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.

KEYWORDS: Phase-space curves, Entropic force, Confinement, Hard
core, Asymptotic freedom, Self-gravitating systems.
1 Introduction

We will study here the classical statistical mechanics of arbitrary phase-space curves $\Gamma$ and unveil some interesting effects, like confinement and hard-cores. Remind 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 curves-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 $[1, 2, 3, 4, 8]$. 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, $[1, 2]$ and references therein). However, Verlinde has argued that gravity can also be understood as an entropic force $[3]$. Same for the Coulomb force $[5]$, etc. For instance, we have an exact solution for the static force between two black holes at the turning points in their binary motion $[6]$ or investigations concerning the entanglement entropy of two black holes and an associated entanglement entropic force $[7]$. 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 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 interesting 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 $\beta$.

$$H(p, q) = p^2 + q^2,$$

where $p$ and $q$ have the same dimensions (that of $H$, obviously). The corresponding partition function is given by [9][10][11]

$$Z(\beta) = \int_{-\infty}^{\infty} e^{-\beta H(p,q)} \, dpdq =$$

$$\pi \int_{0}^{\infty} e^{-\beta U} \, dU = \frac{\pi}{\beta}, \quad (2.2)$$

where we employ the fact that

$$U = p^2 + q^2,$$

and then we use $U$ as a radial coordinate $U = R^2$, integrate over the angle, and set $dU = 2RdR$. For the mean value of the energy we have

$$< U(p, q) > (\beta) = \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} H(p, q)e^{-\beta H(p,q)} \, dpdq =$$

$$\frac{\pi}{Z(\beta)} \int_{0}^{\infty} Ue^{-\beta U} \, dU = \frac{\pi}{\beta^2 Z(\beta)}.$$
and for the entropy

\[
S(\beta) = \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} \left[ \ln Z(\beta) + \beta H(p, q) \right] e^{-\beta H(p, q)} \, dpdq =
\]

\[
\frac{\pi}{Z(\beta)} \int_{0}^{\infty} \{ \ln[Z(\beta)] + \beta U \} e^{-\beta U} \, dU = \frac{\pi}{\beta Z(\beta)} \{ \ln[Z(\beta)] + 1 \} \quad (2.5)
\]

Note that the integrands appearing in (2.2), (2.4), and (2.5) are exact differentials.

3 Path Entropy

Path entropies (phase space curves) have been discussed recently in Ref. [4, 8], 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 \(\Gamma\). The usefulness of such 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 phase-space curves. It will be shown that this endeavor is useful. Thus, generalizing (2.2), (2.4), and (2.5) to curves \(\Gamma\), we define

- The partition function as a function of \(\beta\) and of a curve \(\Gamma\)

\[
Z(\beta, \Gamma) = \pi \int_{\Gamma} e^{-\beta U(p, q)} \, dU(p, q). \quad (3.1)
\]

- The mean energy as

\[
<U(p, q)>(\beta, \Gamma) = \frac{\pi}{Z(\beta, \Gamma)} \int_{\Gamma} U(p, q) e^{-\beta U(p, q)} \, dU(p, q). \quad (3.2)
\]
• Our path entropy is defined according to

\[
S(\beta, \Gamma) = \frac{\pi}{Z(\beta, \Gamma)} \int \{\ln[Z(\beta, \Gamma)] + U(p, q)\} e^{-\beta U(p, q)} \, dU(p, q). \tag{3.3}
\]

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 \( U(0, 0) = 0 \). This can always be the case after an adequate coordinates-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

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

\[
Z(\beta, q_0) = \frac{\pi}{\beta} \left\{ 1 - e^{-\beta U[p(q_0), q_0]} \right\}. \tag{3.4}
\]

2) For the mean value of the energy

\[
<U(p, q) > (\beta, q_0) = \frac{\pi}{Z(\beta, q_0)} \int_0^{q_0} U[p(q), q] e^{-\beta U[p(q), q]} \, dU[p(q), q], \tag{3.5}
\]

which gives

\[
<U(p, q) > (\beta, q_0) = -\frac{\pi}{\beta Z(\beta, q_0)} U[p(q_0), q_0] e^{-\beta U[p(q_0), q_0]} + \frac{\pi}{\beta^2 Z(\beta, q_0)} \left\{ 1 - e^{-\beta U[p(q_0), q_0]} \right\}. \tag{3.6}
\]

3) For the entropy

\[
S = \frac{\pi}{Z(\beta, q_0)} \int_0^{q_0} \{\ln Z(\beta, q_0) + U[p(q), q]\} e^{-\beta U[p(q), q]} \, dU[p(q), q], \tag{3.7}
\]
whose result is

\[ S(\beta, q_0) = \frac{\pi}{\beta Z(\beta, q_0)} \left\{ 1 - e^{-\beta U[p(q_0), q_0]} \right\} \ln[Z(\beta, q_0)] - \frac{\pi}{Z(\beta, q_0)} U[p(q_0), q_0] e^{-\beta U[p(q_0), q_0] + \frac{\pi}{\beta Z(\beta, q_0)} \left\{ 1 - e^{-\beta U[p(q_0), q_0]} \right\}}. \] (3.8)

Note that when \( q_0 \to \infty \) (3.4), (3.6), and (3.8) reduce to (2.2), (2.4), and (2.5), respectively. Note again that the integrands in (3.4), (3.6), and (3.8) are exact differentials. We insist on the fact that i) these integrals become independent of the path \( \Gamma \) (i.e., the same for any \( \Gamma \)), and ii) if one redefines the coordinate-system in such a way that the starting point of \( \Gamma \) 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).

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

\[ <q^2> = \int_{-\infty}^{\infty} \frac{q^2}{Z} e^{-\beta(p^2 + q^2)} dp dq = \pi \int_{0}^{\infty} U e^{-\beta U} dU, \] (4.9)

i.e., along the curve \( \Gamma \)

\[ <q^2> (\beta, \Gamma) = \frac{\pi}{Z} \int \Gamma U e^{-\beta U} dU = \frac{\pi}{Z} \int_{0}^{q_0} U e^{-\beta U} dU = \langle q^2 \rangle (\beta, q_0) = -\frac{\pi}{2\beta Z(\beta, q_0)} U[p(q_0), q_0] e^{-\beta U[p(q_0), q_0]} + \frac{\pi}{2\beta^2 Z(\beta, q_0)} \left\{ 1 - e^{-\beta U[p(q_0), q_0]} \right\} = \frac{<U>(\beta, q_0)}{2}, \] (4.10)

that is,
that, for $q_0 \to \infty$, gives

$$< q^2 > = < p^2 > = \frac{< U >}{2} = \frac{1}{2\beta},$$

that is, classical equipartition.

5 Adiabatic paths

An adiabatic path is one such that $S = \text{constant along it}$. Simplifying (3.8) we obtain

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

$$\frac{\beta U[p(q_0), q_0] e^{-\beta U[p(q_0), q_0]}}{1 - e^{-\beta U[p(q_0), q_0]}} + 1.$$  

The condition $S = \text{constant}$ translates into

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

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

$$p^2 + q^2 = (p + \delta p)^2 + (q + \delta q)^2,$$

i.e.,

$$p\delta p = -q\delta q.$$  

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

$$f(q)f'(q) = -q,$$  

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 (5.17) is obtained after transforming it into
\[ \frac{df^2}{dq} = -2q, \]
\[ f(q)^2 = -q^2 + C \rightarrow p^2 + q^2 = C, \quad (5.18) \]

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 \( g_1(q) + g_2(q) = \text{constant} \).

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

\[ p(q) = aq, \quad (5.19) \]

so that we should have, for two different lines

\[ U = (a^2 + 1)q_0^2 = (a'^2 + 1)q_0'^2. \quad (5.20) \]

If we take

\[ a' < a \]

and

\[ q'_0 = \sqrt{\frac{a^2 + 1}{a'^2 + 1}} q_0, \quad (5.21) \]

then

\[ \Delta S = S(\beta, a', q'_0) - S(\beta, a, q_0) = 0. \quad (5.22) \]

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 \( (5.14) \) is satisfied, the evolution is adiabatic.

### 6 Entropic Force

We arrive here at our main theme. According to \( (5.13) \), the entropic force is given by Eq. (3.3) of [3] that reads \( F_e dx = T dS \). In our case this translates as

\[ F_e dq = \frac{1}{\beta} \frac{\partial S}{\partial q} dq, \quad (6.1) \]
and

\[ F_e = \beta U \frac{\partial U[p(q), q]}{\partial q} e^{-\beta U} \frac{2 - e^{-\beta U}}{(1 - e^{\beta U})^2} \]  \hspace{1cm} (6.2)

where the trajectory’s end-point is free to move in phase-space. For \( \beta U << 1 \) (the quantum limit), Eq. (6.2) simplifies to

\[ F_e = \frac{\partial U[p(q), q]}{\partial q} \left\{ \frac{1}{\beta U[p(q), q]} - \beta U[p(q), q] \right\} \]  \hspace{1cm} (6.3)

or

\[ F_e = 2q \left\{ \frac{1}{\beta U[p(q), q]} - \beta U[p(q), q] \right\} \sim 2q \frac{1}{\beta U[p(q), q]} \]  \hspace{1cm} (6.4)

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

7 Entropic Force on arbitrary phase-space curves

More generally, for \( U = p^2 + q^2 \) and any curve in phase space, one has

\[ F_e = 2q\beta(p^2 + q^2)e^{-\beta(p^2+q^2)} \frac{2 - e^{-\beta(p^2+q^2)}}{[1 - e^{\beta(p^2+q^2)}]^2} \]  \hspace{1cm} (7.5)

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.
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

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

where

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

We plot this total force for, respectively, $\beta = 0.2, 1.0, 5.0$ in Figs. 7, 8, and 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 an infinitesimal work $dW$ generated by a change $dq_0$

$$d < U > = TdS - dW,$$

where $dW$ is the work done ON the system if $dq_0 < 0$. In one dimension, the pressure reduces, of course, to a force. One obtains

$$dW = e^{-\beta U[p(q),q]} \frac{1}{1 - e^{-\beta U[p(q),q]}}^1,$$

and, according to

$$dW = Fdq,$$

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

$$F_{linear}(\Gamma) = \frac{e^{-\beta(p^2+q^2)} \left(2p\frac{dp}{dq} + 2q\right)}{1 - e^{-\beta(p^2+q^2)}}.$$
that, we insist, depends on the curve $\Gamma$ [remember that $p$ and $q$ possess common dimensionality (see Eq. (1))]. Figs. 10, 11, and 12 depict $F_{\text{linear}}$ for, respectively, $\beta = .2, 1, \text{and } 5$, with $\Gamma$ 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 [14]. Indeed, it constitutes the most accepted hypothesis to explain observations dating from the 90's that indicate that the universe is expanding at an accelerating rate. 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.

Finally, the specific heat is easily seen to be

$$C = k_{\text{Boltzmann}} \left\{ 1 - \frac{\beta^2 (p^2 + q^2)e^{-\beta(p^2+q^2)}}{[1 - e^{-\beta(p^2+q^2)}]^2} \right\}, \quad (9.10)$$

independently of the curve $\Gamma$. Figs. 13, 14, and 15 depict $C$ for, respectively, $\beta = .2, 1, \text{and } 5$. 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 heats are perhaps the most distinctive thermodynamic feature of self-gravitating systems [13]. Here, our entropic discourse establishes thereby contact with Verlinde’s work [3].

10 Discussion

We were dealing with a particle attached to the origin by a spring and consider entropic-force effects. Although we focus attention upon arbitrary phase space curves $\Gamma$, most of our effects were independent of the specific path $\Gamma$. 

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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. (3.2) and we saw that the equipartition theorem holds. From Figs. 1-6 we gather 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’s [3].

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.

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Figure 1: Arbitrary curves on phase-space. Entropic force vs. $q, p$ for $\beta = 5$ (low temperature). Note the hard-core barrier and the vanishing of the in a neighborhood of the origin.
Figure 2: Arbitrary curves on phase-space. Level $F_e$—curves in the $q$-$p$ plane (low temperature, $\beta = 5$).
Figure 3: Arbitrary curves on phase-space. Entropic force vs. $q$, $p$ for $\beta = 1$ (intermediate temperature). Note the hard-core barrier and the vanishing of the in a neighborhood of the origin.
Figure 4: Arbitrary curves on phase-space. Level $F_{\epsilon}$-curves in the q-p plane (intermediate temperature, $\beta = 1$).
Figure 5: Arbitrary curves on phase-space. Entropic force vs. $q$, $p$ for $\beta = 0.2$ (high temperature). Note the hard-core barrier, the vanishing of the force at the origin and the attraction/repulsion zones.
Figure 6: Arbitrary curves on phase-space. Level $F_e$—curves in the $q$-$p$ plane for $\beta = 0.2$ (high temperature).

Figure 7: Total force $F_T$ for $\beta = 0.2$. 

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Figure 8: Total force $F_T$ for $\beta = 1.0$.

Figure 9: Total force $F_T$ for $\beta = 5.0$. 
Figure 10: An example of the linear force $F_L$’s behavior for $\beta = 0.2$.

Figure 11: An example of the linear force $F_L$’s behavior for $\beta = 1.0$. 
Figure 12: An example of the linear force $F_L$’s behavior for $\beta = 5.0$.

Figure 13: Specific heat. Level $C-$curves in the q-p plane for $\beta = 0.2$ (high temperature).
Figure 14: Level $C-$curves in the $q$-$p$ plane for $\beta = 1.0$ (intermediate temperature).

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