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Brownian Motion in an External Field Revisited

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Abstract

In many interesting physical examples, the partition function is divergent, as first pointed out in 1924 by Fermi (for the hydrogen-atom case). Thus, the usual toolbox of statistical mechanics becomes unavailable, notwithstanding the well-known fact that the pertinent system may appear to be in a thermal steady state. We tackle and overcome these difficulties hereby appeal to firmly established but not too well-known mathematical recipes and obtain finite values for a typical divergent partition function, that of a Brownian particle in an external field. This allows not only for calculating thermodynamic observables of interest, but for also instantiating other kinds of statistical mechanics' novelties.

Keywords

Divergent Partition Functions, Statistical Mechanics, Fisher Information

1. Introduction

In many interesting physical examples, the partition function is divergent [1] [2] [3] [4]. Thus, the usual toolbox of statistical mechanics becomes unavailable, notwithstanding the well-known fact that the pertinent system may appear to be in a thermal steady state (see, for instance [5] [6] [7] [8] [9]) and references therein]. Our goal here is to deal with a specific divergent partition function, and obtain a finite value for it. This permits to compute new observables of interest and also to develop some hopefully new statistical mechanics' insights.

2. The Central Issue

2.1. Partition Function

We will consider here the partition function for Brownian motion in an external field, given by [4]

$$\mathcal{Z} = \int_{-\infty}^{\infty} \mathrm{e}^{\frac{\beta U_0}{1+x^2}} \mathrm{d}x, \tag{2.1}$$

with $\beta = 1/(k_B T)$ and k_B = Boltzmann's constant. Change now variables to $y = 1 + x^2$. Taking advantage now of well-known features of Schwartz' theory of distributions [10], we can recast the integral that defines $\mathcal{Z}$ in the fashion

$$\mathcal{Z} = \int_{1}^{\infty} (y-1)^{-\frac{1}{2}} \mathrm{e}^{\frac{\beta U_0}{y}} \mathrm{d}y \equiv \lim_{\nu \to 1} \int_{1}^{\infty} y^{\nu-1} (y-1)^{-\frac{1}{2}} \mathrm{e}^{\frac{\beta U_0}{y}} \mathrm{d}y, \tag{2.2}$$

and remember that the limit of an integral equals the integral of the limit. We consult then the Table of Ref. [11] and find that our current integral is a special case of the more general one

$$W = \int_{u}^{\infty} x^{\nu-1} (x-u)^{\mu-1} \mathrm{e}^{\frac{\beta}{x}} \mathrm{d}x = B(1-\mu-\nu, \mu) u^{\mu+\nu-1} \phi\left(1-\mu-\nu; 1-\nu, \frac{\beta}{u}\right). \tag{2.3}$$

Here B is the well-known beta function and ϕ the confluent hypergeometric function, that reads, appealing to the Gamma function Γ,

$$B = \Gamma(1-\mu-\nu)\Gamma(\mu)/\Gamma(1-\nu). \tag{2.4}$$

Comparing integrals, we see at this stage that the right hand side of (2.2) will coincide with W in (2.3) by setting

$$\mu = 1/2; \ \nu = 1; \ u = 1, \tag{2.5}$$

so that these special values are to be inserted in

$$W = \Gamma(1-\mu-\nu)\left[\Gamma(\mu)/\Gamma(1-\nu)\right] u^{\mu+\nu-1} \phi\left(1-\mu-\nu; 1-\nu, \frac{\beta}{u}\right). \tag{2.6}$$

Note also that

$$\Gamma(1/2) = \sqrt{\pi}; \ \Gamma(-1/2) = -2\sqrt{\pi}. \tag{2.7}$$

We have a $\Gamma(0)$ in a denominator now. This induces us to appeal once again to [11] to employ the useful relation

$$\lim_{\gamma \to 0} \phi(\alpha; \gamma; s) = z\alpha\phi(\alpha+1; 2; z), \tag{2.8}$$

so that we can finally arrive at the result

$$\mathcal{Z} = \pi\beta U_0 \phi\left(\frac{1}{2}; 2; \beta U_0\right), \tag{2.9}$$

our desired finite form. We see that we arrive at $\mathcal{Z}$ via a straightforward path. The essential step here is that of consulting an appropriate table of integrals and performing adequate manipulations. Note that at very low temperatures quantum effects raise their head and our treatment becomes invalid. Below it will be shown that one also encounters problems or exceedingly high temperatures. We have found a finite partition function for our Brownian problem and proceed to calculate with it, below, important quantifiers of statistical mechanics.

2.2. Units for Our Graphs

We find it convenient to plot our thermal quantities versus $y = k_B T / U_0$ in the range $0 \le y \le 1$. Given the smallness of k_B, this encompasses an immense T-range, since k_B is of the order of 10^{-23} in its appropriate units. In particular, we plot the logarithm of the partition function in **Figure 1**. We appreciate the fact that it converges to a definite value as T grows.

3. Other Thermal Quantities

3.1. Mean Energy

One has

$$\langle \mathcal{U} \rangle = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}, \tag{3.1}$$

so that

$$\langle \mathcal{U} \rangle = -\frac{1}{\mathcal{Z}}\left[\pi U_0 \phi\left(\frac{1}{2};2;\beta U_0\right) + \frac{\pi \beta U_0^2}{4}\phi\left(\frac{3}{2};3;\beta U_0\right)\right]. \tag{3.2}$$

Note that at very low temperatures quantum effects raise their head and our classical treatment becomes invalid.

3.2. Entropy $\mathcal{S}$

We have

$$S = \frac{\partial\left(k_B T \ln Z\right)}{\partial T}, \tag{3.3}$$

so that

$$\mathcal{S} = \ln\left[\pi \beta U_0 \phi\left(\frac{1}{2};2;\beta U_0\right)\right] - \frac{\beta}{\mathcal{Z}}\left[\pi U_0 \phi\left(\frac{1}{2};2;\beta U_0\right) + \frac{\pi \beta U_0^2}{4}\phi\left(\frac{3}{2};3;\beta U_0\right)\right], \tag{3.4}$$

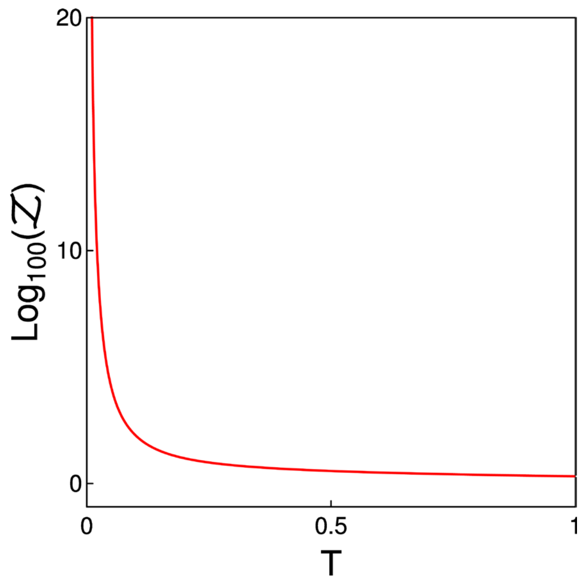

Figure 1. Logarithm of the partition function in appropriate units (see text).

that is plotted in **Figure 2**. Note that at very low temperatures, quantum effects raise their head and our treatment becomes invalid. This is evident whenever S becomes negative at low T. A new effect is observed at very large T. Whenever $T \geq 10^{22}$, the treatment becomes invalid as well. Such high-T outcome is typical of classical self-gravitating systems [12] [13] [14].

3.3. Specific Heat $\mathcal{C}$

One defines it as

$$\mathcal{C} = -\frac{\beta}{T}\frac{\partial\langle\mathcal{U}\rangle}{\partial\beta}, \tag{3.5}$$

so that

$$\begin{aligned}\mathcal{C} = &-\frac{1}{Z^2}\left[\pi U_0\phi\left(\frac{1}{2};2;\beta U_0\right)+\frac{\pi\beta U_0^2}{4}\phi\left(\frac{3}{2};3;\beta U_0\right)\right]\\ &\times\left[\frac{\pi\beta U_0}{T}\phi\left(\frac{1}{2};2;\beta U_0\right)+\frac{\pi\beta^2U_0^2}{4T}\phi\left(\frac{3}{2};3;\beta U_0\right)\right]\\ &+\frac{1}{\mathcal{Z}}\left[\frac{\pi\beta U_0^2}{2T}\phi\left(\frac{3}{2};3;\beta U_0\right)+\frac{\pi\beta^2U_0^3}{8T}\phi\left(\frac{5}{2};4;\beta U_0\right)\right],\end{aligned} \tag{3.6}$$

depicted in **Figure 3**. Note that at very low temperatures, quantum effects raise their head and our treatment becomes invalid. Thus, the third thermodynamics' law is violated here. Interestingly enough there is a Schottky anomaly. This is an effect typical of solid-state physics: the specific heat at low temperature exhibits a peak. When T is high, the specific heat decreases. A new effect is observed at very large T. The specific heat becomes negative. Such outcome is typical of classical self-gravitating systems [12] [13] [15].

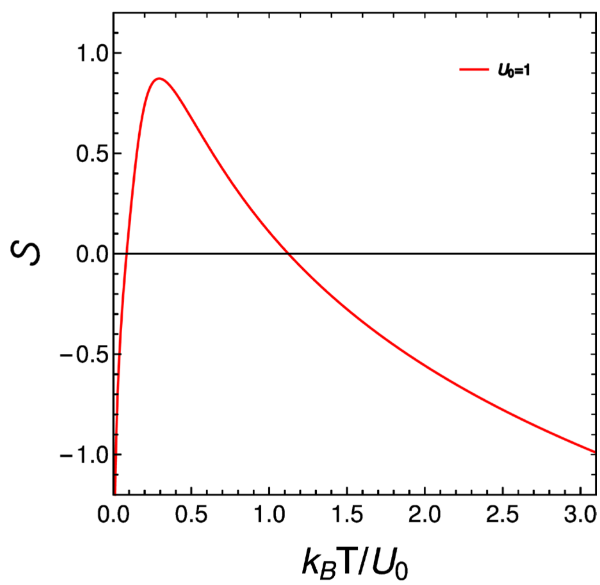

Figure 2. Entropy in appropriate units. Negative values at low T reflect on quantum effects that need to be considered. Those at high $T \geq 10^{22}$ are discussed in the text.

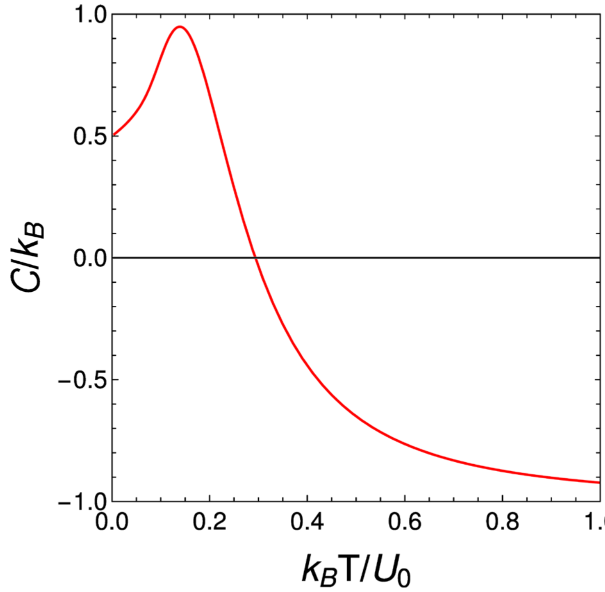

Figure 3. Specific heat in appropriate units. The third thermodynamics' law is violated here because our treatment is classical. A Schottky effect is clearly visible (see text).

4. Moment Generating Functions

We pass to the moment generating function for our extant probability distribution function (PDF) $f(x)$ [consult (2.1)]

$$f(x)=\frac{\mathrm{e}^{\frac{\beta U_0}{1+x^2}}}{\mathcal{Z}}, \tag{4.1}$$

where $\mathcal{Z}$ is given by (2.1). In the naive traditional treatment, these moments diverge. The mean value for x^{2n+1}, $(n=1,2,3,\cdots)$ vanishes by parity. That of x^{2n} becomes

$$\langle x^{2n}\rangle=\frac{1}{\mathcal{Z}}\int_{-\infty}^{\infty} x^{2n}\mathrm{e}^{\frac{\beta U_0}{1+x^2}}\mathrm{d}x. \tag{4.2}$$

Appeal again to the variables change $y=1+x^2$ and face

$$\langle x^{2n}\rangle=\frac{1}{\mathcal{Z}}\int_{1}^{\infty}(y-1)^{n-\frac{1}{2}}\mathrm{e}^{\frac{\beta U_0}{y}}\mathrm{d}y, \tag{4.3}$$

so that, proceeding in a fashion similar to that above we find

$$\langle x^{2n}\rangle=\frac{\beta U_0}{\mathcal{Z}}\Gamma\left(-n+\frac{1}{2}\right)\Gamma\left(n+\frac{1}{2}\right)\phi\left(\frac{1}{2}-n;2;\beta U_0\right), \tag{4.4}$$

Thus, we get for the moment generating function $\mathcal{M}_1(t)$

$$\mathcal{M}_1(t)=\frac{\beta U_0}{\mathcal{Z}}\sum_{n=0}^{\infty}\frac{t^{2n}}{(2n)!}\Gamma\left(\frac{1}{2}-n\right)\Gamma\left(\frac{1}{2}+n\right)\phi\left(\frac{1}{2}-n;2;\beta U_0\right). \tag{4.5}$$

As particular cases, we obtain the values

$$\langle x^2\rangle=-\frac{\pi\beta U_0}{\mathcal{Z}}\phi\left(-\frac{1}{2};2;\beta U_0\right), \tag{4.6}$$

and

$$\left\langle x^4 \right\rangle = \frac{\pi\beta U_0}{\mathcal{Z}}\phi\left(-\frac{3}{2};2;\beta U_0\right). \tag{4.7}$$

The first one is plotted in **Figure 4**. We encounter again here the high temperature effect already reported in [2] [12] [13] (and references therein) and in precedent graphs: a high temperature upper bound, beyond which our treatment becomes invalid. Such bound manifests itself in making negative these types of expectation values at temperatures of the order of 10^{22} Kelvin. For reference, 100 seconds after the Big Bang it is estimated that the temperature is of a billion K-degrees, and 0.0001 seconds after the Big Bang it is of about $T = 10^{13}$ K [16].

5. Fisher Information Measure (FIM)

Given a continuous probability distribution function (PDF) $f(x)$ with $x \in \Delta \subset \mathbb{R}$ and $\int_\Delta f(x)\mathrm{d}x = 1$, its associated *Shannon Entropy* $\mathcal{S}$ is, as we saw above,

$$\mathcal{S}(f) = -\int_\Delta f \ln(f)\mathrm{d}x \tag{5.1}$$

a quantifier of global nature that it is not very sensitive to strong changes in the distribution that may take place in a small-sized region. This is not the case for *Fisher's Information Measure* (FIM) $\mathcal{F}$ [17] [18], which constitutes a quantifier of the gradient content of $f(x)$, being accordingly quite sensitive even to small localized perturbations. One writes

$$F(f) = \int_\Delta \frac{1}{f(x)}\left[\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right]^2 \mathrm{d}x = 4\int_\Delta \left[\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}\right]^2 \tag{5.2}$$

FIM can be interpreted in variegated fashions. 1) As a quantifier of the ability

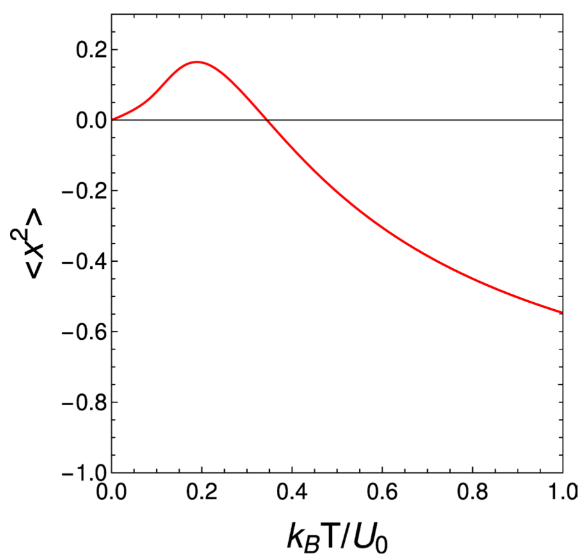

Figure 4. $\langle x^2 \rangle$ values in appropriate units (see text). The unphysical negative values emerge at temperatures higher than 10^{22} Kelvin.

to estimate a parameter. 2) As the amount of information that can be extracted from a set of measurements. 3) A quantifier of the state of disorder of a system or phenomenon [18], and finally, at more recent times 4) As a strict measure of order [19] [20] [21]. In the above definition of FIM the division by $f(x)$ is not desirable if $f(x)\to 0$ at certain *x*-values. We bypass this issue by working with a real probability amplitudes $f(x)=\psi^2(x)$ [17] [18], which is a simpler form (no divisors), while showing that $\mathcal{F}$ simply measures the gradient content of $\psi(x)$. The gradient operator significantly influences the contribution of minute local *f*-changes in FIM's values. Thus, this quantifier is called a local measure [18].

For the *f* of (3.5) one has

$$\mathcal{F}(f)=\frac{2}{\mathcal{Z}}\int_0^\infty \mathrm{e}^{\frac{\beta U_0}{1+x^2}}\left[\frac{\mathrm{d}\mathrm{e}^{\frac{\beta U_0}{1+x^2}}}{\mathrm{d}x}\right]^2\mathrm{d}x, \tag{5.3}$$

or

$$\mathcal{F}(f)=\frac{8\beta^2U_0^2}{\mathcal{Z}}\int_0^\infty \frac{x^2}{\left(1+x^2\right)^2}\mathrm{e}^{\frac{\beta U_0}{1+x^2}}\mathrm{d}x. \tag{5.4}$$

Changing variables in the fashion $y=1+x^2$ we get

$$\mathcal{F}(f)=\frac{4\beta^2U_0^2}{\mathcal{Z}}\int_1^\infty y^{-2}\left(y-1\right)^{\frac{1}{2}}\mathrm{e}^{\frac{\beta U_0}{y}}\mathrm{d}y, \tag{5.5}$$

that after evaluation yields for the Fisher information measure the value

$$\mathcal{F}(f)=2\beta U_0, \tag{5.6}$$

clearly a very large positive number, given the smallness of the Boltzmann constant entering the denominator. Let us look for the Cramer-Rao (CR) product $\left[\mathcal{F}(f)\left\langle x^2\right\rangle_f\right]$, that is always ≥ 1 [18]. The CR relation has been linked to the Heisenberg uncertainty relation (HUR) for the *D*-dimensional quantum central problem [22]. Still further, Frieden has shown that all UHRs can be derived from the CR relation [18].

We need a value for $\left\langle x^2\right\rangle$, that we take from (4.4). The Cramer-Rao product $\left\langle x^2\right\rangle\mathcal{F}$ is then

$$\mathcal{F}(f)\left\langle x^2\right\rangle=-\frac{2\pi\beta^2U_0^2}{\mathcal{Z}}\phi\left(-\frac{1}{2};2;\beta U_0\right). \tag{5.7}$$

The CR product is plotted in **Figure 5**. We see that it is indeed ≥ 1 till we reach a very high temperature, of the order of 10^{22} Kelvin, at which our probability distribution no longer makes sense. We have already encountered above this effect, in connection with $\left\langle x^2\right\rangle$-graph, the entropy, and the specific heat.

6. Conclusions

In deceptively simple fashion, we have regularized the partition function for Brownian functions moving in an external potential, thus solving a very old

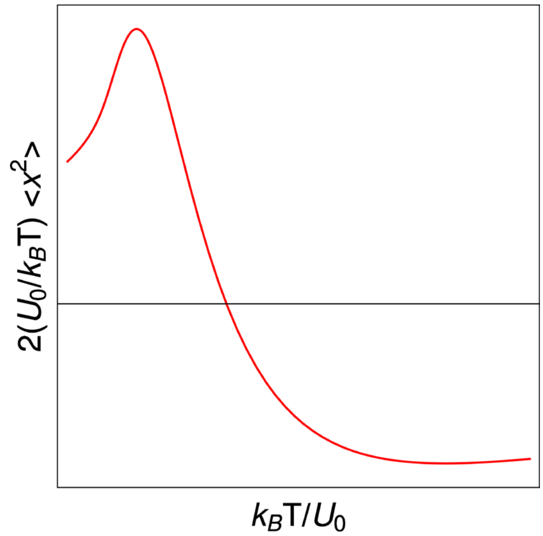

Figure 5. The product of $\langle x^2 \rangle$ times Fisher's information measure (Cramer-Rao) (in appropriate units). The well-known associated bound is seen to be violated for temperatures higher than 10^{22} Kelvin (see text).

problem. Some other special cases were already treated by the present authors. One is that of the Z-expression in the case of Newton's gravity [12], where the divergences are of a different nature from the ones here discussed. A second case is that of Fermi's problem, cited in the Introduction [23]. Our treatment displays two noticeable features.

- Being of a classical nature, it fails at very low temperatures, where quantum effects become predominant.
- At extremely high temperatures, of the order of 10^{22} Kelvin, we face a T-upper bound. This fact has already been reported, in another context, by Refs. [12] [13]. Our partition function is saying to us that the system can not exist at such high temperatures.

Summing up: We were here tackling partition function' divergences, a physically-motivated mathematical problem, that we indeed solved. As for applications, the most we can say at this stage is that we have at our disposal a new canonical probability distribution. Can one use the concomitant partition function Z in a concrete problem? To answer this question, more research is needed. We guess that with this Z some density distribution might be constructed that could describe a quasi-stationary solution in some suitable scenario.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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