

On the origin of power laws in equilibrium

MICHELE CAMPISI¹, FEI ZHAN² and PETER HÄNGGI¹

¹ *Institute of Physics, University of Augsburg - Universitätsstr. 1, D-86159 Augsburg, Germany*

² *International Center for Quantum Materials, Peking University - 100871, Beijing, China*

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Abstract – A particle in the attractive Coulomb field has an interesting property: its specific heat is constant and negative. We show, both analytically and numerically, that when a classical Hamiltonian system stays in weak contact with one such negative specific heat object, its statistics conforms to a fat-tailed power-law distribution with power index given by $C/k_B - 1$, where k_B is the Boltzmann constant and C is the heat capacity.

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Introduction. – In 1968 Lynden-Bell and Wood [1] pointed out an interesting fact: self-gravitating systems have negative specific heats. As Lynden-Bell later on explained [2] this fact seemed quite natural to astronomers, who know for example that when a star gains energy it expands and cools down [3]; but it appeared incongruous, if not completely wrong, to statistical mechanists, who learn from textbooks that specific heats are necessarily positive. The paradox was resolved by Thirring [4]: While it is true that any system *in weak contact with a thermal bath*, hence characterized by the canonical distribution, necessarily has a positive specific heat, isolated systems, characterized by the microcanonical distribution, may well have negative specific heats. Since then, many models showing microcanonical negative specific heats have been reported, see, *e.g.*, [5–11], their statistical mechanics has been discussed [12,13], and negative specific heats have been experimentally measured in thermally isolated small atomic clusters [14,15]. Recently it has also been pointed out that if a system is in *strong* coupling with its environment, likewise it may display negative specific heat [16–23].

Inspired by ref. [24], here we consider an ordinary system S with Hamiltonian $H_S(\mathbf{x}, \mathbf{p})$ and *weakly* couple it via an interaction energy $h(\mathbf{x}, \mathbf{X})$, to a second system with Hamiltonian $H_C(\mathbf{X}, \mathbf{P})$, possessing a *constant* negative microcanonical heat capacity $C < 0$, *i.e.*,

$$H(\mathbf{x}, \mathbf{p}, \mathbf{X}, \mathbf{P}) = H_S(\mathbf{x}, \mathbf{p}) + H_C(\mathbf{X}, \mathbf{P}) + h(\mathbf{x}, \mathbf{X}). \quad (1)$$

For the sake of clarity we recall that the heat capacity C is defined as the derivative of a system's energy with respect

to the temperature, $C = \partial E / \partial T$, while the specific heat c is defined as the heat capacity per unit mass.

The archetypical example of a system with constant negative microcanonical heat capacity is that of a single particle in the gravitational (or the attractive Coulomb) force field, for which $C = -3/2$ [2]. Throughout the paper, temperature is expressed in units of energy. In these units k_B , Boltzmann's constant, is dimensionless and equal to 1, and the heat capacity $C = \partial E / \partial T$ is dimensionless as well.

Our main result is that, provided the *total* system samples the microcanonical ensemble, the system S samples the power-law distribution

$$p(\mathbf{x}, \mathbf{p}) = \frac{[H_S(\mathbf{x}, \mathbf{p}) - E_{\text{tot}}]^{C-1}}{\int d\mathbf{x}d\mathbf{p} [H_S(\mathbf{x}, \mathbf{p}) - E_{\text{tot}}]^{C-1}}, \quad C < 0, \quad (2)$$

where E_{tot} is the (conserved) energy of the total system. To express this result in eq. (2) in the usual set of units, where the temperature is measured in Kelvin, and both the heat capacity and k_B have the dimension of Joule/Kelvin, one should replace C in eq. (2) with the dimensionless ratio C/k_B .

We illustrate this result in fig. 1. A neutral particle, with Hamiltonian $H_S = \mathbf{p}^2 / 2m$, is confined into a box and makes elastic collisions with a particle carrying a charge q subject to the Coulomb field generated by a fixed charge $-q$. The charged particle has constant negative heat capacity $C = -3/2$, and its Hamiltonian reads:

$$H_{C=-3/2}(\mathbf{X}, \mathbf{P}) = \mathbf{P}^2 / 2M - \alpha / |\mathbf{X}|, \quad (3)$$

where $\alpha = q^2 / 4\pi\epsilon_0$ with ϵ_0 the dielectric permittivity of vacuum. According to our main result, eq. (2), since

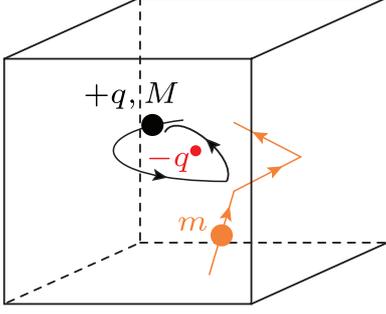


Fig. 1: (Color online) Illustrative example of our main result, eq. (2). A neutral particle (orange) moves freely within a box, making elastic collisions with the box walls and a charged particle (black) immersed in the attractive Coulomb field generated by a fixed point charge (red). Because the heat capacity of the charged (black) particle is $C = -3/2$, the velocity probability distribution function of the neutral (orange) particle conforms to a power law with power index $-3/2 - 1 = -5/2$, eq. (4).

the charged particle has constant negative heat capacity $C = -3/2$, the velocity probability distribution function of the neutral particle is given by the following power law:

$$p(\mathbf{p}) = \frac{(\mathbf{p}^2/2m - E_{\text{tot}})^{-5/2}}{\int d\mathbf{p}(\mathbf{p}^2/2m - E_{\text{tot}})^{-5/2}}. \quad (4)$$

Derivation of the result in eq. (2). – Assuming i) the microcanonical distribution for the total system, and ii) weak coupling h , the system S marginal distribution $p(\mathbf{x}, \mathbf{p})$ can be written as [25–27]

$$p(\mathbf{x}, \mathbf{p}) = \frac{\Omega_C[E_{\text{tot}} - H_S(\mathbf{x}, \mathbf{p})]}{\Omega_{\text{tot}}(E_{\text{tot}})}, \quad (5)$$

where

$$\Omega_C(E) = \int d\mathbf{X} d\mathbf{P} \delta[E - H_C(\mathbf{X}, \mathbf{P})] \quad (6)$$

is the density of states of the negative heat capacity system whose energy is E , and

$$\Omega_{\text{tot}}(E_{\text{tot}}) = \int d\mathbf{X} d\mathbf{P} d\mathbf{x} d\mathbf{p} \delta[E_{\text{tot}} - H(\mathbf{x}, \mathbf{p}, \mathbf{X}, \mathbf{P})] \quad (7)$$

is the density of states of the compound system. Here δ denotes Dirac's delta function.

We note that if a classical system has a constant *negative* microcanonical heat capacity $C < 0$, then its density of states is of the form

$$\Omega_C(E) \propto (-E)^{C-1}, \quad C < 0. \quad (8)$$

For the derivation of this density of states see appendix A. In arriving at eq. (8) we adopt the convention to set the zero of the energy of constant negative heat capacity systems as the lowest energy corresponding to unbound trajectories. Thus, the density of states is only defined for negative E 's, and it diverges for $E \geq 0$.

Using eq. (8) in (5) one arrives at the result in eq. (2). It is important to stress that in eq. (2) the system S

energy has a lower bound, which is conventionally set to zero, and that the total energy E_{tot} must be negative, thus ensuring that the energy $E = E_{\text{tot}} - H_S$ of the system with negative heat capacity is negative at all times. This is necessary in order that the C -system always stays on bounded trajectories and never escapes to infinity.

Numerics. – To corroborate our main result, eq. (2), we simulated the dynamics of the system depicted in fig. 1, using a symplectic integrator [28]. We focussed on the probability density $\rho(E_S)$ of finding the neutral particle (our S system) at energy E_S for a total (negative) simulation energy E_{tot} . According to eq. (4) this is given by

$$\rho(E_S) = \frac{[E_S - E_{\text{tot}}]^{-5/2} E_S^{1/2}}{\int_0^\infty dE_S [E_S - E_{\text{tot}}]^{-5/2} E_S^{1/2}}, \quad (9)$$

where the term $E_S^{1/2}$ derives from the density of states $\Omega_S(E_S) \propto E_S^{3/2-1}$ of the neutral particle. Note that for large E_S , $\rho(E_S) \propto E_S^{-2}$.

Following ref. [27], we chose $h(\mathbf{x}, \mathbf{X}) = V_{LJ}(|\mathbf{x} - \mathbf{X}|)$, where V_{LJ} is the truncated Leonard-Jones potential

$$V_{LJ}(r) = \begin{cases} 0, & |r| > 2^{1/6}\sigma, \\ 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] + \epsilon, & |r| < 2^{1/6}\sigma. \end{cases} \quad (10)$$

We employ the same potential for the walls of the confining cubic box, in which the particle moves freely. In our simulation, we set ϵ , σ , and M (M is the mass of the particle carrying the charge q) as the units of energy, length, and mass, respectively.

Following ref. [27], in order to avoid the singularity of the attractive Coulomb field at $\mathbf{X} = 0$, in the simulation we employ the Plummer potential [29]:

$$\varphi_b(\mathbf{X}) = \frac{-\alpha}{\sqrt{\mathbf{X}^2 + b^2}}. \quad (11)$$

Using this potential in place of the pure Coulombic potential $\varphi(\mathbf{X}) = -\alpha/|\mathbf{X}|$, induces a deviation of the density of states from the pure power-law form $\Omega_{-3/2}(E) = (-E)^{-5/2}$, resulting in a cut-off in the expected power-law distribution $\rho(E_S)$. This cut-off moves to higher energy values as b becomes smaller.

Figure 2 displays the result of our simulation for $b = 10^{-2}$, $E_{\text{tot}} = -1$, a box of side length $L = 10$, $\alpha = 5$, and $m = \sqrt{3}$. The computed energy distribution function for the neutral atom excellently agrees with the expected power-law form in eq. (9) over three decades. At higher energies the distribution displays the expected cut-off due to the truncation in eq. (11). Note that when the neutral atom has high energy the charged particle has low energy and stays close to the bottom of the Plummer potential, eq. (11). The condition $E_{\text{tot}} < 0$ ensures that the energy $E = E_{\text{tot}} - H_S$ of the charged particle is also negative, thus ensuring that its motion remains confined at all times. With our choice of box side length $L = 10$, and $E_{\text{tot}} = -1$, the confinement keeps the charged particle within the box at all times.

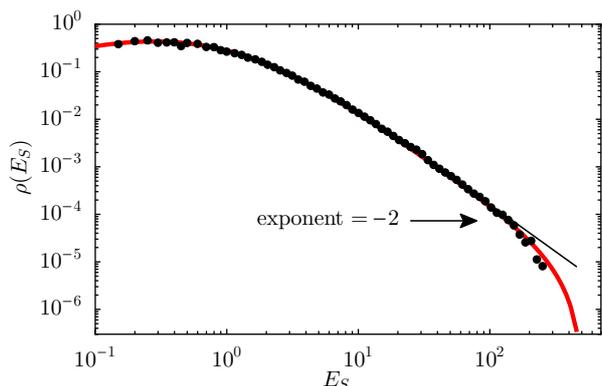


Fig. 2: (Color online) Energy probability density function $\rho(E_S)$ of a neutral particle performing Lennard-Jones collisions, eq. (10), with the walls of a confining box, and with a charged particle in the Plummer potential, eq. (11). Black dots: numerical simulation. Red thick solid line: analytic calculation based on the Plummer potential, eq. (11). Black thin solid line: analytic calculation based on the pure gravitational potential $\varphi(\mathbf{X}) = -\alpha/|\mathbf{X}|$, eq. (9). Simulation parameters: $E_{\text{tot}} = -1$, $b = 10^{-2}$, $L = 10$, $\alpha = 5$, and $m = \sqrt{3}$.

Methods. The simulation was performed by means of an implicit Runge-Kutta symplectic integrator [28]. We simulated the evolution of the whole system with a time step size $\Delta t = 10^{-5}$ and total number of time steps $\mathcal{N} = 1.28 \times 10^{12}$. Note that the units of time are $\sigma\sqrt{M/\varepsilon}$. In order to calculate the statistics, we divided the E_S -axis in 10^4 intervals of size $\Delta E_S = 0.0499$, and counted how many times each interval was visited during the simulation. We adopted a sampling time $\tau = 2 \times 10^5 \Delta t$. The resulting histogram was then normalized and divided by ΔE_S to give an estimate of the probability density. Finally, for better visualization in the log-log plot in fig. 2, the histogram was coarse-grained with a series of intervals with exponentially increasing size, *viz.*, we took $\Delta E_S^{n+1}/\Delta E_S^n = 1.1$, where ΔE_S^n is the size of the n -th interval and $\Delta E_S^0 = \Delta E_S$.

Comparison with the finite bath statistics. – When $C > 0$, one finds the expression $\Omega_C(E) \propto E^{C-1}$ for the densities of states, see appendix A. This differs from eq. (8) by a minus sign in front of E . Note that for constant positive heat capacity systems, whose energy is bounded from below, we adopt the convention that the zero of the energy corresponds to this lower bound. Accordingly, in this case one obtains for the probability density function the same expression as in eq. (2), but with $H_S - E_{\text{tot}}$ replaced by $E_{\text{tot}} - H_S$:

$$p(\mathbf{x}, \mathbf{p}) = \frac{[E_{\text{tot}} - H_S(\mathbf{x}, \mathbf{p})]^{C-1}}{\int d\mathbf{x}d\mathbf{p} [E_{\text{tot}} - H_S(\mathbf{x}, \mathbf{p})]^{C-1}}, \quad C > 0. \quad (12)$$

The statistics in eq. (12) is sometimes referred to as the “finite bath statistics” [26], because it is induced by the weak coupling of the S system with a system with a finite *positive* heat capacity, like, for instance a finite collection

of N free particles, for which $C = 3N/2$. As we will see below, this can also be achieved with one single particle in a properly chosen potential. The finite bath statistics in eq. (12) interpolates between the microcanonical distribution $p(\mathbf{x}, \mathbf{p}) \propto \delta[E_S - H_S(\mathbf{x}, \mathbf{p})]$ and the canonical distribution $p(\mathbf{x}, \mathbf{p}) \propto e^{-H_S(\mathbf{x}, \mathbf{p})/T}$. These two limiting cases are obtained when C approaches 0 and $+\infty$, respectively [26,30,31]. Note that when $C > 0$, $E_{\text{tot}} - H_S$ in eq. (12), is non-negative, as a consequence of the fact that the system S energy may not overcome the total (non-negative) energy E_{tot} . While the negative C distributions in eq. (2) have fat power-law tails, the positive C distributions in eq. (12) exhibits sharp cut-offs at $H_S = E_{\text{tot}}$.

Implementing constant heat capacity systems with single particles. – In three dimensions, constant heat capacity systems can be obtained with a single particle governed by the Hamiltonian:

$$H_C(\mathbf{X}, \mathbf{P}) = \mathbf{P}^2/2M + gC|\mathbf{X}/L|^{6/(2C-3)}, \quad (13)$$

with constants $g, L > 0$ with units of energy and length, respectively, and $C \notin [0, 3/2]$. As shown with explicit calculations in appendix B, the associated density of states is proportional to E^{C-1} for $C > 3/2$, and is proportional to $(-E)^{C-1}$ for $C < 0$. Accordingly, when a system with Hamiltonian H_S bounded from below stays in weak contact with one such constant heat capacity system, its statistics conforms with either eq. (2) or eq. (12), depending on whether $C < 0$ or $C > 3/2$, respectively. The potential in (13) includes many special cases of interest. For C approaching $3/2$ the potential approaches a box potential, namely the system is a particle in a box, which knowingly has a constant heat capacity of $3/2$. For $C = 3$, we have a harmonic oscillator. For $C = -3/2$ we have the $1/r$ case of eq. (3). For $C \rightarrow \pm\infty$, the potential approaches the logarithmic form

$$C|\mathbf{X}|^{6/(2C-3)} \simeq 3\ln|\mathbf{X}| + C, \quad |C| \gg 1, \quad (14)$$

which, as we have shown recently [27], produces the Gibbs distribution. Thus, not only does the canonical ensemble emerge from the coupling to a system with positive infinite heat capacity, but also from the coupling to a system with *negative* infinite heat capacity. The case $C = 0$ is excluded from eq. (13) because it corresponds to an unbound free particle, whose density of states, accordingly, diverges for all energies. For $0 < C < 3/2$, the exponent $6/(2C-3)$ is negative, hence one must chose $g < 0$ to ensure that the potential is attractive. The density of states diverges nonetheless because it involves a divergent integral, see appendix B.

Similar expressions as in eq. (13), but with a different exponent for $|\mathbf{X}|$ can be found in spaces of dimensions other than three.

Conclusions. – We have shown, both analytically and numerically, that weak coupling to a system with constant negative heat capacity leads to the emergence of velocity

probability distributions with fat power-law tails. The power law emerges because the S -system may withdraw indefinitely large amounts of energy from the infinitely deep algebraic potential “well” that systems with constant negative heat capacity possess.

Because of the fat tails it is possible that the negative C distributions may not be normalizable. This happens, for instance, when the S -system density of states goes asymptotically as E_S^α , with $\alpha > -C$. In this case the S -system “wins” over the C -system and the integral of $\Omega_C[E_{\text{tot}} - E_S]\Omega_S[E_S]$, which asymptotically goes like $\propto E_S^{C+\alpha-1}$, diverges. For $\alpha > -C + 1$, $\Omega_C[E_{\text{tot}} - E_S]\Omega_S[E_S]$ asymptotically increases with increasing energies, while for $-C + 1 > \alpha > -C$ it vanishes for $E_S \rightarrow \infty$. As examples, consider the case of fig. 1, but with many neutral particles. With two neutral particles we have $-C + 1 = 5/2 > \alpha = 2 > -C = 3/2$, that is the distribution would not be normalizable but would vanish for large E_S . With three or more neutral particles we have $\alpha \geq 7/2 > 5/2 = -C + 1$, and the distribution would be increasing for large E_S . Arguably the system never reaches equilibrium in such cases.

For our example of a neutral particle making collisions with a particle in the $1/r$ potential field, fig. 1, the energy distribution has a power index -2 , which is very close to the exponent observed in the energy distribution of cosmic rays [32,33]¹. This suggests that the power index $\simeq -2$ of the cosmic ray energy distribution might originate from multiple collisions of the cosmic particles with objects obeying $1/r$ potentials before they reach our instruments. We leave this as an open question.

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Appendix A. Density of states for systems with constant heat capacity. – A classical system has a constant negative microcanonical heat capacity C if and only if its density of states is of the form

$$\Omega_C(E) = f(-E)^{C-1}, \quad C < 0 \quad (\text{A.1})$$

with some constant $f > 0$.

To see this consider the microcanonical heat capacity:

$$C(E) = [\partial T(E)/\partial E]^{-1}, \quad (\text{A.2})$$

¹Typically one looks at the cosmic ray differential spectrum [32,33], which is the derivative of the probability distribution with respect to energy. The cosmic ray spectrum has a power index $\simeq -3$. Accordingly, the energy probability distribution has a power index $\simeq -2$.

where $T(E)$ is the microcanonical temperature. For constant C this implies

$$T(E) = E/C + a, \quad (\text{A.3})$$

with some integration constant a . Using the definition of microcanonical temperature

$$T(E) = [\partial \ln \Phi_C(E)/\partial E]^{-1}, \quad (\text{A.4})$$

one obtains, after a further integration

$$\Phi_C(E) = d[E/C + a]^C, \quad (\text{A.5})$$

with some integration constant d . Here

$$\Phi_C(E) = \int d\mathbf{X}d\mathbf{P}\theta[E - H_C(\mathbf{X}, \mathbf{P})] \quad (\text{A.6})$$

is the phase space volume, and θ denotes Heaviside’s step function. Adopting the convention $\Phi_C(0) = \infty$, sets $a = 0$, hence $\Phi_C(E) = d[E/C]^C$. Recalling that $C < 0$, this can be recast as $\Phi_C(E) \propto (-E)^C$. Using the well-known relation

$$\Omega_C(E) = \partial \Phi_C(E)/\partial E, \quad (\text{A.7})$$

we obtain eq. (A.1).

To see that the reverse is also true, consider eq. (A.7). We have, using eq. (A.1),

$$\Phi_C(E) = \int_{-\infty}^E \Omega_C(E')dE' = -f(-E)^C/C. \quad (\text{A.8})$$

Using (A.4), we obtain

$$T(E) = E/C. \quad (\text{A.9})$$

From eq. (A.2) it then follows that the heat capacity is C .

Likewise, a classical system has a constant positive microcanonical heat capacity C if and only if its density of states is of the form

$$\Omega_C(E) = fE^{C-1}, \quad C > 0 \quad (\text{A.10})$$

with some constant $f > 0$.

To see this the argument proceeds identically to the argument above, with the only difference that in the case $C > 0$ the constant a is set to zero as a consequence of the convention $\Phi_C(0) = 0$.

The argument supporting the reverse implication also proceeds identically as above, with the only difference that now the phase volume reads $\Phi_C(E) = fE^C/C$.

Appendix B. Density of states for the Hamiltonians in eq. (13). – We begin with the case $C < 0$, implying that the exponent

$$\gamma = 6/(2C - 3) \quad (\text{B.1})$$

lies in the interval $-2 < \gamma < 0$. Using eq. (A.6) with eq. (13), recalling that $E, C < 0$, the phase volume reads, after integration over $d\mathbf{P}$

$$\begin{aligned}\Phi_C(E) &= \frac{(2\pi M)^{3/2}}{\Gamma(5/2)} \int d\mathbf{X} [E - gC|\mathbf{X}|^\gamma]^{3/2} \\ &= 4\pi \frac{(2\pi M)^{3/2}}{\Gamma(5/2)} \int_0^{(E/gC)^{1/\gamma}} d\rho \rho^2 [E - gC\rho^\gamma]^{3/2} \\ &= 4\pi \frac{(2\pi M)^{3/2}}{\Gamma(5/2)} \frac{(-E)^{3/2+3/\gamma}}{(-gC)^{3/\gamma}} \int_0^1 dy y^2 [y^\gamma - 1]^{3/2},\end{aligned}\quad (\text{B.2})$$

where we switched to spherical coordinates in the second line and we performed the change of variables $y = \rho(gC/E)^{1/\gamma}$ in the third line. The limit of integration $(E/gC)^{1/\gamma}$ represents the turning point of the closed orbit of negative energy E . In the interval $-2 < \gamma < 0$ the integral converges and can be expressed in terms of the gamma function $\Gamma(x)$, as

$$\int_0^1 dy y^2 [y^\gamma - 1]^{3/2} = \frac{\sqrt{\pi}}{4} \frac{\Gamma(-C)}{\Gamma(3/2 - C)}.\quad (\text{B.3})$$

Note that $3/2 + 3/\gamma = C$. Hence $\Phi_C \propto (-E)^C$. Accordingly, using eq. (A.7), we find that the density of states is of the form $\Omega_C \propto (-E)^{C-1}$.

For $0 < C < 3/2$ it is $\gamma < -2$, hence one must now choose $g < 0$ in order that the potential is attractive. One then arrives at the same expression as for the case $C < 0$. In this case however the integral $\int_0^1 dy y^2 [y^\gamma - 1]^{3/2}$ diverges.

For $C > 3/2$ it is $\gamma > 0$. One can proceed as above, recalling that now $E, C > 0$, to obtain

$$\begin{aligned}\Phi_C(E) &= 4\pi \frac{(2\pi M)^{3/2}}{\Gamma(5/2)} \int_0^{(E/gC)^{1/\gamma}} d\rho \rho^2 [E - gC\rho^\gamma]^{3/2} \\ &= 4\pi \frac{(2\pi M)^{3/2}}{\Gamma(5/2)} \frac{\int_0^1 dy y^2 [1 - y^\gamma]^{3/2}}{(gC)^{3/\gamma}} E^C.\end{aligned}\quad (\text{B.4})$$

The integral in the numerator is well behaved for all $\gamma > 0$, and can be expressed as

$$\int_0^1 dy y^2 [1 - y^\gamma]^{3/2} = \frac{\sqrt{\pi}}{4} \frac{\Gamma(C - 1/2)}{\Gamma(C + 1)}.\quad (\text{B.5})$$

Using eq. (A.7), we find that the density of states is of the form $\Omega_C \propto E^{C-1}$.

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