P}[\mathbf{\Gamma},\mathbf{C}] \tag{4}$$

to quantify the symmetry breaking of the transformation $\mathcal{T}$ for every trajectory $\mathbf{\Gamma}$. For the quantity Δs defined in (4), an integral FT of the form (3) is a mathematical identity,

$$\left\langle \mathrm{e}^{-\Delta s/k_\mathrm{B}}\right\rangle = \int \mathcal{D}[\mathbf{\Gamma}] P[\mathbf{\Gamma},\mathbf{C}]\mathrm{e}^{-\Delta s/k_\mathrm{B}} = \int \mathcal{D}[\mathbf{\Gamma}]\tilde{P}[\mathbf{\Gamma},\mathbf{C}] = 1$$

The path integration $\int \mathcal{D}[\mathbf{\Gamma}]$ covers all continuous functions $\mathbf{\Gamma}$, weighted by the probability $P[\mathbf{\Gamma},\mathbf{C}]$.

We are interested in a fluctuation theorem that quantifies the irreversibility of the stochastic process. This is why we choose the transformation $\mathcal{T}$ to be time reversal,[2]

$$\begin{aligned}&\tilde{P}[\mathbf{\Gamma},\mathbf{C}] = P[\tilde{\mathbf{\Gamma}},\tilde{\mathbf{C}}]\\ &\text{with } \tilde{\mathbf{\Gamma}}(+t) = \mathbf{\Gamma}(-t)\\ &\text{and } \tilde{\mathbf{C}}(+t) = \mathbf{C}(-t) \quad \text{for all } t\end{aligned}$$

To get a result on the total entropy production, the transformation $\mathcal{T}$ acts globally by reversing both the stochastic system trajectory $\mathbf{\Gamma}$ and the time dependence of the environment $\mathbf{C}$.

The probability $P[\mathbf{\Gamma},\mathbf{C}]$ of observing a stochastic trajectory $[\mathbf{\Gamma}]_{-\tau}^{+\tau}$ in the time interval $(-\tau,+\tau)$ depends on the initial conditions, which are given by $\mathbf{\Gamma}(-\tau)$ for a Markov process or by the history $[\mathbf{\Gamma}]_{-\tau-T}^{-\tau}$ for a system with memory time T (which may be infinite):

[2] If $\mathbf{\Gamma}$ is the phase space vector $(\mathbf{x},\mathbf{p})$, the momenta are inverted, $\tilde{\mathbf{\Gamma}}(t) = (\mathbf{x}(-\mathbf{t}), -\mathbf{p}(-t))$.

$$P[\mathbf{\Gamma},\mathbf{C}] = P_{\text{in}} P_{\text{F}} \tag{5}$$
$$\text{with } P_{\text{in}} = \begin{cases} P(\mathbf{\Gamma},\mathbf{C})|_{-\tau}, & \text{if Markovian} \\ P[\mathbf{\Gamma},\mathbf{C}]_{-\tau-T}^{-\tau}, & \text{if with memory} \end{cases}$$
$$\text{and } P_{\text{F}} = P([\mathbf{\Gamma},\mathbf{C}]_{-\tau}^{+\tau}|\text{in})$$

We refer to the initial state or the history as the in-state of the system, which is distributed according to the first factor P_{in} in (5). The second factor P_{F} is the (forward) propagator on the time interval $(-\tau, +\tau)$ under the influence of the thermal environment. Analogously, the time-reversed probability is written as

$$\tilde{P}[\mathbf{\Gamma},\mathbf{C}] = \tilde{P}[\tilde{\mathbf{\Gamma}},\tilde{\mathbf{C}}] = P_{\text{out}} P_{\text{R}} \tag{6}$$

Inserting (5) and (6) in (4), Δs decomposes into the sum

$$\Delta s = \Delta s_{\text{s}} + \Delta s_{\text{e}} \tag{7}$$
$$\text{with } \Delta s_{\text{s}} = -k_{\text{B}} \ln P_{\text{out}} + k_{\text{B}} \ln P_{\text{in}} \tag{8}$$
$$\text{and } \Delta s_{\text{e}} = k_{\text{B}} \ln \frac{P_{\text{F}}}{P_{\text{R}}} \tag{9}$$

The first term (8) is the change of the system entropy $s_{\text{s}} = -k_{\text{B}} \ln P_j$ as the system state changes from '$j = \text{in}$' to '$j = \text{out}$'. The expression $s_{\text{s}}(P_j) = -k_{\text{B}} \ln P_j$ for the system entropy was suggested in [13] for a Markov process and is a widely accepted definition because s_{s} resembles the Boltzmann entropy and $S_{\text{s}} = \langle s_{\text{s}} \rangle = -k_{\text{B}} \langle \ln P_j \rangle$ coincides with the Gibbs entropy of the ensemble P_j.

The second term (9) is a Crooks relation [24] defined by the forward and reversed time evolution under the stochastic influence of the thermal environment. We have to show that Δs_{e} as introduced in (9) equals exactly the entropy produced in the thermal environment, so that $\Delta s = \Delta s_{\text{s}} + \Delta s_{\text{e}}$ is the total entropy production. It is the objective of this article to evaluate (9) for a thermal environment at relativistic energies to adjudicate on the physical interpretation as environmental entropy.

For Markov processes, such as the relativistic Brownian motion discussed in the next section, the forward and reverse propagators are infinite products of transition probabilities,

$$P_{\text{F}} = \lim_{n\to\infty} \prod_{k=1}^{n} P_{\text{trans}}^{\Delta t_k}\big(\mathbf{\Gamma}_{k-1} \mapsto \mathbf{\Gamma}_k, \mathbf{C}(\Delta t_k)\big) \quad \text{and}$$
$$P_{\text{R}} = \lim_{n\to\infty} \prod_{k=1}^{n} P_{\text{trans}}^{\Delta t_k}\big(\mathbf{\Gamma}_{k} \mapsto \mathbf{\Gamma}_{k-1}, \mathbf{C}(\Delta t_k)\big)$$

so that entropy production is local in time: For the environmental entropy follows

$$\Delta s_{\text{e}} = \int_{-\tau}^{+\tau} \dot{s}_{\text{e}}(t)\,\mathrm{d}t \quad \text{with}$$
$$\dot{s}_{\text{e}}(t)\,\mathrm{d}t = k_{\text{B}} \ln \frac{P_{\text{trans}}^{\mathrm{d}t}(\mathbf{\Gamma}^- \mapsto \mathbf{\Gamma}^+, \mathbf{C}(t))}{P_{\text{trans}}^{\mathrm{d}t}(\tilde{\mathbf{\Gamma}}^- \mapsto \tilde{\mathbf{\Gamma}}^+, \mathbf{C}(t))} \tag{10}$$

and the change in system entropy is $\Delta s_{\text{s}} = s_{\text{s}}(+\tau) - s_{\text{s}}(-\tau)$ with $s_{\text{s}}(t) = -k_{\text{B}} \ln P(\mathbf{\Gamma}(t), \mathbf{C}(t))$. The probability density $P(\mathbf{\Gamma}, t) = P(\mathbf{\Gamma}, \mathbf{C}(t))$ evolves according to the continuity equation,

$$\partial_t P(\mathbf{\Gamma}, t) + \nabla_{\mathbf{\Gamma}} \circ \mathbf{j}(\mathbf{\Gamma}, t) = 0 \tag{11}$$

with the probability current

$$\mathbf{j}(\mathbf{\Gamma}, t) = \sum_{n=0}^{\infty} \frac{(-\nabla_{\mathbf{\Gamma}})^n}{n!} \circ \mathbf{M}_{n+1}(\mathbf{\Gamma}, t) P(\mathbf{\Gamma}, t) \tag{12}$$

The Helfand moments $\mathbf{M}_n$ are tensors of order n which are related to the transition probability $P_{\text{trans}}^{\mathrm{d}t}$ by [25]

$$\mathbf{M}_n(\mathbf{\Gamma}, t)\,\mathrm{d}t = \int (\mathbf{\Gamma}' - \mathbf{\Gamma})^n P_{\text{trans}}^{\mathrm{d}t}\big(\mathbf{\Gamma} \mapsto \mathbf{\Gamma}', \mathbf{C}(t)\big)\,\mathrm{d}\mathbf{\Gamma}'$$

The higher moments are present only if the heat bath in which the system is embedded is out of equilibrium. A possible system for relativistic Brownian motion is an electron which couples by Compton scattering to a gas of photons. We assume that such a heat bath is in local equilibrium so that we have a well-defined temperature $T(\mathbf{x},t)$ yielding an isotropic diffusion $\mathbf{M}_2 \propto T\mathbb{1}$ with vanishing higher moments, $\mathbf{M}_n = 0$ for $n > 2$. Eq. (11) then reduces to the Fokker–Planck equation and the transition probabilities are Gaussian.

2.2. *The detailed fluctuation theorem*

While the integral FT derived above holds for arbitrary environmental conditions $\mathbf{C}$, the stronger detailed FT (2) holds if the deterministic protocol is invariant under time-reversal, $\mathbf{C} = \tilde{\mathbf{C}}$. The general derivation for the quantity Δs defined in (4) is also done conveniently by path integration. The probability to observe a production of entropy $\Delta s = ak_\mathrm{B}$ is

$$\begin{aligned}
\mathrm{Prob}(\Delta s = ak_\mathrm{B}) &= \int P[\boldsymbol{\Gamma},\mathbf{C}]\delta\big(\Delta s[\boldsymbol{\Gamma},\mathbf{C}] = ak_\mathrm{B}\big)\mathcal{D}[\boldsymbol{\Gamma}] \\
&= \int P[\tilde{\boldsymbol{\Gamma}},\tilde{\mathbf{C}}]\mathrm{e}^{\Delta s/k_\mathrm{B}}\delta\big(\Delta s[\boldsymbol{\Gamma},\mathbf{C}] = ak_\mathrm{B}\big)\mathcal{D}[\boldsymbol{\Gamma}] \\
&= \mathrm{e}^{a}\int P[\tilde{\boldsymbol{\Gamma}},\tilde{\mathbf{C}}]\delta\big(\Delta s[\boldsymbol{\Gamma},\mathbf{C}] = ak_\mathrm{B}\big)\mathcal{D}[\boldsymbol{\Gamma}] \\
&= \mathrm{e}^{a}\int P[\tilde{\boldsymbol{\Gamma}},\tilde{\mathbf{C}}]\delta\big(\Delta s[\tilde{\boldsymbol{\Gamma}},\tilde{\mathbf{C}}] = -ak_\mathrm{B}\big)\mathcal{D}[\boldsymbol{\Gamma}]
\end{aligned}$$

In the second and last equality we exploited Eq. (4). Using the trivial fact that the path integration can be reordered in time, we arrive at

$$\mathrm{Prob}(\Delta s = ak_\mathrm{B}) = \mathrm{e}^{a}\int P[\boldsymbol{\Gamma},\tilde{\mathbf{C}}]\delta\big(\Delta s[\boldsymbol{\Gamma},\tilde{\mathbf{C}}] = -ak_\mathrm{B}\big)\mathcal{D}[\boldsymbol{\Gamma}]$$

Comparing this result with the probability

$$\mathrm{Prob}(\Delta s = -ak_\mathrm{B}) = \int P[\boldsymbol{\Gamma},\mathbf{C}]\delta\big(\Delta s[\boldsymbol{\Gamma},\mathbf{C}] = -ak_\mathrm{B}\big)\mathcal{D}[\boldsymbol{\Gamma}]$$

of observing a reduction $\Delta s = -ak_\mathrm{B}$, yields the detailed FT (2) for any symmetric protocol, $\mathbf{C} = \tilde{\mathbf{C}}$. Therefore the detailed FT holds not only in the steady state, which the system reaches under time-independent forcing, $\mathbf{C}(t) = \text{const}$, but also, for example, in periodically changing conditions that are symmetric with respect to the observed time-frame $(-\tau, +\tau)$.

We conclude this general derivation of FTs with the remark that the formulation presented gives a unifying perspective on the distinct FTs of [13] and [26]. Eq. (6) in [26] is generalized by Eq. (4), while Eqs. (8) and (9) correspond to the decomposition of entropy according to Eqs. (5) and (14) in [13], respectively.

3. Relativistic Brownian motion

The derivation of the FTs (2) and (3) in Section 2 uses the abstract expression (10) for the entropy production $\dot{s}_\mathrm{e}$ in the embedding heat bath. As emphasized before, this expression has to be evaluated for a physical process to allow for a physical interpretation as entropy. An instructive process is relativistic Brownian motion.

To minimize technicalities, we consider first the one-dimensional special-relativistic motion of a particle with rest mass m in a heat bath at temperature T. The generalization to higher spatial dimensions is straightforward. Even if we would allow the particle to equilibrate with its environment, the mean squared velocity may not obey the non-relativistic law $\langle v^2\rangle = k_\mathrm{B}T/m$ in the high temperature limit, since the finite speed of light defines an insurmountable upper bound. The special-relativistic nonequilibrium Brownian motion, giving rise to bounded velocity distributions, has been set forth in [17–19] using both, the language of stochastic differential equations (relativistic Langevin equations) and the language of probability densities (relativistic Fokker–Planck equations). Simulations of this relativistic stochastic process have been applied to analyze scattering experiments of quark–gluon plasma [27]. As in the familiar non-relativistic case [25], a deterministic force F_d acts on the particle in the rest frame of the heat bath,

$$\mathrm{d}p_\mathrm{d} = F_\mathrm{d}\,\mathrm{d}t = -\nu p\,\mathrm{d}t \tag{13}$$

so that the time scale of dissipation is $1/\nu$. In the relativistic generalization (13), the non-relativistic momentum mv is replaced by $p = p^1 = mv/\sqrt{1-v^2/c^2}$, which is the spatial component of the relativistic momentum vector p^α. As usual, Greek indices refer to temporal ($\alpha = 0$) and spatial components. The signature of the Minkowski metric tensor is $\eta_{\alpha\beta} = \eta^{\alpha\beta} = \mathrm{diag}(-1, 1)$. Moreover, Einstein's summation convention is invoked throughout. Since the rest mass is not altered in elastic collisions, $p^\alpha p_\alpha = -(mc)^2 = \mathrm{const}$, the change in the momentum vector $\mathrm{d}p^\alpha$ is always 'orthogonal' to p_α in the sense of

$$p_\alpha\,\mathrm{d}p^\alpha = 0 \tag{14}$$

This means that the classical particle cannot leave its mass shell $p^\alpha p_\alpha = -(mc)^2$, which is nothing but its dispersion relation,

$$E = p^0 c = \sqrt{\left(mc^2\right)^2 + (pc)^2} \tag{15}$$

The general solution of (14) is the projection $\mathrm{d}p^\alpha = (\delta^\alpha_\beta + p^\alpha p_\beta/(mc)^2)\xi^\beta$ of an arbitrary Lorentz vector ξ^β. It is readily confirmed that the choice

$$\mathrm{d}p^\alpha_\mathrm{d} = -m\nu\left(\delta^\alpha_\beta + \frac{p^\alpha p_\beta}{(mc)^2}\right)v^\beta_\mathrm{bath}\,\mathrm{d}\tau \tag{16}$$

reduces to Eq. (13) in the rest frame of the bath with the bath velocity vector $v^\alpha_\mathrm{bath} = (c, 0)$ and the particle's proper time τ. Hence, Eq. (16) is the generalized Lorentz-invariant deterministic part of the Brownian motion.[3]

The description of relativistic Brownian motion is completed by Lorentz-invariant stochastic changes $\mathrm{d}p^\alpha_\mathrm{s}$ of the momentum caused by the impacts of the surrounding heat bath at temperature T. The derivation is guided by two principles: first, the relativistic momentum is the proper quantity performing a Wiener process, since it is physically exchanged and additive, whereas the velocity is well-known not to be additive in special relativity. The second postulate demands that the distribution is Gaussian in the instantaneous rest frame of the particle. This connects the relativistic Brownian motion to the non-relativistic case. These principles determine the exchanged momenta $\mathrm{d}p^\alpha_\mathrm{s}$ to be distributed according to (cf. Eq. (35c) in [18])

$$P_\mathrm{coll}(p^\mu, \mathrm{d}p^\nu_\mathrm{s}) = \frac{mc\delta(p_\beta\,\mathrm{d}p^\beta_\mathrm{s})}{2\sqrt{\pi}\,\mathcal{D}\,\mathrm{d}\tau}\exp\left(-\frac{\mathrm{d}p^\alpha_\mathrm{s}\,\mathrm{d}p_{\mathrm{s}\alpha}}{4\mathcal{D}\,\mathrm{d}\tau}\right) \tag{17}$$

The Dirac distribution $\delta(p_\beta\,\mathrm{d}p^\beta_\mathrm{s})$ in (17) guarantees that the mass-shell condition (14) is also fulfilled by the stochastic impacts, since they are elastic. While the relativistic momentum p is additive and unbounded, the velocity is restricted to the open interval $(-c, +c)$. This can be seen by the elegant relation $v/c^2 = p/E$ in the rest frame of the bath, which is equivalent to

$$\mathrm{d}x = \frac{pc}{\sqrt{(mc)^2 + p^2}}\,\mathrm{d}t \tag{18}$$

As mentioned before in the context of the general Kramers–Moyal expansion (12), the bath temperature T is defined by the Einstein relation,

$$\mathcal{D} = k_\mathrm{B} T m\nu \tag{19}$$

with the momentum diffusion constant $\mathcal{D}$ (cf. Eq. (59) in [18]).

[3] Eq. (16) in [18] contains an identically vanishing term.

4. Relativistic fluctuation theorem

We have now the manifestly Lorentz-invariant Langevin equation

$$\mathrm{d}p^\alpha = \mathrm{d}p_\mathrm{d}^\alpha + \mathrm{d}p_\mathrm{s}^\alpha \tag{20}$$

with the deterministic part given by (16) and the stochastic part described by (17) at hand. Specifying (20) to the rest frame of the bath yields

$$\mathrm{d}p = -\nu p\,\mathrm{d}t + \mathrm{d}p_\mathrm{s} \tag{21}$$

The probability density of the exchanged momenta $\mathrm{d}p_\mathrm{s}$ is found by integrating out the $\mathrm{d}p_\mathrm{s}^0$-component in (17), cf. [18]:

$$P_{\mathrm{coll}}(p, \mathrm{d}p_\mathrm{s}) = \frac{\exp(-\mathrm{d}p_\mathrm{s}^2/(4\mathcal{D}\sqrt{1+\frac{p^2}{(mc)^2}}\,\mathrm{d}t))}{2\sqrt{\pi\mathcal{D}\,\mathrm{d}t}\,\sqrt[4]{1+\frac{p^2}{(mc)^2}}} \tag{22}$$

This exhibits the discretization dilemma: A discretization rule has to be imposed on (22) since relativistic invariance does not determine whether p in (22) refers to the particle momentum p_- before the collision (pre-point rule of Itô), to the post-point $p_+ = p_- + \mathrm{d}p$ (Hänggi–Klimontovich), or to the midpoint $(p_- + p_+)/2$ (Fisk–Stratonovich).

Eqs. (18), (21) and (22) establish the relativistic stochastic motion of the Brownian particle in phase space. The corresponding transition probability is uniquely determined by the discretization rule:

$$P_{\mathrm{trans}}^{\mathrm{d}t}\begin{pmatrix} x \mapsto x+\mathrm{d}x \\ p \mapsto p+\mathrm{d}p \end{pmatrix} = \frac{\delta(\mathrm{d}x - \frac{pc^2}{E}\,\mathrm{d}t)}{2\sqrt{\pi\mathcal{D}E\,\mathrm{d}t/mc^2}} \times \exp\left(-\frac{(\mathrm{d}p + \nu p\,\mathrm{d}t - (1-\kappa)\frac{\mathcal{D}}{mc^2}\frac{\mathrm{d}E}{\mathrm{d}p}\,\mathrm{d}t)^2}{4\mathcal{D}E\,\mathrm{d}t/mc^2}\right) \tag{23}$$

The discretization is contained in the parameter κ, $0 \leqslant \kappa \leqslant 1$. Hänggi–Klimontovich, Fisk–Stratonovich, or Itô correspond to the values $\kappa = 0, \frac{1}{2}$, or 1 respectively.

Let us now investigate the consequences for entropy production arising out of the special-relativistic discretization dilemma. As derived in Section 2, the total entropy is a sum of the particle intrinsic entropy $s_\mathrm{s} = -k_\mathrm{B}\ln P$ with the particle's nonequilibrium phase space density $P(x,p,t)$, and the external entropy s_e of the ambient heat bath at temperature T.

Inserting the probability current (12) in momentum space

$$j_p(x,p,t) = -\left(\nu p + \kappa\frac{\mathcal{D}}{mc^2}\frac{\mathrm{d}E}{\mathrm{d}p}\right)P(x,p,t) - \frac{\mathcal{D}E}{mc^2}\frac{\partial P(x,p,t)}{\partial p} \tag{24}$$

in the differential $\mathrm{d}s_\mathrm{s}$ of the particle entropy $s_\mathrm{s}(t) = -k_\mathrm{B}\ln P(x(t), p(t), t)$ we find the equation of motion (generalizing Eq. (7) in [13]) for s_s,

$$\mathrm{d}s_\mathrm{s} = \mathrm{d}s_\mathrm{s}|_{\kappa=0} + \kappa k_\mathrm{B}\,\mathrm{d}\ln E \tag{25}$$

Here we have isolated the second term which depends on the discretization rule applied.

The entropy production $\mathrm{d}s_\mathrm{e}$ in the bath follows by contrasting the transition probabilities of the trajectory $\mathbf{\Gamma} = (x,p)$ with its time-reverse $\tilde{\mathbf{\Gamma}} = (\tilde{x}, -\tilde{p})$ to extract the irreversible part, $\ln P_{\mathrm{trans}}^{\mathrm{d}t}(\mathbf{\Gamma}^- \mapsto \mathbf{\Gamma}^+) - \ln P_{\mathrm{trans}}^{\mathrm{d}t}(\tilde{\mathbf{\Gamma}}^- \mapsto \tilde{\mathbf{\Gamma}}^+)$, causing the dissipation (10). From a brief computation we find:

$$\mathrm{d}s_\mathrm{e} = k_\mathrm{B}\ln\frac{P_{\mathrm{trans}}^{\mathrm{d}t}\begin{pmatrix} x \mapsto x+\mathrm{d}x \\ p \mapsto p+\mathrm{d}p \end{pmatrix}}{P_{\mathrm{trans}}^{\mathrm{d}t}\begin{pmatrix} x+\mathrm{d}x \mapsto x \\ -p-\mathrm{d}p \mapsto -p \end{pmatrix}} = -\frac{\mathrm{d}E}{T} - \kappa k_\mathrm{B}\,\mathrm{d}\ln E \tag{26}$$

Eqs. (25) and (26) reveal that although the relativistic Brownian motion is physically inequivalent depending on κ, the fluctuations of the total entropy $s = s_\mathrm{s} + s_\mathrm{e}$ are independent of κ. Explicitly, the change of the total entropy is

$$\frac{\mathrm{d}s}{k_\mathrm{B}} = -\frac{\partial\ln P}{\partial t}\,\mathrm{d}t - \frac{\partial\ln P}{\partial x}\,\mathrm{d}x + \frac{mc^2 j_p}{\mathcal{D}EP}\,\mathrm{d}p$$

Two technical comments are here in order. First, when computing $\mathrm{d}s_\mathrm{e}$ in (26) the notation has to carefully distinguish between initial $\mathbf{\Gamma}^-$ and finale state $\mathbf{\Gamma}^+$, and one should consider the quotient $P(\mathbf{\Gamma}^- \to \mathbf{\Gamma}^- + \mathrm{d}\mathbf{\Gamma})/P(\mathbf{\Gamma}^- + \mathrm{d}\mathbf{\Gamma} \to \mathbf{\Gamma}^-)$ as done in (26). Writing the back transition in the numerator in the form $P(\mathbf{\Gamma}^+ \to \mathbf{\Gamma}^+ - \mathrm{d}\mathbf{\Gamma})$ would be correct yet unfavorable for evaluation, because common $\mathbf{\Gamma}^-$-factors could not be cancelled out. In transforming $P(\mathbf{\Gamma}^+ \to \mathbf{\Gamma}^+ - \mathrm{d}\mathbf{\Gamma})$ to $P(\mathbf{\Gamma}^- + \mathrm{d}\mathbf{\Gamma} \to \mathbf{\Gamma}^-)$ the known spurious drift of the multiplicative coupling has to be taken into account [25]. Second, the discretization term in (26) can be absorbed by defining a more complicated fluctuation-dissipation theorem, however in this article we use exclusively the Einstein relation (19).

The path integration of the results (25) and (26) according to Section 2 yields the detailed FT (2) for time-symmetric environments, and the integral FT (3) for arbitrary environmental conditions, with entropy fluctuations Δs observed over finite time. Thus we have proven relativistic FTs that are unaffected by the discretization dilemma.

Furthermore, we are now in a position to address the physical choice of κ by virtue of the FT. Because of energy conservation, the energy $-\mathrm{d}E$ in (26) lost by the particle equals the heat $\mathrm{d}Q$ gained by the ambient bath:

$$\mathrm{d}s_\mathrm{e} = \frac{\mathrm{d}Q}{T} - \kappa k_\mathrm{B}\,\mathrm{d}\ln E \tag{27}$$

In the non-relativistic regime the particle energy $E = mc^2 + E_\mathrm{kin}$ is dominated by the energy of the rest mass m so that the second term in (27) vanishes for $mc^2 \gg E_\mathrm{kin}$,

$$\mathrm{d}\ln E = \frac{E_\mathrm{kin}}{mc^2 + E_\mathrm{kin}}\,\mathrm{d}\ln E_\mathrm{kin}$$

and we recover the non-relativistic FTs [13]. At arbitrary relativistic energies (15) the Hänggi–Klimontovich rule, $\kappa = 0$, entails the correct expression for the entropy

$$\mathrm{d}s_\mathrm{e} = \frac{\mathrm{d}Q}{T} \tag{28}$$

which is produced in the heat bath.

4.1. Generalizations in the framework of special relativity

To generalize the FTs to n spatial dimensions, momentum and force in Eq. (13) are simply substituted by their spatial vectors and the Greek indices in the Lorentz-invariant Eqs. (16) and (17) take values up to n. After integrating out the temporal component p^0, the distribution (22) is found to contain a quadratic form $\mathbf{A}$ instead of the square in the exponent (cf. Eq. (15) in [19]) with tensor components

$$A_{ij} = \delta_{ij} - \frac{c^2}{E^2} p_i p_j \tag{29}$$

The FTs follow using the fact that $\mathbf{p}$ is an eigenvector of $\mathbf{A}$. No complications are caused by allowing an inhomogeneous heat bath, where the temperature T and the dissipation rate ν vary in space. As far as the integral FT (3) is concerned, a bath temperature evolving in time is also permitted (as part of the environmental condition $\mathbf{C}(t)$ in Section 2). Since the time-asymmetric part enters (28), the dissipation rate ν may be an even function of the momentum, $\nu(\mathbf{p}) = \nu(-\mathbf{p})$. This is of physical relevance since ν is known not to be constant even for most non-relativistic processes [28]. As mentioned in the general derivation of Section 2, an arbitrary time-dependent external force $F_\mathrm{e}(t)$ (being also part of the environmental condition $\mathbf{C}(t)$ defined in the rest frame of the bath) does not pose a problem. After adding $F_\mathrm{e}(t)$ to the deterministic force F_d in (13) we find the expression $\mathrm{d}s_\mathrm{e} = \mathrm{d}Q/T$ with the heat $\mathrm{d}Q = -\mathrm{d}E + F_\mathrm{e}\,\mathrm{d}x$. This is the first law of thermodynamics stated in the frame of the bath.

4.2. The commuting Brownian particle

We give (to the author's knowledge) the first example where the non-Gaussian fluctuations of particle entropy Δs_s, environmental entropy Δs_e, and total entropy Δs can be evaluated exactly. A complementary method which allows the general numerical computation of fluctuations by iteration will be proposed in Section 5.3.

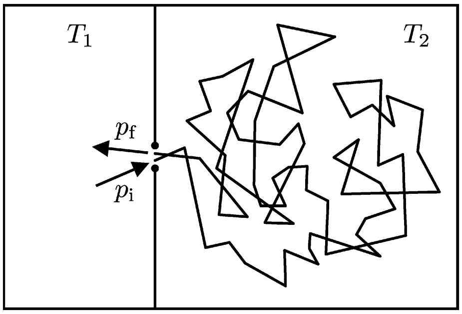

Fig. 1. A Brownian particle commuting between different thermal environments. The non-Gaussian fluctuations of entropy occurring in this system can be evaluated analytically (cf. Figs. 2 and 3).

Consider two heat baths at temperatures T_1 and T_2 with a Brownian particle moving initially in T_1. After the equilibration time, its momentum p_i (in units of mc) will be distributed according to the Jüttner–Maxwell distribution $\varphi(p_\mathrm{i}, T_1)$ [29], where

$$\varphi(p,T) = C^{-1}\mathrm{e}^{-E(p)/T} = C^{-1}\mathrm{e}^{-\sqrt{1+p^2}/T} = \frac{\mathrm{e}^{-p^2/(T+T\sqrt{1+p^2})}}{Z(T)} \tag{30}$$

is the equilibrium solution of the Brownian motion presented in Section 3. The last formulation in (30) (following from $\sqrt{1+p^2}-1 = p^2/(1+\sqrt{1+p^2})$) is convenient for the low momentum limit. To keep formulas concise, we measure heat in units of mc^2 and entropy in units of k_B, so that temperature T is measured in units of mc^2/k_B. The relativistic partition sum $Z(T)$ equals

$$Z(T) = 2\exp(1/T)K_1(1/T) \tag{31}$$

with K_1 being the first modified Bessel function of the second kind. The Brownian particle can pass to the bath T_2 through an opening (cf. Fig. 1). This opening is small enough to keep the baths at different temperatures and to ensure that the Brownian particle spends enough time in T_2 before returning to T_1. So its momentum p_f on return has become uncorrelated to the initial value p_i and is distributed according to $\varphi(p_\mathrm{f}, T_2)$. The change of the particle entropy Δs_s and the environmental entropy Δs_e during the relaxation of the Brownian particle in T_2 can be expressed using φ:

$$\Delta s_\mathrm{s} = s_\mathrm{s}(t_\mathrm{f}) - s_\mathrm{s}(t_\mathrm{i}) = \ln\frac{\varphi(p_\mathrm{i}, T_1)}{\varphi(p_\mathrm{f}, T_2)} \tag{32a}$$

$$\Delta s_\mathrm{e} = \frac{\Delta Q}{T_2} = \ln\frac{\varphi(p_\mathrm{f}, T_2)}{\varphi(p_\mathrm{i}, T_2)} \tag{32b}$$

$$\Delta s_{=} \Delta s_\mathrm{s} + \Delta s_\mathrm{e} = \ln\frac{\varphi(p_\mathrm{i}, T_1)}{\varphi(p_\mathrm{i}, T_2)} \tag{32c}$$

The total entropy Δs in (32c) follows from the above definitions of particle entropy (32a) and environmental entropy[4] (32b). From the resulting expression (32c) we find the macroscopic Gibbs entropy,

$$\Delta S = \langle \Delta s\rangle = \int \varphi(p_\mathrm{i}, T_1)\ln\frac{\varphi(p_\mathrm{i}, T_1)}{\varphi(p_\mathrm{i}, T_2)}\,\mathrm{d}p_\mathrm{i}$$

to equal the relative entropy of the baths,

$$\Delta S = S_\mathrm{KL}(T_1 \| T_2) \tag{33}$$

which is also known as the Kullback–Leibler distance [30].

[4] Aside from the physical expression $\Delta Q/T$ used in (32b), the expression $\ln(\varphi(p_\mathrm{f}, T)/\varphi(p_\mathrm{i}, T))$ in terms of the equilibrium distribution φ is directly related to the definition (10) by the principle of detailed balance, $\varphi(p_\mathrm{i}, T)P^{(\Delta t)}_\mathrm{trans}(p_\mathrm{i} \mapsto p_\mathrm{f}, T) = \varphi(p_\mathrm{f}, T)\, P^{(\Delta t)}_\mathrm{trans}(p_\mathrm{f} \mapsto p_\mathrm{i}, T)$, because the baths themselves are in local equilibrium.

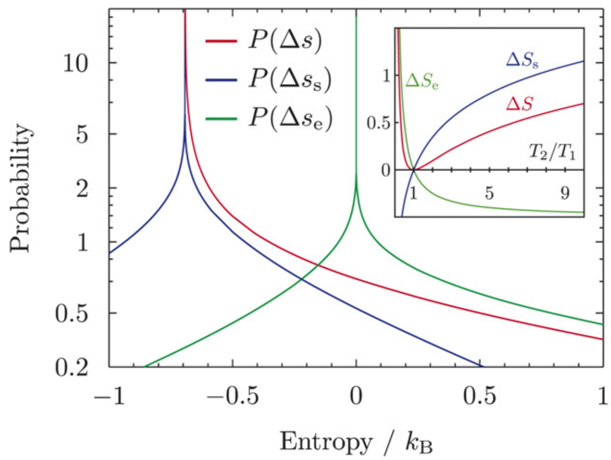

Fig. 2. The exact expressions (34a) for the distribution of particle entropy Δs_s (blue), environmental entropy Δs_e (green), and total entropy $\Delta s = \Delta s_s + \Delta s_e$ (red). The plot is for $T_1 = 4T_2 \ll mc^2/k_B$. The inset shows the dependence on the temperature ratio for the macroscopic entropies (35): $\Delta S_s = \langle \Delta s_s \rangle$, $\Delta S_e = \langle \Delta s_e \rangle$, and $\Delta S = \Delta S_s + \Delta S_e$ which is non-negative according to the second law of thermodynamics (1).

The trajectory entropies (32) depend only on the pair (p_i, p_f) of initial and end points in momentum space. Therefore the distributions $P(\Delta s)$, $P(\Delta s_s)$ and $P(\Delta s_e)$ follow not from path integrals but ordinary integrals such as $P(\Delta s_e) = \int \varphi(p_i, T_1)\varphi(p_f, T_2)\delta(\Delta s_e - \Delta s_e(p_i, p_f))\,\mathrm{d}p_i\,\mathrm{d}p_f$, where the expression $\Delta s_e(p_i, p_f)$ (32b) is inserted in the Dirac delta function to sum over all trajectories yielding a certain entropy increment Δs_e. Because of its physical relevance, we begin with the explicit non-relativistic results, $T \ll mc^2/k_B$, when φ (30) becomes the Maxwell–Boltzmann distribution:

$$P(\Delta s) = \frac{\Theta(A(\Delta s - s_0))}{\sqrt{\pi A(\Delta s - s_0)}}\mathrm{e}^{-\frac{\Delta s - s_0}{A}} \tag{34a}$$

$$P(\Delta s_s) = \frac{K_0(|\Delta s_s - s_0|)}{\pi} \tag{34b}$$

$$P(\Delta s_e) = \frac{\sqrt{\alpha}}{\pi}\mathrm{e}^{\Delta s_e \frac{1-\alpha}{2}} K_0\left(|\Delta s_e|\frac{1+\alpha}{2}\right) \tag{34c}$$

The abbreviations $A = \alpha^{-1} - 1$ and $s_0 = \frac{1}{2}\ln\alpha$ contain the dependence on the temperature ratio $\alpha = T_2/T_1$. The Heaviside step function is denoted by Θ. The distribution functions (34a) are plotted in Fig. 2. With the Bessel function K_0 appearing in (34a), the distributions for Δs_s and Δs_e have logarithmic divergences at s_0 and 0 respectively. The distribution of Δs has the stronger inverse square root divergence as Δs approaches s_0 from above and vanishes below s_0. From (34a) the integral FT (3) can be verified directly, while the detailed FT (2) is obviously not fulfilled (as it has to be since the embedding temperature for the Brownian particle changes randomly with time). We remark that (34a) is not simply the convolution of (34b) and (34b) because Δs_s and Δs_e are highly correlated.

The macroscopic entropies $\Delta S_s = \langle \Delta s_s \rangle$, $\Delta S_e = \langle \Delta s_e \rangle$, and $\Delta S = \langle \Delta s \rangle = \Delta S_s + \Delta S_e \geqslant 0$ are the mean values of the distributions (34a):

$$\Delta S_s = s_0 = \frac{\ln\alpha}{2} \tag{35a}$$

$$\Delta S_e = \frac{\alpha^{-1} - 1}{2} \tag{35b}$$

After the Brownian particle has visited both reservoirs once, the total macroscopic entropy increment has the symmetric form

$$\Delta S(T_1 \to T_2 \to T_1) = \Delta S(T_2 \to T_1 \to T_2) = \frac{(T_1 - T_2)^2}{2T_1T_2} > 0 \tag{36}$$

In the relativistic regime, mc^2 defines a third energy scale, so that the results no longer depend only on the ratio of temperatures. The singularity at $\Delta s = s_0$ is shifted to the position

$$s_0 = \ln \frac{Z(T_2)}{Z(T_1)} \tag{37}$$

in terms of the partition sum (31). The first relativistic correction of the partition sum is

$$Z(T) = \sqrt{2\pi T}\left(1 + \frac{3}{8}T + \mathcal{O}\big(T^2\big)\right) \tag{38}$$

so that s_0 depends on the temperature difference $\Delta T = T_2 - T_1$ in first order:

$$s_0 = \frac{1}{2}\ln\frac{T_2}{T_1} + \frac{3}{8}\Delta T + \mathcal{O}\big(T_1^2, T_2^2\big) \tag{39}$$

In the ultra-relativistic regime, $T \gg mc^2/k_B$, the partition sum becomes linear in T,

$$Z(T) = 2T + 2 + \mathcal{O}(1/T) \tag{40}$$

so that the position s_0 of the singularity depends on the ratio of temperatures as in the non-relativistic limit and reaches twice its non-relativistic value,

$$\lim_{k_B T \gg mc^2} s_0 = 2 \lim_{k_B T \ll mc^2} s_0 = \ln\frac{T_2}{T_1} \tag{41}$$

The relativistic distribution functions are sums of Bessel functions. For example the system entropy Δs is distributed at arbitrary temperatures T_1 and T_2 according to

$$P(\Delta s_s) = \frac{1}{N(T_1, T_2)}\begin{cases} f(T_1, T_2, |\Delta s_s - s_0|), & \Delta s > s_0 \\ f(T_2, T_1, |\Delta s_s - s_0|), & \Delta s < s_0 \end{cases} \tag{42}$$

The normalization factor in (42) is

$$N(T_1, T_2) = \frac{Z(T_1)Z(T_2)}{2\sqrt{T_1 T_2}} \tag{43}$$

and the function f in (42) is defined by the integral

$$f(a, b, z) = e^{-z}\int_0^\infty dx\, \frac{e^{-x}}{\sqrt{x}\sqrt{x+2z}}\,\frac{1 + ax/2}{\sqrt{1 + ax/4}}\,\frac{1 + b(x/2 + z)}{\sqrt{1 + b(x/4 + z/2)}} \tag{44}$$

The non-relativistic limit (34b) follows from $f(0, 0, z) = K_0(z)$ and $N(0, 0) = \pi$. The first relativistic corrections are

$$P(\Delta s) = g_0(\Delta s_s - s_0) + \overline{T} g_1(\Delta s_s - s_0) + \Delta T g_2(\Delta s_s - s_0) + \mathcal{O}\big(T_1^2, T_2^2, T_1 T_2\big) \tag{45}$$

with the mean temperature $\overline{T} = (T_1 + T_2)/2$ and the temperature difference $\Delta T = T_2 - T_2$. We remark that the functions

$$g_0(z) = \frac{K_0(|z|)}{\pi} \tag{46a}$$

$$g_1(z) = \frac{3}{4\pi}\big(|z| K_1\big(|z|\big) - K_0\big(|z|\big)\big) \tag{46b}$$

$$g_2(z) = \frac{3}{8\pi} z K_0\big(|z|\big) \tag{46c}$$

exhibit the symmetry $T_1 \leftrightarrow T_2$ of the system, $g_1(-z) = g_1(z)$, $g_2(-z) = -g_2(z)$, and preserve the normalization at any order, $\int_{-\infty}^{\infty} g_j(z)\,dz = \delta_{0,j}$.

In the ultra-relativistic limit, we find $N \to 2\sqrt{T_1 T_2}$ (43) and $f(T_1, T_2, z) \to \sqrt{T_1 T_2} e^{-z}$ (44), so that

$$P(\Delta s_s) = \frac{e^{-|\Delta s_s - s_0|}}{2} \tag{47}$$

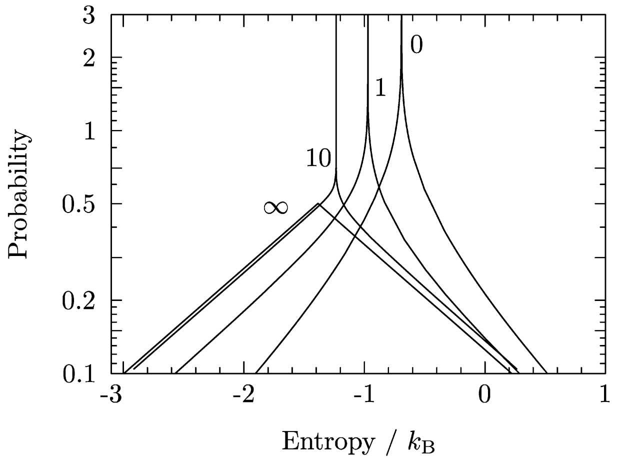

Fig. 3. This plot shows the distribution of system entropy, $P(\Delta s_s)$, as we pass from the non-relativistic regime to the ultra-relativistic regime. The parameter attached to each graph is $k_B\sqrt{T_1T_2}/(mc^2)$ which assumes the values zero (non-relativistic limit), 1, 10 and ∞ (ultra-relativistic limit). As we approach the ultra-relativistic limit, the mean doubles and the spread of fluctuations widens, but does not diverge. The logarithmic peak reduces to a kink. Note that we are discussing the classical relativistic regime. Quantum corrections, depending on the particle spin, are expected when pair creation sets in.

is an exponential distribution. It is only in the ultra-relativistic limit that the logarithmic divergence at s_0 vanishes in favor of a kink (cf. Fig. 3). In the intermediate relativistic regime ($k_BT \approx mc^2$) the distribution $P(\Delta s_s)$ has skewness. The exact distribution (42) is shown for a fixed temperature ratio $T_1 = 4T_2$ as the geometric mean $\sqrt{T_1T_2}$ is increased form zero (non-relativistic limit) to infinity (ultra-relativistic limit) in Fig. 3.

5. Generalizations in the framework of general relativity

The monotonic increase of entropy is a fundamental principle of physics and the universe is known to expand, as was discovered by E. Hubble in 1929. The discussion whether there is a direct connection between these observations has never stopped [3–7]. Therefore we aspire to a formulation of the FT consistent with general relativity, but we restrict ourselves to the class of Friedmann–Lemaître models, which describe a spatially homogenous and isotropic, expanding or contracting universe. The corresponding line element (given by the Robertson–Walker metric) is $-\mathrm{d}t^2 + \mathrm{d}r^2$. The important difference compared to special relativity is that the spatial part, $\mathrm{d}r^2$, is scaled by a time dependent factor $R(t)$ describing the expansion or contraction of the universe:

$$\mathrm{d}r^2 = R^2(t)h_{ij}(\xi)\,\mathrm{d}\xi^i\,\mathrm{d}\xi^j \tag{48}$$

The Latin indices describe spatial components numbered by 1 to 3. We do not have to deal with the details of the metric tensor $\mathbf{h}$ describing the spatial curvature. The result will be valid for all possible geometries. The expansion rate $H(t) = \dot{R}(t)/R(t)$, named the Hubble function, is one of the most important quantities in cosmology and its present value is a direct observable [31]. The typical frame for a cosmic heat bath is the frame of the cosmic microwave background.

5.1. Cosmological fluctuation theorem

In general relativity, the correct equations of motion include the covariant differential $\mathrm{D}p$ of the momentum. (Denoting by p the 4-vector, the components of $\mathrm{D}p$ are $\mathrm{D}p^\alpha = \mathrm{d}p^\alpha + \Gamma^\alpha_{\mu\nu}p^\mu\,\mathrm{d}x^\nu$.) Its spatial components replace the left hand side of (21) and can be split up into a spatially covariant part, ${}^{(3)}\mathrm{D}\mathbf{p}$, and a contribution due to the time-dependent scaling:

$$\mathrm{D}\mathbf{p} = {}^{(3)}\mathrm{D}\mathbf{p} + H(t)\mathbf{p}\,\mathrm{d}t \tag{49}$$

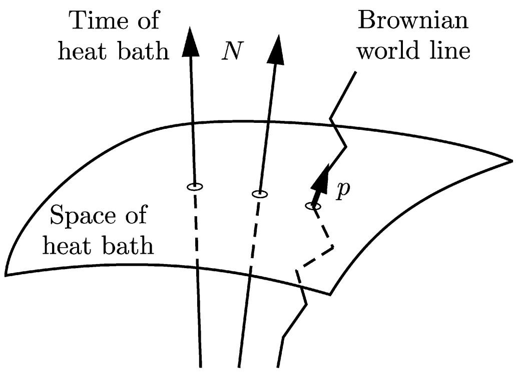

Fig. 4. A sketch of spacetime showing a spatial slice of the heat bath at fixed time and the world line of a Brownian particle in a (locally) expanding universe.

Therefore the covariant Langevin equation, generalizing Eq. (21) to be valid in an expanding or contracting universe of arbitrary spatial geometry, reads

$$^{(3)}\mathrm{D}\mathbf{p} = -\big[\nu(\mathbf{p},t) + H(t)\big]\mathbf{p}\,\mathrm{d}t + {}^{(3)}\mathrm{D}\mathbf{p}_\mathrm{s} \tag{50}$$

Herein, H enters as an additional damping term, which has caused the cooling during the expansion of our universe and is responsible for the cosmological red shift. The distribution of the stochastic impacts $^{(3)}\mathrm{D}\mathbf{p}_\mathrm{s}$ is found after substituting h_{ij} for the Euclidean metric δ_{ij} in (29). Applying the time-reversal map, we find that Eq. (28) gains a second term due to the cosmic expansion:

$$\mathrm{d}s_\mathrm{e} = -\frac{\mathrm{d}E}{T} - \frac{\|\mathbf{p}\|^2}{ET}\,\mathrm{d}\ln R = -\frac{\mathrm{d}E}{T} - H\frac{(\mathbf{p},\mathrm{d}\mathbf{r})}{T} = \mathrm{d}s_\mathrm{e}^{(\text{particle})} + \mathrm{d}s_\mathrm{e}^{(\text{cosmic})} \tag{51}$$

The numerator $(\mathbf{p},\mathrm{d}\mathbf{r})$ in (51) is the canonical line integral (canonical one-form) in phase space. The integral FT (3) extends to an expanding ($H > 0$) or contracting ($H < 0$) spacetime when this second term is taken into account. It has a clear geometric interpretation: the Hubble function is the external curvature of space,

$$\mathrm{D}N = H\,\mathrm{d}\mathbf{r} \tag{52}$$

with N being the time-like normal vector to the space of the heat bath as depicted in Fig. 4. This permits the second term in (51) to be written as

$$\mathrm{d}s_\mathrm{e}^{(\text{cosmic})} = -\frac{(p,\mathrm{D}N)}{T}$$

Since the particle energy $E = p^0 = -p_0 = -(p,N)$ is the zero component of the 4-vector p, the first term in (51) equals the differential

$$\mathrm{d}s_\mathrm{e}^{(\text{particle})} = \frac{\mathrm{d}(p,N)}{T} = \frac{(\mathrm{D}p,N) + (p,\mathrm{D}N)}{T}$$

such that the sum of both terms is

$$\mathrm{d}s_\mathrm{e} = \frac{(\mathrm{D}p,N)}{T} \tag{53}$$

It is natural to think of the numerator $(\mathrm{D}p,N)$ as the heat $\mathrm{d}Q = T\,\mathrm{d}s_\mathrm{e}$ exchanged with the bath, since it is the projection of the exchanged 4-momentum $\mathrm{D}p$ on the local energy component N of the heat bath.

Cosmology is an example for the breaking of the first law, $-\mathrm{d}E = \mathrm{d}(p,N) \neq (\mathrm{D}p,N) = \mathrm{d}Q$, by non-static metrics. So we find ourselves in a remarkable situation: There is no first law in cosmology, while the second law and, furthermore, the integral FT hold.

The isolated cosmological entropy term $\mathrm{d}s_\mathrm{e}^{(\text{cosmic})}$ in (51) would indeed undergo a change of sign if the expansion turned into contraction. However, in the entire bath entropy (53) the geodesic flow N enters as a projection, which does not imply a change of sign if N was to contract. Eventually, a decreasing total entropy $s = s_\mathrm{s} + s_\mathrm{e}$ is always exponentially unlikely as expressed by the integral FT (3).

5.2. Additional theorems for the Einstein–de Sitter universe

So far, we applied the time-reversal transformation to arrive at $\langle e^{-\Delta s}\rangle = 1$. As emphasized at the outset of the general derivation in Section 2, we are free to choose any other transformation from the mathematical point of view. Then the function in the exponent will no longer equal the entropy Δs. For instance, if the system is invariant under the chosen transformation, we will get the trivial result $\langle e^0\rangle = 1$. However, for physically sensible transformations, the FT will remunerate us with non-trivial relations. In order to derive a FT that contains the cosmic expansion rate H, let us choose a local time-reversal transformation, which acts only on the local particle dynamics and leaves the sign of the global cosmic expansion rate H unchanged. Repeating the computation of Section 5.1 with the transformation $\tilde{H} = H$ (local time reversal) instead of $\tilde{H} = -H$ (global time reversal) yields

$$\left\langle e^{-(\Delta s+\Delta h)}\right\rangle = 1, \quad \text{with } \Delta h = \frac{AH}{T} \tag{54}$$

The additional term Δh is proportional to the Hubble constant, the inverse temperature and the action $A = \int((\mathbf{p},\mathbf{v}) - \Delta E)\,dt$ of the energy change $\Delta E = \dot{E}/\nu$.

This demonstrates that the FT is an efficient technique to design relations that include those physical observables, which are most interesting for a given system or experiment. The second general relativistic FT (54) holds in addition to (3). At first glance one might be surprised that there is an infinity of FTs, all constraining the fluctuations of Δs. But since the distribution function $P(\Delta s)$ is a point in the infinite dimensional (Banach) space of integrable functions, there has to be an infinity of physical constraints to determine $P(\Delta s)$ uniquely.

In many interesting stages of the cosmic evolution, such as the early (hypothetical) inflationary phase and the future phase of accelerated expansion, the size of the universe grows exponentially with time so that H is constant. During these periods the cosmic impact on the local relativistic Brownian motion with (49) is time-independent. We can therefore immediately infer from the general derivation in Section 2.2, that for these phases of the cosmic evolution the stronger detailed formulations of the FT hold as well.

5.3. The expanding universe

The cosmological FTs of Sections 5.1 and 5.2 restrict the entropy fluctuations Δs caused by a relativistic particle. In this section we compute the detailed distribution of fluctuations explicitly for evolving cosmic environments.

The entropy change $ds = ds_s + ds_e^{(\text{particle})} + ds_e^{(\text{cosmic})}$ has contributions of the system entropy, $s_s = -\ln P$, and by heat exchange, $ds_e = dQ/T$. Since there is no first law, $dE + dQ \neq 0$, for the time dependent cosmic metric, the heat contribution ds_e splits up in a term due to the change of particle energy, $ds_e^{(\text{particle})} = -dE/T$, and a cosmological term, $ds_e^{(\text{cosmic})} = -p^2 H\,dt/(ET)$, as derived in Eq. (51). The method to compute distributions of fluctuations will be presented for the particle term, $s_e^{(\text{particle})}$, which we abbreviate by s_p. It is straight forward to apply the method to the other terms.

To compute the distribution $P(\Delta s_p, \Delta t)$ of produced entropy Δs_p, we have to sum up $ds_p = -dE/T(t)$ over the observation time Δt. Therefore we have to evolve the process $p(t)$ while book keeping the change of entropy s_p. This is done by extending the Fokker–Planck equation to evolve the joint distribution $P(p, s_p, t)$. The evolution of entropy s_p is directly related to the dynamical variable p by the differential $ds_p = -dE(p)/T(t)$, since relativistic Brownian motion is restricted to the mass-shell (15). The similar evolution of $P(p, E, t)$ is easily determined. One method is to include the Helfand moments $\langle dE\rangle$, $\langle dE^2\rangle$, and $\langle dE\,dp\rangle$ into the probability current (12), from which we find the Fokker–Planck equation $\partial_t P + \partial_p j_p + \partial_E j_E = 0$ for $P(p, E, t)$. The correlation $\langle dE\,dp\rangle$ is important because dE is not independent from dp on the mass-shell. Equivalently, we can proceed using the Fokker–Planck equation $\partial_t P + \partial_p j_p = 0$ for $P(p, t)$ with the current (24) and substitute every differentiation ∂_p by $\partial_p + \frac{\partial E}{\partial p}\partial_E$ so that the probability current is tangential to the mass-shell. After identifying $\partial_{s_e} = -T\partial_E$ (28) we arrive at the Fokker–Planck equation

$$\frac{1}{\nu}\partial_t P = F_0\left(\partial_p - \frac{E'(p)}{T}\partial_{s_p}\right)P = \left[F_0(\partial_p) - F_1(\partial_p)\partial_{s_p} + F_2\cdot\partial_{s_p}^2\right]P \tag{55}$$

for the distribution $P(p, s_p, t)$. The momentum operator is

$$F_0(\partial_p) = \lambda + (\lambda + T/E)p\partial_p + ET\partial_p^2$$

The entropic extensions of the Fokker–Planck equation (55) are

$$F_1(\partial_p) = 1 + \lambda F_2 + 2p\partial_p \quad \text{and} \quad F_2 = p^2/(ET)$$

The function $\lambda(t) = 1 + H(t)/\nu$ contains the cosmic driving by expansion. This function of time is deterministic since we can safely neglect the back reaction of our tiny system on the cosmic evolution. The entropy fluctuations $P(\Delta s_\mathrm{p}, \Delta t)$ follow from (55) when solved for the initial condition

$$P(p, s_\mathrm{p}, t)|_{t=0} = \delta(s_\mathrm{p}) P_0(p) \tag{56}$$

and after integrating out the momentum p:

$$P(\Delta s_\mathrm{p}, \Delta t) = \int_{\mathbb{R}} P(p, \Delta s_\mathrm{p}, \Delta t)\,\mathrm{d}p \tag{57}$$

The Fokker–Planck equation (55) is solved by orthogonal functions. We expand the distribution $P(p, s_\mathrm{p}, t)$ in a series of Hermite polynomials with respect to the entropy dependence, so that the two-dimensional Fokker–Planck (55) for $P(p, s_\mathrm{p}, t)$ reduces to an one-dimensional system for the coefficients $a_k(p, t)$. The coefficients $a_k(p, t)$ are simple linear combinations of the moments $M_l(p, t)$,

$$M_l(p, t) = \int P(p, s_\mathrm{p}, t) s_\mathrm{p}^l \,\mathrm{d}s_\mathrm{p}$$

so that the singular initial condition (56) are represented by $M_0(p, 0) = P_0(p)$ and $M_l(p, 0) = 0$ for all $l > 0$ in a regular way. From (55) follows after integrating by parts a hierarchy of differential equations for the moments $M_l(p, t)$:

$$\frac{1}{\nu}\partial_t M_l = F_0(\partial_p) M_l + l F_1(\partial_p) M_{l-1} + l(l-1) F_2 M_{l-2} \tag{58}$$

The case $l = 0$ reduces to the Fokker–Planck equation for the momentum, $M_0(p, t) \equiv P(p, t)$. Since (58) is a parabolic differential equation, numerical solutions for the $M_l(p, t)$ can be obtained by standard techniques. Integrating p, we have the moments $m_l(\Delta t) = \int M_l(p, \Delta t)\,\mathrm{d}p$ for the distribution of entropy (57). After computing iteratively a sufficient number of moments m_l, the probability distribution for the entropy (57) can be reconstructed by the algorithm presented in Appendix A.

Let us illustrate (57) for a universe undergoing a transient inflation as sketched in the inset of Fig. 5. Such a transition of the scale factor ranging from R_i to R_f according to

$$R(\tau) = \frac{R_\mathrm{i} \mathrm{e}^{-\tau} + R_\mathrm{f} \mathrm{e}^{\tau}}{\mathrm{e}^{-\tau} + \mathrm{e}^{\tau}}$$

is a common toy-model for particle creation in quantum field theory [32]. The peak of the Hubble function shall be $H_{\max}$, so that $\tau = t H_{\max}/I$. The inflation factor is $I = 2(\sqrt{R_\mathrm{f}} - \sqrt{R_\mathrm{i}})/(\sqrt{R_\mathrm{f}} + \sqrt{R_\mathrm{i}})$. Neglecting quantum effects, the thermal heat bath, which may consist of photons or other massless particles, cools proportional to the inverse scale factor [33],

$$T(t) = \frac{T_\mathrm{mean}}{R_\mathrm{i}^{-1} + R_\mathrm{f}^{-1}} \frac{2}{R(t)}$$

We choose the mean temperature T_mean in the relativistic regime, $k_\mathrm{B} T_\mathrm{mean} = 10mc^2$. The universe inflates by the factor $R_\mathrm{f}/R_\mathrm{i} = 2$. The cosmic forcing of the system depends on the ratio of the relaxation rate ν and the expansion rate $H_{\max}$. For the nonequilibrium distribution of the particle entropy Δs_p shown as solid line in Fig. 5 the dimensionless control parameter $H_{\max}/\nu$ equals 100. As reference, the symmetric distribution of the relativistic equilibrium with $H_{\max} = 0$ is plotted in dashed line. When $H_{\max}/\nu$ assumes the values 1, 10 and 100, the width σ_{s_p} of the distribution $P(\Delta s_\mathrm{p})$ increases monotonically, being equal to 1.45, 1.48 and 1.64 respectively. In contrast, the mean ΔS_p is not monotonic and assumes the values 0.68, 0.69 and 0.15 respectively. Five moments have been computed to construct Fig. 5.

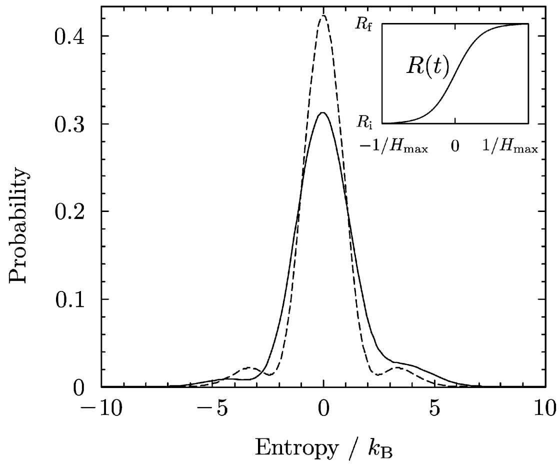

Fig. 5. The distribution of particle entropy Δs_p is shown for a cosmic inflationary phase. The system starts in equilibrium at time $t = -1/\nu$ with temperature T_i, undergoes a period of inflation centered at $t = 0$ (cf. the inset), and equilibrates again until the time $1/\nu$ with the lower bath temperature T_f. The maximum of the Hubble function is $H_{max} = 100\nu$ for the distribution shown in solid line. The case of a static universe with zero mean entropy is plotted in dashed line. This system is described completely by the ratio H_{max}/ν of the cosmic expansion rate and the thermal relaxation rate, the temperature to mass ratio $k_B T_{mean}/(mc^2) = 10$, and the inflation factor $R_f/R_i = 2$.

6. Conclusions

Relativistic FTs have been established that remain valid for high temperatures or low masses, $mc^2 \ll k_B T$. The integral FT, $\langle e^{-\Delta s} \rangle = 1$, was found to hold also in the framework of general relativity as far as the cosmic expansion is concerned.

With the additional FT $\langle e^{-\Delta s - \Delta h} \rangle = 1$ and the numerical example of Section 5.3 we can answer the question raised in the introduction: yes, the cosmic expansion has an influence on the total entropy fluctuations Δs, and the mean values of individual terms such as the particle contribution $\Delta s_e^{(particle)}$ can undergo a change of sign for cosmic contraction. However the relation $\langle e^{-\Delta s} \rangle = 1$ implies the second law, $\Delta S = \langle \Delta s \rangle > 0$, so that for a macroscopic system the sign of ΔS is independent of the cosmological evolution.

On the theoretical road ahead, one may expect integral FTs to hold for arbitrary time-dependent and inhomogeneous fields, such as gravitational waves, when the concise expression (53) is applied. For the process originally introduced in [17], the weaker inequality (1) has been proven recently [34] under general conditions.

Experimentally, the change of the environmental entropy $\Delta s_e = -\Delta E/T$ can be measured by detecting single particles after a sequence of elastic collisions, i.e. collisions without decay or excitation of internal degrees of freedom. Such collisions are observed for heavy quarks (for instance the charm quark) which traverse the expanding quark–gluon plasma created by heavy-ion collisions. Nonequilibrium thermodynamical descriptions are common for these relativistic media [27]. The relativistic FT is not only subject of high energy physics and cosmology. The special-relativistic FT can be tested with a high-precision spectroscopy experiment by shining a laser on an excited granulate of glass or reflecting steal beads, so that the granulate serves as a heat bath and the photons are the ultra-relativistic 'Brownian' particles. The environmental entropy $\Delta s_e = -\Delta E/T$ then follows from the measurement of the frequency shift $\Delta\nu = \Delta E/h$.

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Appendix A. The truncated moment problem

When reconstructing a distribution function we are interested in an efficient algorithm that generates uniquely out of $n \geqslant 2$ given moments m_k a continuous and non-negative function f on the real line, such that

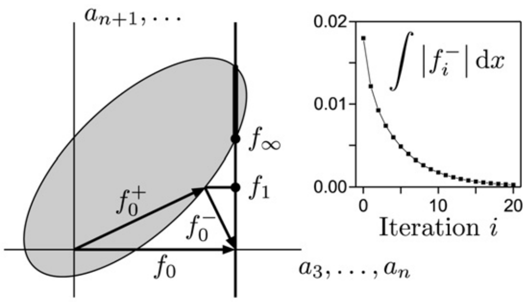

Fig. 6. A sketch of the space spanned by the functions (A.3). The first n coefficients $a_3, \ldots, a_n$ are predetermine by the known moments (vertical line). The higher coefficients $a_{n+1}, \ldots$ are determined iteratively. The shaded region represents the non-linear (convex) space of non-negative functions. The inset shows the rapid convergence of the algorithm.

$$\int_{\mathbb{R}} f(x) x^k \, \mathrm{d}x = m_k \quad \text{for } k \leqslant n, \quad \text{and} \tag{A.1}$$

$$\left| \int_{\mathbb{R}} f(x) H_k \, \mathrm{d}x \right| = \text{minimal} \quad \text{for } k > n \tag{A.2}$$

In (A.2) the Hermite polynomials $H_k(y) = \sum_{l=0}^{k} h_{kl} y^l$ are written in the variable $y = (x - m_1)/\sqrt{2}\sigma$ rescaled by the width $\sigma = \sqrt{m_2 - m_1^2}$. The truncated moment problem (A.1) has to be augmented by the complementary condition (A.2) for uniqueness. Functions solving Eqs. (A.1) are readily given by

$$f(x) = \frac{\mathrm{e}^{-y^2}}{\sqrt{2\pi}\sigma} \left(1 + \sum_{k=3}^{\infty} \frac{a_k}{2^n n!} H_k(y) \right) \tag{A.3}$$

By virtue of the orthogonality of the Hermite polynomials, the first n coefficients

$$a_k = \langle H_k \rangle_f = \int f H_k \, \mathrm{d}x = \sum_{l=0}^{k} h_{kl} m_l$$

are directly determined by the known moments m_l. If one was to truncate the series (A.3) after the n's coefficient, the resulting function f_0 may take negative values. If so, we use this negative part $f_0^- = f_0 \Theta(-f_0)$ of the function $f_0 = f_0^+ + f_0^-$ to determine the higher coefficients to be $a_k = -\langle H_k \rangle_{f_0^-}$ for $k > n$. This yields a new function $f_1 = f_1^+ + f_1^-$ with a smaller negative part f_1^-. Iteratively one approaches the desired solution f_∞ with arbitrary precision (cf. Fig. 6).

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