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Thermodynamic framework for compact q-Gaussian distributions

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HIGHLIGHTS

- A consistent thermodynamic framework is presented for systems of particles interacting repulsively.
- The thermodynamics applies to an entropic form of Tsallis type, s_ν, with $\nu > 1$ ($\nu = 2 - q$).
- A basic requirement concerns a cutoff in the equilibrium distribution $P_{eq}(x)$.
- An effective temperature θ, conjugated to the entropy s_ν, is defined.
- Thermodynamic potentials, Maxwell relations, and response functions are obtained.

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ABSTRACT

Recent works have associated systems of particles, characterized by short-range repulsive interactions and evolving under overdamped motion, to a nonlinear Fokker–Planck equation within the class of nonextensive statistical mechanics, with a nonlinear diffusion contribution whose exponent is given by $\nu = 2 - q$. The particular case $\nu = 2$ applies to interacting vortices in type-II superconductors, whereas $\nu > 2$ covers systems of particles characterized by short-range power-law interactions, where correlations among particles are taken into account. In the former case, several studies presented a consistent thermodynamic framework based on the definition of an effective temperature θ (presenting experimental values much higher than typical room temperatures T, so that thermal noise could be neglected), conjugated to a generalized entropy s_ν (with $\nu = 2$). Herein, the whole thermodynamic scheme is revisited and extended to systems of particles interacting repulsively, through short-ranged potentials, described by an entropy s_ν, with $\nu > 1$, covering the $\nu = 2$ (vortices in type-II superconductors) and $\nu > 2$ (short-range power-law interactions) physical examples. One basic requirement concerns a cutoff in the equilibrium distribution $P_{eq}(x)$, approached due to a confining external harmonic potential, $\phi(x) = \alpha x^2/2$ ($\alpha > 0$). The main results achieved are: (a) The definition of an effective temperature θ conjugated to the entropy s_ν; (b) The construction of a Carnot cycle, whose efficiency is shown to be $\eta = 1 - (\theta_2/\theta_1)$, where θ_1 and θ_2 are the effective temperatures associated with two isothermal transformations, with $\theta_1 > \theta_2$; (c) Thermodynamic potentials, Maxwell relations, and response functions. The

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present thermodynamic framework, for a system of interacting particles under the above-mentioned conditions, and associated to an entropy s_ν, with $\nu > 1$, certainly enlarges the possibility of experimental verifications.

1. Introduction

An appropriate thermodynamic description for a system of interacting particles represents a fundamental intent in physics and may become a great challenge in many cases [1–3]. Depending on the particular type of interactions, the outstanding framework of statistical mechanics may turn intractable, at least from the analytical point of view, in such a way that numerical approaches emerged as important tools in the recent years. The elegant connection between the microscopic world (described by statistical mechanics) and the macroscopic one (described by thermodynamics) occurs usually through the entropy concept, so that the knowledge of the entropy associated to a given system becomes a crucial step in this pathway. Although the standard procedure should be applied for systems at equilibrium, the connection of the entropy concept with dynamics represents a remarkable result of nonequilibrium statistical mechanics [2–4]. The statistical entropy s is defined as a functional depending only on the probabilities of a physical system [2], i.e., $s \equiv s\{P_i(t)\}$, for a discrete set of states, where $P_i(t)$ represents the probability for finding the system in a state i, at time t, while $s \equiv s[P(x, t)]$, for continuous states, where x usually denotes the position in a one-dimensional space. The association with dynamics may occur by means of the following procedures: (i) The statistical entropy may be extremized under certain constraints, in order to yield an equilibrium probability that coincides with the stationary-state distribution obtained from some equations describing the time evolution of the probabilities (e.g., a Fokker–Planck equation [5]); (ii) An H-theorem, which may be proven by considering the statistical entropy and a given equation for the time evolution of the probabilities [2–5].

These connections among entropies and dynamics were extended for generalized entropic forms, mostly by making use of nonlinear Fokker–Planck equations (NLFPEs) [6]; a typical NLFPE, relevant for the present work, is given by

$$\mu \frac{\partial P(x,t)}{\partial t} = -\frac{\partial [A(x)P(x,t)]}{\partial x} + \nu D \frac{\partial}{\partial x}\left\{[\lambda P(x,t)]^{\nu-1}\frac{\partial P(x,t)}{\partial x}\right\} + kT\,\frac{\partial^2 P(x,t)}{\partial x^2}\,, \tag{1.1}$$

where μ stands for a friction coefficient, ν a real number, and λ represents a characteristic length of the system. One should notice that, due to the normalization condition, the probability $P(x, t)$ presents dimension $[\text{length}]^{-1}$ and consequently, the characteristic length λ was introduced in the nonlinear diffusion term for dimensional reasons. Moreover, the diffusion constant D may result from a coarse-graining procedure (see, e.g., Refs. [7–9]), being directly related to particle–particle interactions, thus depending on the physical system under investigation. The above equation also takes into account the effects of a heat-bath at a temperature T (with k standing for the Boltzmann constant), whose contribution may be obtained in the standard way, through the introduction of a thermal noise in the system [3]. Additionally, $A(x) = -d\phi(x)/dx$ corresponds to an external force derived from a confining potential $\phi(x)$, being fundamental for the approach to equilibrium, as well as for the resulting form of the probability distribution in the long-time limit. The particular case $\nu = 2$ has been much explored recently, being shown to be directly related to a system of interacting vortices, relevant for type-II superconductors [7–17]; in this application, λ represents the London penetration length, and it was shown that $D \gg kT$, so that thermal effects could be neglected [12]. Herein, we will be concerned with physical systems for which this approximation applies, leading to,

$$\mu \frac{\partial P(x,t)}{\partial t} = -\frac{\partial [A(x)P(x,t)]}{\partial x} + \nu D \frac{\partial}{\partial x}\left\{[\lambda P(x,t)]^{\nu-1}\frac{\partial P(x,t)}{\partial x}\right\}\,, \tag{1.2}$$

corresponding to the NLFPE introduced in Refs. [18,19], being associated with Tsallis entropy [20], through the identification $\nu = 2 - q$, where q represents the well-known entropic index. The above equation became an useful tool for dealing with a wide range of natural phenomena, like those related to anomalous diffusion [21–23].

Generalized forms of the H-theorem, making use of NLFPEs, were developed by many authors in the recent years [24–34]; particularly, the NLFPE in Eq. (1.2) was shown to be associated to Tsallis' entropy,

$$s_\nu[P] = \frac{k}{\nu - 1}\left\{1 - \lambda^{\nu-1}\int_{-\infty}^{\infty} dx\,[P(x,t)]^\nu\right\}\,, \tag{1.3}$$

through a well-defined sign for the time derivative of the free-energy functional, i.e., $(df/dt) \leq 0$, where

$$f[P] = u[P] - \theta s_\nu[P]\,; \qquad u[P] = \int_{-\infty}^{\infty} dx\,\phi(x)P(x,t)\,. \tag{1.4}$$

It is important to remind that the characteristic length λ appearing in Eq. (1.3) follows from an H-theorem [proven by making use of Eq. (1.2)] and it leads to the correct dimension for the entropy. Moreover, the time-dependent solution of Eq. (1.2), for