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Statistical mechanics of phase–space curves

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ABSTRACT

We study the classical statistical mechanics of a phase–space curve. This unveils a mechanism that, via the associated entropic force, provides us with a simple realization of effects such as confinement, hard core, and asymptotic freedom. Additionally, we obtain negative specific heats, a distinctive feature of self-gravitating systems, and negative pressures, typical of dark energy.

1. Introduction

We will study here the classical statistical mechanics of arbitrary phase–space curves Γ and unveil some interesting effects, like confinement and hard-cores. Recall that by confinement one understands the physics phenomenon that impedes isolation of color charged particles (such as quarks), that cannot be isolated singularly. Therefore, they cannot be directly observed. In turn, asymptotic freedom is a property of some gauge theories that causes bonds between particles to become asymptotically weaker as distance decreases. Finally, in the case of a "hard core" repulsive model, each particle (usually molecules, atoms, or nucleons) consists of a hard core with an infinite repulsive potential.

Our curve-analysis will provide, in classical fashion, a simple entropic mechanism for these three phenomena. The so-called entropic force is a *phenomenological* one arising from some systems' statistical tendency to increase their entropy [1–5]. No appeal is made to any particular underlying microscopic interaction. The text-book example is the elasticity of a freely-jointed polymer molecule (see, for instance, Refs. [1,2] and references therein). However, Verlinde has argued that gravity can also be understood as an entropic force [3]. The same applies for the Coulomb force [6], etc. For instance, we have an exact solution for the static force between two black holes at the turning points in their binary motion [7] or investigations concerning the entanglement entropy of two black holes and an associated entanglement entropic force [8]. A causal path entropy (causal entropic forces) has been recently appealed to for links between intelligence and entropy [4].

Here we appeal to an extremely simple model to show that confinement can be shown to arise from entropic forces. Our model involves a quadratic Hamiltonian in phase–space.

Quadratic Hamiltonians are well known both in classical mechanics and in quantum mechanics. In particular, for them the correspondence between classical and quantum mechanics is exact. However, explicit formulas are not always trivial. Moreover, a good knowledge of quadratic Hamiltonians is useful in the study of more general quantum Hamiltonians (and

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their associated Schroedinger equations) for the semiclassical regime. Quadratic Hamiltonians are also important in partial differential equations, because they give non trivial examples of wave propagation phenomena. Quadratic Hamiltonians are also of utility because they help to understand properties of more complicated Hamiltonians used in quantum theory.

We wish here to appeal to quadratic Hamiltonians in a classical context in order to discern whether some interesting features are revealed concerning the entropic force along phase–space curves. We will see that the answer is in the affirmative.

2. Preliminaries

We consider a typical, harmonic oscillator-like Hamiltonian in thermal contact with a heat-bath at the inverse temperature β, that will be kept constant throughout:

$$H(p,q) = p^2 + q^2, \tag{1}$$

where p and q have the same dimensions (natural units, those of H, obviously; we wish to avoid dealing with a tensor g_{ij}).

The corresponding partition function is given by Refs. [9–11]

$$\begin{aligned} Z(\beta) &= \int_{-\infty}^{\infty} \mathrm{e}^{-\beta H(p,q)} \mathrm{d}p\mathrm{d}q \\ &= \pi \int_0^{\infty} \mathrm{e}^{-\beta U}\, \mathrm{d}U = \frac{\pi}{\beta}, \end{aligned} \tag{2}$$

where we employ the fact that the total microscopic energy is

$$U = p^2 + q^2 \tag{3}$$

and then we make the change of variable $p = \sqrt{U - q^2}$. Evaluating the resulting integral, first in the variable q and then in the variable U, we have for the mean value of the energy

$$\begin{aligned} \langle U(p,q)\rangle(\beta) &= \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} H(p,q) \mathrm{e}^{-\beta H(p,q)}\, \mathrm{d}p\mathrm{d}q \\ &= \frac{\pi}{Z(\beta)} \int_0^{\infty} U \mathrm{e}^{-\beta U}\, \mathrm{d}U = \frac{\pi}{\beta^2 Z(\beta)}, \end{aligned} \tag{4}$$

and for the entropy

$$\begin{aligned} S(\beta) &= \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} [\ln Z(\beta) + \beta H(p,q)] \mathrm{e}^{-\beta H(p,q)}\, \mathrm{d}p\mathrm{d}q \\ &= \frac{\pi}{Z(\beta)} \int_0^{\infty} \{\ln[Z(\beta)] + \beta U\} \mathrm{e}^{-\beta U}\, \mathrm{d}U = \frac{\pi}{\beta Z(\beta)} \{\ln[Z(\beta)] + 1\}. \end{aligned} \tag{5}$$

Note that the integrands appearing in (2), (4) and (5) are exact differentials.

3. Path entropy

Remember that we are in contact with a reservoir at the fixed inverse temperature β.

Path entropies (phase space curves) have been discussed recently in Refs. [4,5], for instance. We will be concerned here with a *related but not identical notion* and deal with a particle moving in phase space, focusing attention on its entropy evaluated as it moves along some phase space path Γ that starts at the origin and ends at some arbitrary point $(p_o(q_o), q_o)$. The path Γ is thus parameterized by the phase–space variable q. The usefulness of such a construct will become evident in the forthcoming sections. Also, as we will show below, some of the associated paths are adiabatic.

Accordingly, our purpose in this section is to define the thermodynamic variables of Section 2 *on these phase–space curves* Γ. It will be shown that this endeavor is useful. Remark that all our calculations here are of a microscopic character. No macrostates are to be dealt with at all! Thus, generalizing the exact differentials–integrands (2), (4) and (5) to curves Γ, we define the following.

- The partition function as a function of β and of a curve Γ

$$Z(\beta, \Gamma) = \pi \int_{\Gamma} \mathrm{e}^{-\beta U(p,q)}\, \mathrm{d}U(p,q). \tag{6}$$

- The mean energy as

$$\langle U(p,q)\rangle(\beta, \Gamma) = \frac{\pi}{Z(\beta,\Gamma)} \int_{\Gamma} U(p,q) \mathrm{e}^{-\beta U(p,q)}\, \mathrm{d}U(p,q). \tag{7}$$

- Our path entropy is defined according to

$$S(\beta, \Gamma) = \frac{\pi}{Z(\beta, \Gamma)} \int_{\Gamma} \{\ln[Z(\beta, \Gamma)] + U(p, q)\} e^{-\beta U(p,q)} \, dU(p, q). \tag{8}$$

We consider curves, parameterized as a function of the independent variable q, passing through the origin, for which we have $p(0) = 0$ and $q = 0$ and, as a consequence, at any temperature $U(0, 0) = 0$. This can always be the case after an adequate coordinate-change. Moreover, if we take into account that (i) the integrands are exact differentials and (ii) the integrals are independent of the curve's shape and only depend on their end-points q_0, we have the following.

(1) For the partition function

$$Z(\beta, q_0) = \pi \int_0^{q_0} e^{-\beta U[p(q),q]} \, dU[p(q), q]$$

and evaluating the integral

$$Z(\beta, q_0) = \frac{\pi}{\beta}\{1 - e^{-\beta U[p(q_0),q_0]}\}. \tag{9}$$

(2) For the mean value of the energy

$$\langle U(p, q)\rangle(\beta, q_0) = \frac{\pi}{Z(\beta, q_0)} \int_0^{q_0} U[p(q), q] e^{-\beta U[p(q),q]} \, dU[p(q), q], \tag{10}$$

which gives

$$\langle U(p, q)\rangle(\beta, q_0) = -\frac{\pi}{\beta Z(\beta, q_0)} U[p(q_0), q_0] e^{-\beta U[p(q_0),q_0]} + \frac{\pi}{\beta^2 Z(\beta, q_0)}\{1 - e^{-\beta U[p(q_0),q_0]}\}. \tag{11}$$

(3) For the entropy

$$S = \frac{\pi}{Z(\beta, q_0)} \int_0^{q_0} \{\ln Z(\beta, q_0) + U[p(q), q]\} e^{-\beta U[p(q),q]} \, dU[p(q), q], \tag{12}$$

the result of which is

$$\begin{aligned} S(\beta, q_0) = {} & \frac{\pi}{\beta Z(\beta, q_0)} \left\{1 - e^{-\beta U[p(q_0),q_0]}\right\} \ln[Z(\beta, q_0)] \\ & - \frac{\pi}{Z(\beta, q_0)} U[p(q_0), q_0] e^{-\beta U[p(q_0),q_0]} + \frac{\pi}{\beta Z(\beta, q_0)} \left\{1 - e^{-\beta U[p(q_0),q_0]}\right\}. \end{aligned} \tag{13}$$

Note that when $q_0 \to \infty$ (9), (11) and (13) reduce to (2), (4) and (5), respectively. Note again that the integrands in (9), (11) and (13) are *exact differentials*. As a consequence these integrals become independent of the path Γ. If one redefines the coordinate-system in such a way that the starting point of Γ coincides with the origin, their values will depend only on the end-point q_0 of the path. Thus, they are functions of the microscopic state (at least for the HO-Hamiltonian, at this stage). We can refer to the entropy and the mean energy evaluated above as *microscopic thermodynamic potentials* (for the HO). Remember that we are in contact with a reservoir at the fixed inverse temperature β.

The simplest possible path-forms are straight lines connecting the origin with $(p_o(q_o), q_o)$.

4. Equipartition

In order to ascertain that our thermodynamics along phase–space curves does make physical sense we look now for an equipartition theorem. We encounter that

$$\langle q^2\rangle = \int_{-\infty}^{\infty} \frac{q^2}{Z} e^{-\beta(p^2+q^2)} \, dp \, dq = \frac{\pi}{2Z} \int_0^{\infty} U e^{-\beta U} \, dU, \tag{14}$$

i.e., along the curve Γ

$$\begin{aligned} \langle q^2\rangle(\beta, \Gamma) &= \frac{\pi}{2Z} \int_{\Gamma} U e^{-\beta U} \, dU = \frac{\pi}{2Z} \int_0^{q_0} U e^{-\beta U} \, dU \\ &= \langle q^2\rangle(\beta, q_0) = -\frac{\pi}{2\beta Z(\beta, q_0)} U[p(q_0), q_0] e^{-\beta U[p(q_0),q_0]} \\ &\quad + \frac{\pi}{2\beta^2 Z(\beta, q_0)}\{1 - e^{-\beta U[p(q_0),q_0]}\} = \frac{\langle U\rangle(\beta, q_0)}{2}, \end{aligned} \tag{15}$$

that is,

$$\langle q^2\rangle(\beta, q_0) = \langle p^2\rangle(\beta, q_0) = \frac{\langle U\rangle(\beta, q_0)}{2} \tag{16}$$

which, for $q_0 \to \infty$, gives

$$\langle q^2\rangle = \langle p^2\rangle = \frac{\langle U\rangle}{2} = \frac{1}{2\beta}, \tag{17}$$

that is, classical equipartition.

5. Adiabatic paths

An adiabatic path is one such that $S =$ constant along it. Simplifying (13) we obtain

$$S(\beta, q_0) = \ln\left\{\frac{\pi}{\beta}\left[1 - \mathrm{e}^{-\beta U[p(q_0), q_0]}\right]\right\} - \frac{\beta U[p(q_0), q_0]\mathrm{e}^{-\beta U[p(q_0), q_0]}}{1 - \mathrm{e}^{-\beta U[p(q_0), q_0]}} + 1. \tag{18}$$

The condition $S =$ constant translates into

$$\beta = C_1 \quad U[p(q_0), q_0] = C_2, \quad \text{independently of } q_0. \tag{19}$$

$C_1 = \beta$ is constant by the very reservoir notion. For the curve $p = f(q)$ this entails, for our Hamiltonian, that

$$p^2 + q^2 = (p + \delta p)^2 + (q + \delta q)^2, \tag{20}$$

i.e.,

$$p\delta p = -q\delta q. \tag{21}$$

For the curve $p = f(q)$ one has $p\delta p = pf'(q)\delta q$ and

$$f(q)f'(q) = -q \tag{22}$$

is the equation that yields an adiabatic path $f(q)$ (indeed, an infinite family of paths since an integration constant C will emerge in solving the pertinent equation). The solution of (22) is obtained after transforming it into

$$\frac{\mathrm{d}f^2}{\mathrm{d}q} = -2q,$$

$$f(q)^2 = -q^2 + C \to p^2 + q^2 = C, \tag{23}$$

which is intuitively obvious. We may dare to conjecture that for any Hamiltonian of the form $H = g_1(q) + g_2(q)$ the end points of the adiabatic paths might be of the form $g_1(q) + g_2(q) = constant$.

A slightly different question is that of finding two straight-line paths (passing trough the origin) with the same entropy. They are found as follows:

$$p(q) = aq, \tag{24}$$

so that we should have, for two different lines,

$$U = (a^2 + 1)q_0^2 = (a'^2 + 1)q_0'^2. \tag{25}$$

If we take

$$a' < a$$

and

$$q_0' = \sqrt{\frac{a^2 + 1}{a'^2 + 1}}q_0, \tag{26}$$

then

$$\Delta S = S(\beta, a', q_0') - S(\beta, a, q_0) = 0. \tag{27}$$

If the evolution of the system starts from the line $p = aq$, ends in the line $p = a'q'$, and crosses all the space between the two lines then, whenever (19) is satisfied, the evolution is adiabatic.

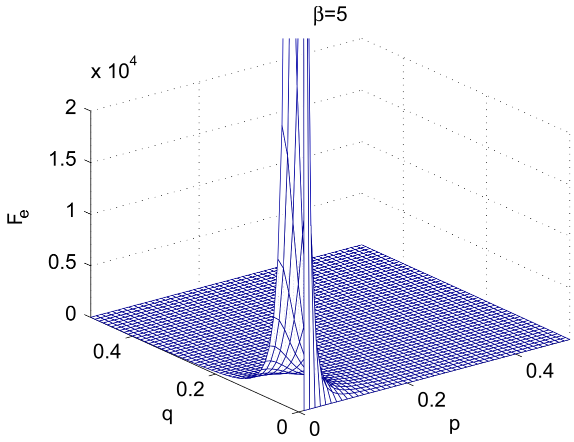

Fig. 1. Arbitrary curves on phase–space. Entropic force versus q, p for $\beta = 5$ (low temperature). Note the hard-core barrier and the vanishing of the force in a neighborhood of the origin.

6. Entropic force

We arrive here at our main theme. According to (18), the entropic force is given by Eq. 3.3 of Ref. [3] which reads $F_e \mathrm{d}x = T\mathrm{d}S$. In our case this translates as

$$F_e \mathrm{d}q = \frac{1}{\beta}\frac{\partial S}{\partial q}\mathrm{d}q, \tag{28}$$

and

$$F_e = \beta U \frac{\partial U[p(q), q]}{\partial q} \mathrm{e}^{-\beta U} \frac{2 - \mathrm{e}^{-\beta U}}{(1 - \mathrm{e}^{\beta U})^2} \tag{29}$$

where the trajectory's end-point is free to move in phase–space. For $\beta U \ll 1$, Eq. (29) simplifies to

$$F_e = \frac{\partial U[p(q), q]}{\partial q}\left\{\frac{1}{\beta U[p(q), q]} - \beta U[p(q), q]\right\} \tag{30}$$

or

$$F_e = 2q\left\{\frac{1}{\beta U[p(q), q]} - \beta U[p(q), q]\right\} \sim 2q\frac{1}{\beta U[p(q), q]}. \tag{31}$$

Thus, there is a strong repulsion; actually, a hard core at $q = 0$. We are dealing with a particle attached via a spring to the origin, that cannot be reached due to the entropic force.

7. Entropic force on arbitrary phase–space curves

More generally, for $U = p^2 + q^2$ one has

$$F_e = 2q\beta(p^2 + q^2)\mathrm{e}^{-\beta(p^2+q^2)}\frac{2 - \mathrm{e}^{-\beta(p^2+q^2)}}{[1 - \mathrm{e}^{\beta(p^2+q^2)}]^2}. \tag{32}$$

We present 3-dimensional plots and F_e-level curves for three temperature regimes, namely,

- low temperatures, $\beta = 5$ (Figs. 1–2),
- intermediate temperatures, $\beta = 1$ (Figs. 3–4),
- high temperatures, $\beta = 0.2$ (Figs. 5–6).

We see that there is an infinitely repulsive barrier (hard core) near (but not at) the origin. In the immediate vicinity of the origin the force vanishes. It also tends to zero at long distances from the hard core. The conjunction between these facts yields both confinement and asymptotic freedom via a simple classical mechanism.

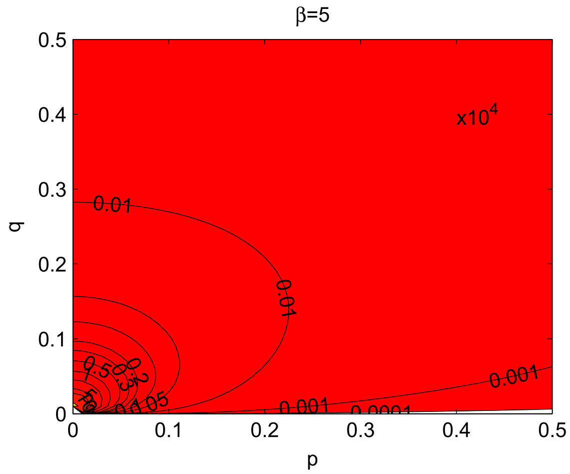

Fig. 2. Arbitrary curves on phase–space. Level F_e-curves in the q–p plane (low temperature, $\beta = 5$).

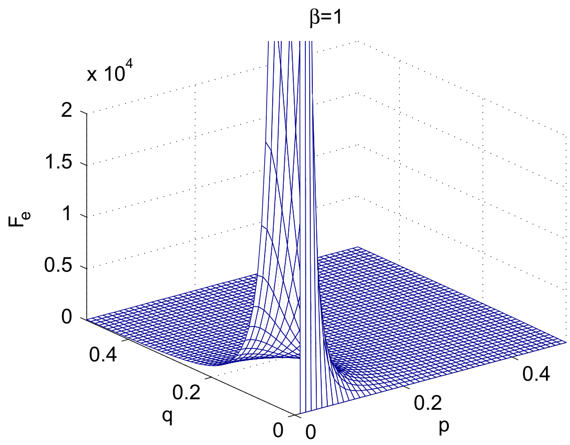

Fig. 3. Arbitrary curves on phase–space. Entropic force versus q, p for $\beta = 1$ (intermediate temperature). Note the hard-core barrier and the vanishing of the force in a neighborhood of the origin.

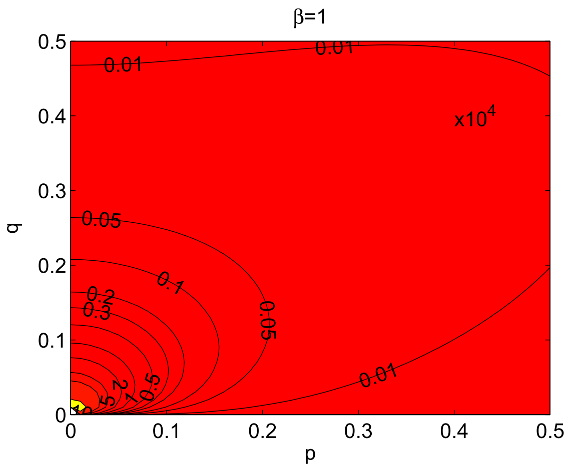

Fig. 4. Arbitrary curves on phase–space. Level F_e-curves in the q–p plane (intermediate temperature, $\beta = 1$).

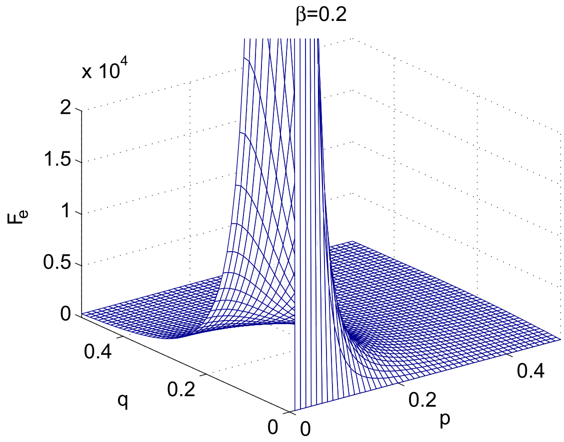

Fig. 5. Arbitrary curves on phase–space. Entropic force versus q, p for $\beta = 0.2$ (high temperature). Note the hard-core barrier, and the vanishing of the force at the origin.

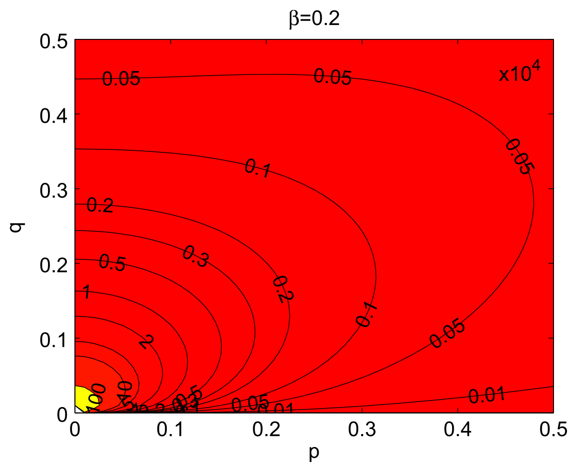

Fig. 6. Arbitrary curves on phase–space. Level F_e-curves in the q–p plane for $\beta = 0.2$ (high temperature).

8. The total well that our particle feels

Of course, our particle not only feels the F_e-influence but also that of the negative gradient of the HO potential. Thus, it is affected by a total force $F_{Tot} = F_e + F_{HO}$. The pertinent expression is

$$F_T = q[1 + 3\beta(p^2 + q^2) - e^{-\beta(p^2+q^2)} - 2\beta(p^2 + q^2)e^{-\beta(p^2+q^2)}]\frac{e^{-\beta(p^2+q^2)}}{[1 - e^{-\beta(p^2+q^2)}]^2}, \tag{33}$$

where

$$F_{HO} = q[1 - \beta(p^2 + q^2) - e^{-\beta(p^2+q^2)}]\frac{e^{-\beta(p^2+q^2)}}{[1 - e^{-\beta(p^2+q^2)}]^2}. \tag{34}$$

We plot this total force for, respectively, $\beta = 0.2$, 1.0, and 5.0 in Figs. 7–9. It is seen that the essential features described in the preceding section do not suffer any appreciable qualitative change.

9. Clausius relation and specific heat

Let us now consider, for infinitesimal work dW generated by a change dq_0 in the end-point of our path Γ,

$$d\langle U\rangle = T dS - dW,$$

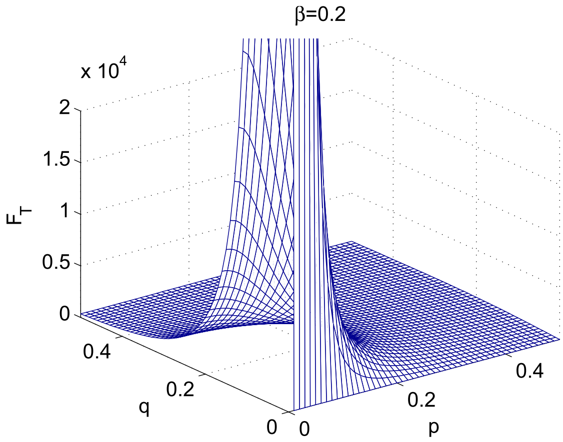

Fig. 7. Total force F_T for $\beta = 0.2$.

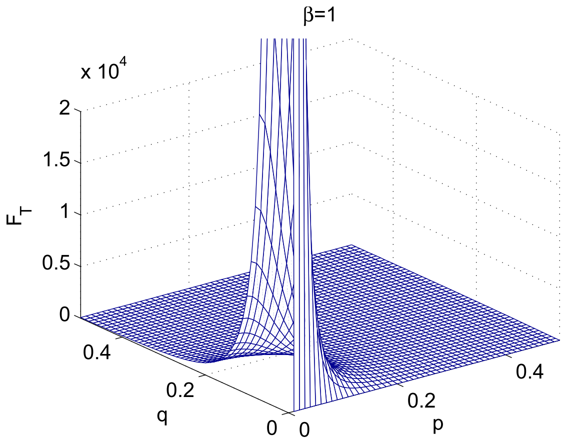

Fig. 8. Total force F_T for $\beta = 1.0$.

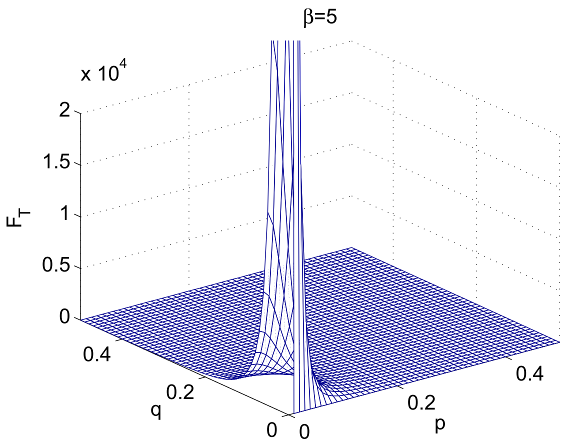

Fig. 9. Total force F_T for $\beta = 5.0$.

where dW is the microscopical mechanical work (no macrostates in this paper!) done ON the system if d$q_0 < 0$ [12]. In one dimension, the pressure reduces, of course, to a force. One obtains

$$\mathrm{d}W = \frac{\mathrm{e}^{-\beta U[p(q),q]}}{1 - \mathrm{e}^{-\beta U[p(q),q]}}, \tag{35}$$

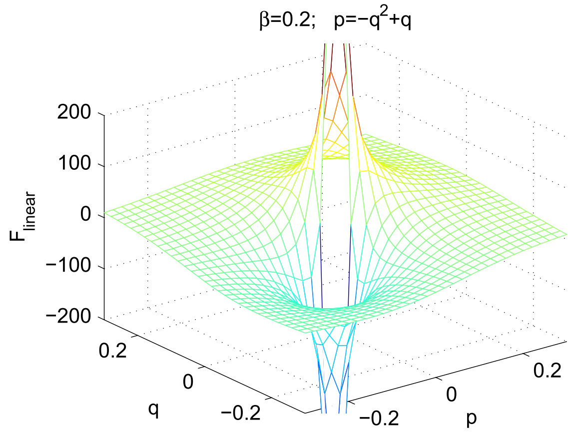

Fig. 10. An example of the linear force F_L's behavior for $\beta = 0.2$.

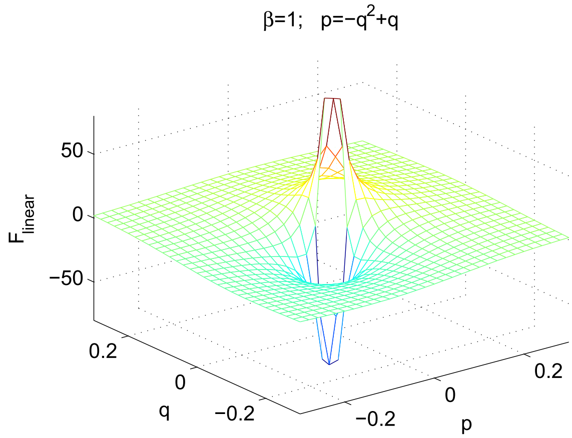

Fig. 11. An example of the linear force F_L's behavior for $\beta = 1.0$.

and, according to

$$dW = F dq,$$

for the linear force (pressure in one dimension) F_{linear} we see that it is Γ-dependent and given by

$$F_{linear}(\Gamma) = \frac{e^{-\beta(p^2+q^2)}\left(2p\frac{dp}{dq} + 2q\right)}{1 - e^{-\beta(p^2+q^2)}}, \tag{36}$$

which, we insist, depends on the curve Γ (remember that p and q possess common dimensionality (see Eq. (28))). Figs. 10–12 depict F_{linear} for, respectively, $\beta = 0.2$, 1, and 5, with Γ being given by $p = -q^2 + q$. The force vanishes almost everywhere. There is a clear transition near the hard core and, significantly enough, it becomes negative on one side of it.

Now, negative pressures (linear force in our case) are a distinctive property of dark energy, a hypothetical form of energy that permeates all of space and tends to accelerate the expansion of the universe [13]. Indeed, it constitutes the most accepted hypothesis to explain observations dating from the 1990s that indicate that the universe is expanding at an accelerating rate. Thus, dark energy may be described as a fluid with negative pressure. We say that this negative pressure counteracts gravity and accelerates the expansion of the universe. Now consider, for example, a star. Gravity contracts the star, but positive (thermal) pressure counteracts the collapse. Note here that, independently from its actual nature, dark energy would need to have a strong negative pressure (acting repulsively) in order to explain the observed acceleration in the expansion rate of the universe. According to General Relativity, the pressure within a substance contributes to its gravitational attraction for other things just as its mass density does. This happens because the physical quantity that causes matter to generate gravitational effects is the stress–energy tensor, which contains both the energy (or matter) density of a substance and its pressure and viscosity.

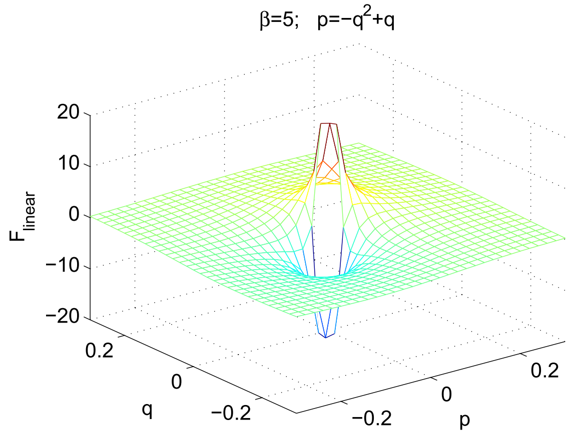

Fig. 12. An example of the linear force F_L's behavior for $\beta = 5.0$.

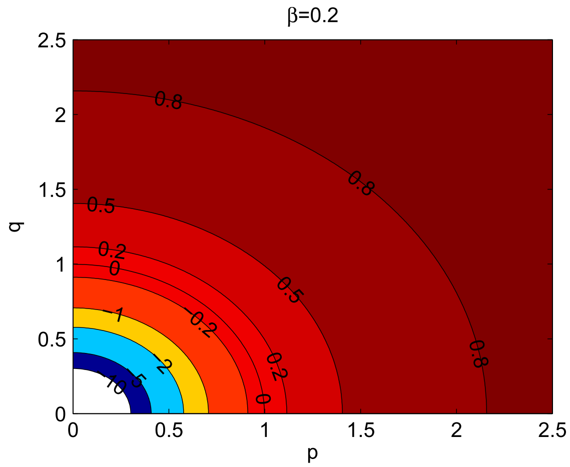

Fig. 13. Specific heat. Level C-curves in the q–p plane for $\beta = 0.2$ (high temperature).

Finally, the *specific heat*, that is, the derivative of the mean energy with respect to the temperature at constant volume, is easily seen to be ($k =$ Boltzmann's constant)

$$C = k\left\{1 - \frac{\beta^2(p^2+q^2)e^{-\beta(p^2+q^2)}}{\left[1-e^{-\beta(p^2+q^2)}\right]^2}\right\}, \tag{37}$$

independently of the curve Γ. Figs. 13–15 depict C for, respectively, $\beta = 0.2$, 1, and 5. The hard core generates a phase transition. The specific heat changes sign and becomes negative near it, and drops rapidly near the origin. Negative specific heat is perhaps the most distinctive thermodynamic feature of self-gravitating systems [14]. Here, our entropic discourse establishes thereby contact with Verlinde's work [3]. In Fig. 16 we plot C/k versus U for several values of β in order to better appreciate the change of sign mentioned above.

10. Discussion

We were dealing with a particle attached to the origin by a spring and considered entropic-force effects. Although we focused attention upon arbitrary phase space curves Γ, most of our effects were independent of the specific path Γ. Our statistical mechanics-along-curves concept is seen to make sense because the equipartition theorem is valid for it.

We considered the entropic construct of Eq. (7) and we saw that the equipartition theorem holds. From Figs. 1–6 we gather that the entropic force diverges at short distances from the origin (hard-core effect), but vanishes both just there and at infinity, so that, with some abuse of language, one may speak of "asymptotic freedom". The entropic force is repulsive. As stated above, at long distances from the origin the entropic force tends to vanish. The negative specific heat we encounter near the hard core links our work to that of Verlinde [3].

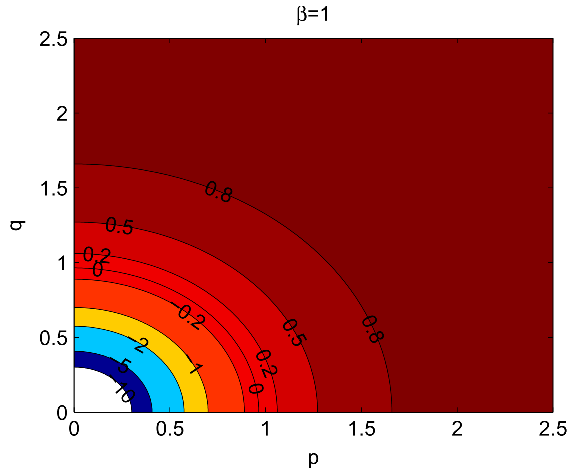

Fig. 14. Level C-curves in the q–p plane for $\beta = 1.0$ (intermediate temperature).

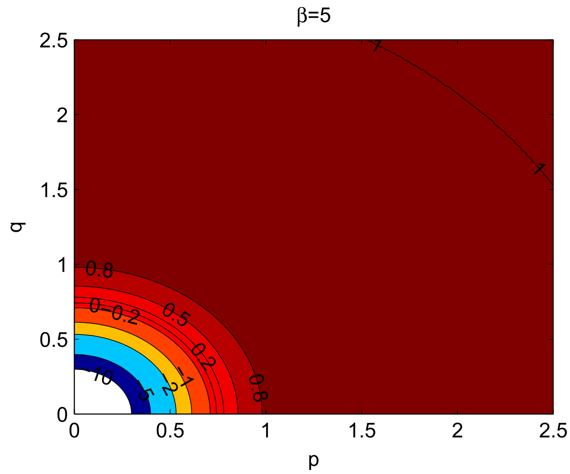

Fig. 15. Level C-curves in the q–p plane for $\beta = 5.0$ (low temperature).

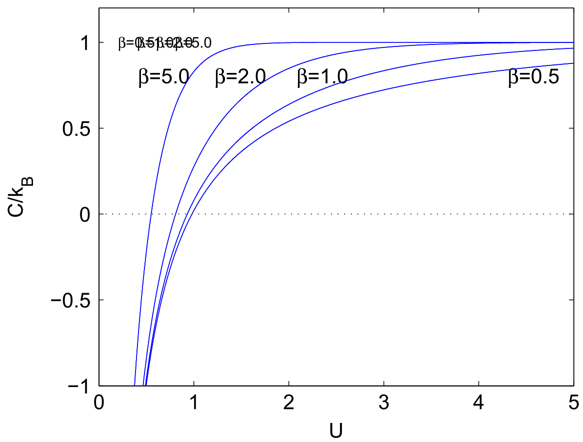

Fig. 16. C/k versus U for $\beta = 0.5, 1.0, 2.0$, and 5.0. See the change of sign of the specific heat.

Entropic confinement is the most remarkable effect that our classical entropic force-model exhibits. Independently of whether our model is realistic or not, it does provide a classical confinement mechanism. The present considerations should encourage non-classical explorations regarding the entropic force.

Finally, when we couple the entropic force effects with those of the HO-potential we are not able to discern significant new features. We have presented here somewhat counter-intuitive results. Further work should try to incorporate the interesting entropic notions developed by Sadhukhan and Bhattacharjee in Ref. [15]. Further work will be extended to other types of curves with different dependences $p(q)$.

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