BERNSTEIN POLYNOMIALS: A BRIDGE BETWEEN THE WEIERSTRASS THEOREM AND A LANDAU TEMPERATURE FLUCTUATION PROBLEM

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Abstract

We address a Landau temperature fluctuation problem by applying Bernstein polynomials and the Weierstrass approximation theorem. We consider the problem detailed in [X. Wang and Q.H. Liu, *Temperature fluctuations for a finite system of classical spin-1/2 particles*, Annals of Physics 322 (2007), 2168-2178] in which temperature fluctuations diverge as the temperature of a particle system tends to 0. An application of Bernstein polynomials allows us to solve this issue by proving that the m'th moment of the configurational temperature of a finite particle system tends to the temperature of the surroundings, implying the fluctuations in the temperature must tend to 0.

1 Introduction

Throughout history, pure math and theoretical physics have gone hand-in-hand. Frequently, pure math will discover an important principle that seems disconnected from reality, but upon further inspection, there is a profound application in physics. For example, group theory was developed hundreds of years ago and, upon the invention of quantum mechanics, found an application in describing the spin states of elementary particles through the special unitary group. This illustrates a deep connection between physics and pure math; even the most abstract idea in math can find an incredible application in describing reality.
Another aspect of theoretical physics that can see an application of pure math is the Landau thermodynamic problem. In the standard examination of particle systems, theory predicts a strange occurrence: as the temperature of the surrounding system drops to 0 K, the fluctuations in the temperature grow without bound. This seems to be dissonant with a physical interpretation of a spin system, for temperature fluctuations growing infinitely large has no real meaning. By utilizing Bernstein polynomials, a topic rooted firmly in analysis, we may be able to solve this problem, justifying the much more reasonable idea that the temperature fluctuations tend to 0 as the temperature tends to 0. X. Wang and Q.H. Liu [3] were the first to document this method of solving the problem. This paper provides the mathematical rigor behind their solution. We first must review their work before stating our main theorem.

If we are to assume a system of practically infinite ($N > 10^{23}$), spin-1/2 particles, the temperature fluctuation is defined as

$$\overline{(\Delta T)^2} = \frac{kT_{\text{can}}^2}{C_B} \tag{1}$$

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where k is the Boltzmann constant, T_{can} is the fixed temperature of the surrounding system, and C_B is the heat capacity for the system. This heat capacity is

$$C_B = Nk\left(\frac{\epsilon}{kT_{\text{can}}}\right)^2 \operatorname{sech}^2\left(\frac{\epsilon}{kT_{\text{can}}}\right) \tag{2}$$

where ϵ is the energy quantum of independent, spin-1/2 nuclei in a magnetic field B in thermal equilibrium. From this, it can be seen that

$$\overline{(\Delta T)^2} = \frac{k^2 T_{\text{can}}^4}{\epsilon^2 N}\cosh^2\left(\frac{\epsilon}{kT_{\text{can}}}\right) \tag{3}$$

This is where the Landau temperature fluctuation problem arises. Equation (3) shows that $\overline{(\Delta T)^2} \to \infty$ as the temperature, T_{can}, tends to 0; a result of the hyperbolic cosine function diverging as the argument grows infintely large. As seen in Landau and Lifshitz's statisitcal mechanics textbook [1], deriving these equations implicitly presumes the temperature fluctuations are small, and so the result requires statistical methods when the fluctuations diverge.

To attempt to solve this problem, let's introduce a system A of a finite number N particles. Consider this system as a small fraction of a much larger closed one A_0, where the rest of the closed system, A_b, makes up the surrounding environment with M particles. So the full system $A_0 = A \oplus A_b$. Using this definition, when $T_{\text{can}} = 0$ K, all of the particles are spin-up. When $T_{\text{can}} \neq 0$, there are n_0 spin-down particles among the $M + N$ total particles. In such a system, we can define the temperature T_{can} as

$$T_{\text{can}} = \frac{2\epsilon}{k}\left[\ln\left(\frac{M+N}{n_0} - 1\right)\right]^{-1} \tag{4}$$

Since this temperature is the temperature of the surrounding environment A_b, every particle has the same probability p to be spin-down, with p given by

$$p \equiv \frac{n_0}{M+N} = \frac{\exp\left(-\frac{\epsilon}{kT_{\text{can}}}\right)}{\exp\left(-\frac{\epsilon}{kT_{\text{can}}}\right) + \exp\left(\frac{\epsilon}{kT_{\text{can}}}\right)} \tag{5}$$

Since the temperature of the system A is not T_{can} if N is relatively small, we can assume $n_0 > N$, implying the number M is so large that $n_0 = p(M+N) > N$ can be satisfied.

If we assume that at an instant t, there is a configuration of n spin-down particles and $N - n$ spin up particles, then the configuration appears with probability

$$\binom{N}{n} p^n (1-p)^{N-n} \tag{6}$$

by using the binomial probability distribution. Then, as specified in the standard treatment [1], the configurational finite N temperature $T(n, N)$ is defined as

$$T(n,N) = \begin{cases} 0 & n = 0, N \\ 0 & n = \frac{N}{2} \text{when } N \text{ is even} \\ \frac{2\epsilon}{k}(\ln(\frac{N-n}{n}))^{-1} & \text{otherwise} \end{cases} \tag{7}$$

This definition suffers from a discontinuity when N is even. A similar situation happens when the number of particles N is odd. When N is odd, we get

$$T(n,N) = \begin{cases} 0 & n = 0, N \\ \frac{2\epsilon}{k}(\ln(\frac{N-n}{n}))^{-1} & \text{otherwise} \end{cases} \tag{8}$$

In this ensemble, the mean value of a quantity $f(n, N)$ is defined as

$$\overline{f}(p,N) = \sum_{n=0}^{N} f(n,N)\binom{N}{n} p^n (1-p)^{N-n} \tag{9}$$

and so the mth moment of the configurational temperature is

$$\overline{T^m}(p,N) = \sum_{n=0}^{N}(T(n,N))^m \binom{N}{n} p^n (1-p)^{N-n} := T \tag{10}$$

We now arrive at our main theorem.

Theorem 1. *If* $\overline{T^m}(p,N)$ *is given by (10), then*

$$\lim_{N\to\infty} \overline{T^m}(p,N) = \left(\frac{2\epsilon}{k}\frac{1}{\ln(\frac{1}{p}-1)}\right)^m = (T_{can})^m \tag{11}$$

When $m = 1$, we recover the probability given by the Maxwell-Boltzmann distribution through algebraic manipulations. This shows that, in the thermodynamic limit, temperature fluctuations do not diverge. In other words,

$$\lim_{N\to\infty} \overline{(\Delta T)^2} = 0 \quad (0 < T_{\text{can}} < \infty) \tag{12}$$

The key behind proving equation (11) is modifying a proof of the Weierstrass approximation theorem. The proof in question hinges on the idea of a Bernstein polynomial. We define this polynomial now [2].

Definition 1 (Bernstein Polynomial)**.** *A polynomial of the form*

$$B_{n,k}(x) = \binom{n}{k} x^k (1-x)^{n-k}, \;\; k \in \{0,...,n\} \tag{13}$$

This polynomial is very reminiscent of the probability mass function of a binomial random variable X with parameters n trials, k successes, and a probability of success x. This implies the polynomial is always nonnegative (as probability distributions are always nonnegative) and implies that the sum over the entire polynomial is 1, for a fixed x.

$$\sum_{k=0}^{n} \binom{n}{k} x^k (1-x)^{n-k} = 1 \tag{14}$$

Some special values related to the binomial random variable are the expectation and variance. These can come in handy when proving things using these polynomials. The expectation is defined as

$$E(B_{n,k}(x)) = \sum_{k=0}^{n} k B_{n,k}(x) = nx \tag{15}$$

while the variance is

$$\sigma^2 = nx(1-x) \tag{16}$$

These values come from the standard definition of the expectation and variance of a random variable. There's an interesting point, see [2] for example. By manipulating equations (15) and (16), we can see

$$\sum_{k=0}^{n} \frac{k}{n} B_{n,k}(x) = x \tag{17}$$

and

$$\sum_{k=0}^{n} \left(\frac{k}{n} - x\right)^2 B_{n,k}(x) = \frac{x(1-x)}{n} \tag{18}$$

This is akin to assigning $B_{n,k}$ as the probability to the 'events' $\frac{k}{n}$ and taking the expectation and variance. These equations will be more useful to us.

2 Proof of the Weierstrass Theorem and Landau's Temperature Fluctuation Law

We are now sufficiently equipped to prove the Weierstrass approxmation theorem and Landau's temperature fluctuation law. A modification of the proof of the former will give us the proof of the latter. The following proof is given in a note by M. Loss [2]:

Theorem 2 (Weierstrass Approximation Theorem). *Let $f : [0,1] \to \mathbb{R}$ be a continuous function. Define the polynomial*

$$B_n(f)(x) := \sum f\left(\frac{k}{n}\right) B_{n,k}(x). \tag{19}$$

Then for any $\epsilon > 0$, there exists N such that $\forall n > N$ and all $x \in [0,1]$, $|B_n(f)(x) - f(x)| < \epsilon$.

This theorem claims this polynomial will approximate a function f to arbitrary accuracy on an interval where f is continuous.

Proof. Since f is continuous on the closed interval, it is uniformly continuous. This means for every $\epsilon > 0$, there exists some $\delta > 0$, depending only on ϵ, such that $|f(x) - f(y)| < \frac{\epsilon}{2}$ when $|x - y| < \delta$. Then consider the following quantity:

$$B_n(f)(x) - f(x) = \sum_{k=0}^{n} f\left(\frac{k}{n}\right) B_{n,k}(x) - f(x) \sum_{k=0}^{n} B_{n,k}(x) \tag{20}$$

$$= \sum_{k=0}^{n} \left[f\left(\frac{k}{n}\right) - f(x) \right] B_{n,k}(x) \tag{21}$$

where the first step follows from the fact that a sum over the entirety of a probability distribution is 1. Then consider splitting the sum at $|\frac{k}{n} - x|$, depending on when it's above and below δ. Our goal is to bound the following distance by some ϵ.

$$|B_n(f)(x) - f(x)| \leq \sum_{|\frac{k}{n}-x|<\delta} \left| f\left(\frac{k}{n}\right) - f(x) \right| B_{n,k}(x) + \sum_{|\frac{k}{n}-x|\geq\delta} \left| f\left(\frac{k}{n}\right) - f(x) \right| B_{n,k}(x) \tag{22}$$

This step uses the fact that the polynomial is nonnegative. Now we use the fact that f is uniformly continuous on the interval to obtain

$$|B_n(f)(x) - f(x)| \leq \frac{\epsilon}{2} \sum_{|\frac{k}{n}-x|<\delta} B_{n,k}(x) + 2\max|f(x)| \sum_{|\frac{k}{n}-x|\geq\delta} B_{n,k}(x) \tag{23}$$

In the second term of equation (23), we note the distance between any two values of f can't be greater than twice the maximum value of f, $2\max|f(x)|$. So we have

$$\sum_{|\frac{k}{n}-x|\geq\delta} B_{n,k}(x) = \sum_{|\frac{k}{n}-x|\geq\delta} \frac{|\frac{k}{n}-x|^2}{|\frac{k}{n}-x|^2} B_{n,k}(x) \leq \frac{1}{\delta^2} \sum_{|\frac{k}{n}-x|\geq\delta} \left|\frac{k}{n} - x\right|^2 B_{n,k}(x) \leq \frac{x(1-x)}{n\delta^2} \tag{24}$$

The second to last step uses the uniform continuity of f, while the last step uses the formula for the variance given in equation (18). Then in the distance inequality we are examining, we obtain

$$|B_n(f)(x) - f(x)| \leq \frac{\epsilon}{2} \sum_{|\frac{k}{n}-x|<\delta} B_{n,k}(x) + 2\max|f(x)| \frac{x(1-x)}{n\delta^2} \leq \frac{\epsilon}{2} + \frac{\max|f(x)|}{2n\delta^2} \tag{25}$$

The last step comes from the fact that the $x(1-x) \leq \frac{1}{4}$ on the interval $[0,1]$. So by choosing $n > \frac{\max|f(x)|}{\epsilon\delta^2}$, we arrive at

$$|B_n(f)(x) - f(x)| \leq \frac{\epsilon}{2} + \frac{\max|f(x)|}{2n\delta^2} \leq \epsilon \tag{26}$$

yielding the theorem. □

This theorem is quite interesting. The concept of approximating any continuous function with a polynomial is very enticing, especially in physics. To apply this to our problem, we need to make some modifications. From the definition of the configuational temperature (8), it's clear to see we don't have a continuous function. However, we have a way around this.
We can now mathematically show the configurational temperature of a finite N particle system will tend to T_{can} as $N \to \infty$. This provides a solution to the problem described by Landau.

Proof of Theorem 1. Let's define the function γ as follows:

$$\gamma(x) = \left(\frac{2\epsilon}{k} \left(\ln \left(\frac{1}{x} - 1 \right) \right)^{-1} \right)^m \tag{27}$$

This function has three points of discontinuity: 0, $\frac{1}{2}$, and 1. Since $\lim_{x\to 0^+} \gamma(x) = 0$ and $\lim_{x\to 1^-} \gamma(x) = 0$, the discontintuities at 0 and 1 are removable. Let's define γ to be 0 at these points. The discontinuity at $\frac{1}{2}$ is not removable, since both the left and right sided limits of γ do not exist. So consider a closed sub-interval $[a, b] \subset [0, 1]$ such that γ is continuous on $[a, b]$. This amounts to considering a closed sub-interval of $[0, 1]$ that does not contain $\frac{1}{2}$.
Let's consider the distance $|\overline{T^m}(p, N) - \gamma(p)|$ where $p \in [a, b]$. We know

$$\begin{aligned} |\overline{T^m}(p, N) - \gamma(p)| &= \left| \sum_{n=0}^{N} \left(T(n, N)^m \binom{N}{n} p^n (1-p)^{N-n} \right) - \gamma(p) \sum_{n=0}^{N} \binom{N}{n} p^n (1-p)^{N-n} \right| && (28) \\ &= \left| \sum_{n=0}^{N} \left(T(n, N)^m B_{N,n}(p) \right) - \gamma(p) \sum_{n=0}^{N} B_{N,n}(p) \right| && (29) \\ &\leq \sum_{n=0}^{N} \left| T(n, N)^m - \gamma(p) \right| B_{N,n}(p) && (30) \end{aligned}$$

where the third line follows from the fact that Bernstein polynomials are strictly non-negative. Now since γ is continuous at p, we know for every $\epsilon > 0$, there exists some $\delta > 0$ such that $|\gamma(x) - \gamma(p)| < \frac{\epsilon}{2}$ when $|x - p| < \delta$. Let's split (30) according to when $|\frac{n}{N} - p|$ is less than or greater than δ.

$$|\overline{T^m}(p, N) - \gamma(p)| \leq \sum_{|\frac{n}{N} - p| < \delta} \left| \gamma\left(\frac{n}{N}\right) - \gamma(p) \right| B_{N,n}(p) + \sum_{|\frac{n}{N} - p| \geq \delta} \left| T(n, N)^m - \gamma(p) \right| B_{N,n}(p) \tag{31}$$

Now the distance in the first sum of (31) will be less than $\frac{\epsilon}{2}$. Now we need to examine the righthand sum of (31). We will break this up into two cases; one where $|\frac{n}{N} - \frac{1}{2}| < \delta$ and one where $|\frac{n}{N} - \frac{1}{2}| \geq \delta$. Let's first assume $|\frac{n}{N} - \frac{1}{2}| < \delta$. We note the following asymptotic behavior: when $N \to \infty$,

$$B_{N,n}(p) \sim b_{\text{approx}}(p) = \frac{1}{\sqrt{2\pi n(1 - \frac{n}{N})}} e^{-\frac{(Np-n)^2}{2n(1-\frac{n}{N})}} \tag{32}$$

as a result of the normal distribution approximation to the binomial distribution using the central limit theorem. Using (32), we can see that $|T(n, N)^m| B_{N,n}(p) \sim |T(n, N)^m| b_{\text{approx}}(p)$. We can also see that since $|\frac{n}{N} - \frac{1}{2}| < \delta$, we have $|T(n, N)^m - \gamma(p)| \leq 2|T(n, N)^m|$ due to the singularity of $T(n, N)^m$. If $T(n, N)$ is 0, then (32) dominates $\gamma(p)$. Let's split the right hand sum in (31) into the following:

$$\begin{aligned} \sum_{|\frac{n}{N} - p| \geq \delta} \left| T(n, N)^m - \gamma(p) \right| B_{N,n}(p) = &\sum_{\substack{|\frac{n}{N} - p| \geq \delta \\ |\frac{n}{N} - \frac{1}{2}| < \delta}} \left| T(n, N)^m - \gamma(p) \right| B_{N,n}(p) \\ &+ \sum_{\substack{|\frac{n}{N} - p| \geq \delta \\ |\frac{n}{N} - \frac{1}{2}| \geq \delta}} \left| T(n, N)^m - \gamma(p) \right| B_{N,n}(p) \end{aligned} \tag{33}$$

Now utilizing the facts above, we can transform this first portion in (33).

$$\sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|<\delta}} |T(n,N)^m - \gamma(p)|\, B_{N,n}(p) \leq 2 \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|<\delta}} |T(n,N)^m|\, b_{\text{approx}}(p) \tag{34}$$

So we have this $|T(n,N)^m| b_{\text{approx}}(p)$ term in the sum. In the summands, we have $|\frac{n}{N} - p| \geq \delta$, so $b_{\text{approx}}(p) \leq \frac{1}{\sqrt{N}} e^{-2N\delta^2}$ and due to the restriction $|\frac{n}{N} - \frac{1}{2}| < \delta$, we have $T(n,N)^m \leq (\ln(\frac{2N}{N\pm1} - 1))^{-m}$ as the worst term. We can also see that (34) has around δN terms. This means we have:

$$2 \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|<\delta}} |T(n,N)^m|\, b_{\text{approx}}(p) \leq 2N\delta \left(\ln\left(\frac{2N}{N\pm1} - 1 \right) \right)^{-m} \frac{1}{\sqrt{N}} e^{-2N\delta^2} \tag{35}$$

We can see that as $N \to \infty$, the right hand side of (35) tends to 0. So the first sum in the right hand side of (33) can be ignored. This means we get the following

$$\sum_{|\frac{n}{N}-p|\geq\delta} |T(n,N)^m - \gamma(p)|\, B_{N,n}(p) \to \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} |T(n,N)^m - \gamma(p)|\, B_{N,n}(p), \quad N \to \infty \tag{36}$$

Since we are working in a closed interval where γ is continuous, the extreme value theorem will tell us that γ is bounded above by some M. So the distance in the right-hand side of (36) is guaranteed to be less than $2M$. From this we achieve

$$|\overline{T^m}(p,N) - \gamma(p)| \leq \sum_{|\frac{n}{N}-p|<\delta} |T(n,N)^m - \gamma(p)|\, B_{N,n}(p) + \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} |T(n,N)^m - \gamma(p)|\, B_{N,n}(p) \tag{37}$$

$$\leq \frac{\epsilon}{2} \sum_{|\frac{n}{N}-p|<\delta} B_{N,n}(p) + 2M \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} B_{N,n}(p) \tag{38}$$

Now examining the second sum in (38), we can perform the following manipulation:

$$\sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} B_{N,n}(p) = \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} \frac{|\frac{n}{N} - p|^2}{|\frac{n}{N} - p|^2} B_{N,n}(p) \tag{39}$$

$$\leq \frac{1}{\delta^2} \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} \left| \frac{n}{N} - p \right|^2 B_{N,n}(p) \tag{40}$$

$$\leq \frac{p(1-p)}{N\delta^2} \tag{41}$$

The last step follows from substituting the variance given in (18). Now we can see

$$|\overline{T^m}(p,N) - \gamma(p)| \leq \frac{\epsilon}{2} \sum_{|\frac{n}{N}-p|<\delta} B_{N,n}(p) + 2M \sum_{\substack{|\frac{n}{N}-p|\geq\delta \\ |\frac{n}{N}-\frac{1}{2}|\geq\delta}} B_{N,n}(p) \leq \frac{\epsilon}{2} + \frac{2Mp(1-p)}{N\delta^2} \tag{42}$$

Since the quantity $p(1-p)$ is always less than $\frac{1}{4}$ on the interval $[0,1]$, this must also be true for the sub-interval $[a,b]$. So

$$|\overline{T^m}(p,N) - \gamma(p)| \leq \frac{\epsilon}{2} + \frac{2Mp(1-p)}{N\delta^2} \leq \frac{\epsilon}{2} + \frac{M}{2N\delta^2} \tag{43}$$

So by choosing $n_0 > \frac{M}{\epsilon\delta^2}$, we can see that when $N > n_0$,

$$|\overline{T^m}(p, N) - \gamma(p)| \le \frac{\epsilon}{2} + \frac{M}{2N\delta^2} \le \epsilon \tag{44}$$

□

This means we arrive at the following statement:

$$\forall \epsilon > 0,\ \exists n_0 \text{ s.t. } |\overline{T^m}(p, N) - \gamma(p)| < \epsilon,\ \forall N > n_0 \tag{45}$$

This precisely means $\lim_{N\to\infty} \overline{T^m}(p, N) = \gamma(p) = (T_{\text{can}})^m$ for p in the sub-interval $[a, b]$. Since this is an arbitrary sub-interval of $[0, 1]$ not including $\frac{1}{2}$, we can say $\overline{T^m}(p, N)$ converges to $\gamma(p) = (T_{\text{can}})^m$ on the set $[0, \frac{1}{2}) \cup (\frac{1}{2}, 1]$. The influence of the proof of Theorem 2 is apparent. The main change that is required is examining closed sub-intervals of the interval where γ is defined. This proof also gives insight into why the temperature fluctuations tend to 0 as N grows large. The configuational temperature of the system A, as the number of particles grows large, will tend to the temperature of the surroundings. A rewording of the last statement of the above proof can describe this more clearly:

$$\forall \epsilon > 0,\ \exists n_0 \text{ s.t. } |\overline{T}(p, N) - T_{\text{can}}| < \epsilon,\ \forall N > n_0,\ m = 1 \tag{46}$$

Any fluctuation in temperature will be reflected in the value $\overline{T}(p, N)$. Since we have determined that the distance between this temperature and the temperature of the surroundings T_{can} must be bounded, any fluctuation in temperature must also be bounded. Furthermore, as $\overline{T}(p, N)$ gets closer to T_{can}, the fluctuations will necessarily get smaller, implying the fluctuations tend to 0 as N grows large.

3 Discussions and Conclusions

The main result of this paper is a mathematical proof of (11), as X. Wang and Q.H. Liu [3] presented. We aimed to reconcile the dissonance between the current models of a spin system and the supposed infinite temperature fluctuations that are predicted. Our proof provides a rigorous connection between the Landau thermodynamic problem and analysis, specifically by using Bernstein polynomials to understand why the temperature fluctuations of a finite particle system tend to 0, even as the temperature of the surrounding heat bath tends to 0 K.

This paper provides a rigorous foundation for the newly proposed ensemble, thereby further validating the previous physics-based work on the subject.

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