Reflections on Gibbs: From Statistical Physics to the Amistad

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abstract

J. Willard Gibbs, the younger was the first American theorist. He was one of the inventors of statistical physics. He introduced and developed the concepts of phase space, phase transitions, and thermodynamic surfaces in a remarkably correct and elegant manner. These three concepts form the basis of different areas of physics. The connection among these areas has been a subject of deep reflection from Gibbs' time to our own. This talk therefore tries to celebrate Gibbs by talking about modern ideas about how different parts of physics fit together.

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How do theories fit together?

Older ideas suggest physical theories merge via a limiting process in which some parameter smoothly approaches its final value. Thus classical mechanics might emerge as a limit of quantum mechanics as S goes to zero. This view seems just a bit tame, and not quite right. A newer view, which I describe as a theory of "singular connections" is suggested by the work of Michael Berry and explicitly put forward by Robert Batterman. This view replaces the metaphor of limits by one based upon the applied mathematics ideas of asymptotic behavior and of singular perturbations.

Singular Connections

Consider the relation between quantum theory and classical mechanics. The metaphors of singularity and asymptotics permits and encourages us to think that three different conceptualizations might be needed to describe in the two limiting cases and, in addition, the territory in between.

I shall describe the singular connections approach using two examples close to Gibbs: the Gibbs phenomenon in Fourier series and the relations among the parts of statistical physics.

At the end of the talk, I shall get to a more personal note. Our own J. Willard Gibbs had all his achievements concentrated in science. His father, also J. Willard Gibbs, also a Professor at Yale, had one great achievement that remains unmatched in our day. I shall describe it.

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Sources

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J. Willard Gibbs' Scientific Contributions

He was a theorist interested in the mathematical and theoretical structure of his problems. He was extremely careful to publish and utter only true things about physics and mathematics.

minor idea: dot and cross products in vector calculus.

not so minor: Apparently Gibbs held to the modern idea that a vector was a thing in itself, while others confused the components with the object.

The "Gibbs Phenomenon" in Fourier Theory.(Stokes?)

Statistical Mechanics
Invented phase space and ensemble theory

Thermodynamics
Invented thermodynamic surfaces and chemical potentials. Recognized that thermodynamics is true independent of micro models.

Phase Transitions
Invented the 'phase rule' which described the equilibrium among phases. Recognized that phase transitions only happen in infinite systems.

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Gibbs struggled with connecting different parts of statistical physics

See, Yale Conference Volume

A.S. Wightman p.34

> There is one aspect of the thermodynamic limit that Gibbs does not emphasize. That is the appearance of phase transitions between distinct thermodynamic phases. [S]harp phase transitions do not occur in finite systems. A little more pedagogical zeal by Gibbs could have saved some of the generations that followed considerable time. [...] Gibbs could have told them that it was pointless to discuss [phase transitions] except in the thermodynamic limit.

The technical word used by both physicists and philosophers for this process of connection is reduction. Unfortunately one group would insist that quantum theory reduces to classical while the other would suggest that reductions works in just the opposite sense. I'll stick with the word connection which is more neutral.

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Simple Limiting Process

Sometimes the connections are very simple. The pendulum's motion becomes identical to that of a simple harmonic oscillator whenever the pendulum oscillates weakly and remains close to its equilibrium position. The connection involves a low-energy limit of the pendulum and a limiting process just about as simple as the one by which the calculus' derivative operation is defined. The concept of a limit is not fully transparent to an unprepared mind. (Think of the troubles of Bishop Berkeley with derivatives, or of many generations with the limiting processes involved in Achilles catching up with and then passing the tortoise.) However, it is now familiar and direct, so that all theory connections which involve only the simple version of the concept of limits may be said to be well understood.

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Something Missing/Extra

But the concept of a simple limit does not seem to describe the kinds of limiting process which really occur in relating different domains of physical science. In doing a simple limit, you don't get anything really new, the old thing morphs smoothly into its limiting form. However think of our usual examples of theory connection as exemplified by the following table: (display table)\

In short the limiting theories do not talk the same language, and neither talk the language of the intermediate case.

Michael Berry (physicist and applied mathematician) and Robert Batterman (philosopher) have addressed the general question of connections, while many many other people have looked at connections in individual instances. I shall spend a while describing their approach.

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first theory/ typical concept	second theory/ concept	intermediate case/concept
classical mechanics/ determinate motion	quantum mechanics/ probabilities	quasi-classical/ quantum chaos
thermodynamics [=of infinite systems] /phase transitions--discontinuities	finite N statistical mechanics/ smooth variation of everything	finite size scaling/ power law scaling
infinitely large system/entropy always increases deterministic	finite system/reversible behavior statistical prediction	Dynamical Systems theory/ chaos and determinacy coexist bifurcations catastrophes

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Connections

Batterman and Berry and everyone accepts that connections are done with limiting process, like taking □ to zero. However B&B argue that the right ideas of limits are borrowed from the concepts of singular limits and asymptotics of 20C math, not the simple limits of Newton and Liebnitz.

Concept I: singular perturbation: sometimes even a little □ is a lot. Example

$x-1 = 0$ one solution $x=1$. but perturbation problem has TWO solutions

$x-1 = \square x^2$ first solution $x=1+\square+2\square^2 + \dots$

second solution $x=\square^{-1}+1 +\square^2+\dots$

Here the small parameter controls the number of solutions. (A singular perturbation is identified whenever the highest order term in an equation is multiplied by a small parameter.)

Typically the interesting connection processes among different theories arise from singular perturbations.

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Concept II. The Asymptotic Expansion.

Usual power series like the familiar one

$e^{x} =1 +x +x^{2}/2! +...+ x^{n}/n! + ...$

define a interesting but a smooth behavior.You use the expansion by computing successive terms and adding them up. The more terms you add, the better is your answer. There is nothing left over, hard work will give you the whole function.

Consider in contrast a typical asymptotic expansion like the Sterling approximation to n!,

$\ln (n-1)! = n \ln n -n +0.5 \ln n - \ln (2 \pi)^{1/2} +O(1/n) +...$

For all n you get a pretty good answer from the first term. For higher n, you get a better answer by including more terms. But for each n, you should stop somewhere: there is an optimal number of terms to compute. If you go further you get a worse answer. (a story) An asymptotic analysis is accurate, as far as it goes, but can leave out something. For example, in the expansion of $\ln (n^{2}+ n!)$, we would never see the n^{2} in the asymptotic analysis because there are an Infinity of larger terms.

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A story

Tony Houghton and I were doing a renormalization group calculation very early in the history of such calculations. We had developed a theory and we were calculating a critical index called ν which described how the correlation exponent diverged as the temperature approached the critical temperature in the two-dimensional Ising model.

Our zeroth order theory gave $\nu_0=0.7$. The exact answer, according to the Onsager exact calculation was $\nu_{exact}=1$. Not too awful. After some work we got a first order result $\nu_1=0.9$. Not bad. More work gave $\nu_2=0.99$, better! Then, after much work we got the third order $\nu_3=0.999$. Great! We saw that we could, by working very hard, just accomplish the next order. We did it and finished the calculation, by finding $\nu_4=1.7$ .... We had found an asymptotic expansion! Some physics was left out, and that left-out physics prevented us from ever getting to the exact right answer.

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So ?

Typically singular perturbations describe situations in which there is very different behavior for different values of the small parameter. Typically, they can be effectively analyzed by using different asymptotic expansion in different regions of the behavior. Each expansion catches a part of the truth for that problem and leaves out another part.

In contrast ordinary power series expansions describe smooth behavior and contain all the physics in one go.

The right metaphor for connecting phase transition to the statistical mechanics of finite systems is not the power series expansion and the smooth approach to limits.   According to Berry and Batterman and much contemporary thought it is the asymptotic expansion which is demanded in the analysis of singular perturbations.

Berry showed this for waves and quantum chaos. Batterman developed a philosophical discourse on this subject. Let me give a little analysis of a simple problem, due to J. Willard Gibbs, the younger.

Gibbs' Error

J. Willard Gibbs, Nature Vol LIX p. 200 Dec. 29,1898.

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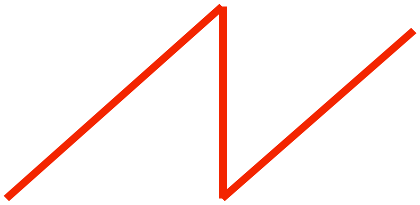
Consider the Fourier Series

$$f_N(x) = -2\sum_{n=1}^{N}\frac{(-1)^n}{n}\sin nx$$

cut off for large but not infinite values of N. Think of the analysis of this function as a simple example of a physics theory. Since the function in question is the Fourier series expansion of the periodically repeated function

$$g(x) = \begin{cases} x & \text{for} \quad -\pi < x < \pi \\ x - 2\pi & \text{for} \quad \pi < x < 3\pi \\ \quad \dots & \end{cases}$$



we might wish and expect to get "different" theories, for each interval, (-π,π), (π,3π), ...

Gibbs looks at the curves $y=f_N(x)$ for the different values of N. He then says that the curves approach the curve $y=g(x)$ as N goes to infinity. This is an error, as Gibbs soon recognized. show overshoot curves,

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Gibbs’ erratum appeared as

J. Willard Gibbs, Nature LIX p. 606 April. 27, 1899.

In this paper, Gibbs pointed to the overshoot (now called the Gibbs overshoot) and recognized that his statement about the approach of curves was wrong.

We would now analyze this situation as one that could be described by different “theories”,e.g.

1. x in $(-\pi,\pi)$ except very close to the ends, $f_N(x)$ is equal to x, except for small rapidly wiggling terms which go to zero as N goes to infinity.

2. x in $(\pi,3\pi)$ except very close to the ends, $f_N(x)$ is equal to $x-2\pi$, except for small terms at the boundaries. These are the analog of two similar but different theories which hold for different ranges of the parameters.

3. Very close to the boundary a third kind of theory is required, a scaling theory with very different concepts for the above. As, say, $x-\pi$ gets small we have

$H_N(z) = f_N(\pi + N z) \;\; H_\infty(z)$ (show scaling plot)

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Gibbs' analysis (?)

let x=π+y so that critical point is at y=0

$$f_N'(\pi + y) = \square 2 \sum_{n=1}^{N} \cos(ny)$$

$$= \square \frac{\sin(n+1)y}{\sin(y/2)}$$

use the variable z=ny to focus upon critical point

then

$$f_N'(\pi + nz) = \square \frac{\sin(1+1/n)z}{\sin(z/2n)}$$

$$\approx \square \frac{\sin z}{z/2n}$$

Here we have said that z is of order 1 and n is very large.The maximum of f nearest to the singularity occurs at z=π/2, i.e. x= π +π/(2n). Integrate the derivative to find the value at the maximum.

$$f_N(\pi + \pi/(2n)) \,\square\, f_N(\pi) \approx \int_0^{\pi/2} dz \frac{\sin z}{z/2} > 1$$

Note the overshoot and note that it is independent of n in the limit of large n.

Conclusion

From Gibbs' own example: A "theory" of the "physical" process of convergence of this Fourier series requires different behaviors and different conceptualizations in different regions. This is because the N goes to infinity limit produces, in essence, a singular perturbation and requires an asymptotic analysis.

In a much more sophisticated sense, this same story describes the connection between wave optics and ray optics (Michael Berry) and among a wide class of other problems (Robert Batterman).

In a slightly different sense, the modern theory of fluctuation-dominated phase transition behavior is an intermediate asymptotics between Gibbs' theory of thermodynamic phases for infinite systems and Gibbs' probablisitic and ensemble related theory of statistical equilibrium in finite dimensional phase space.

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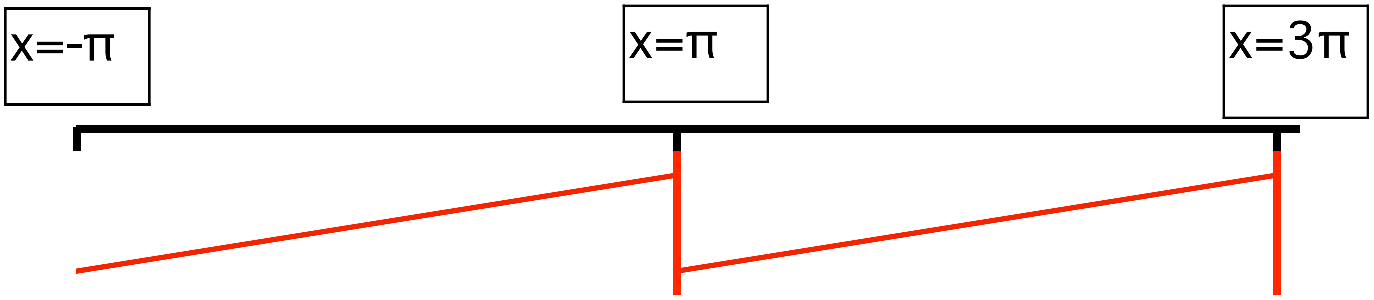
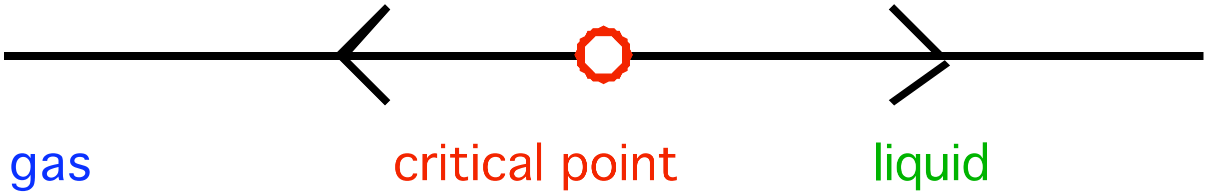
Pictures: From Analysis to Metaphor

Gibb’s Fourier Series: Asymptotic Analysis



enables us to analyze different regions of behavior

Phase Transitions: Renormalization group flow



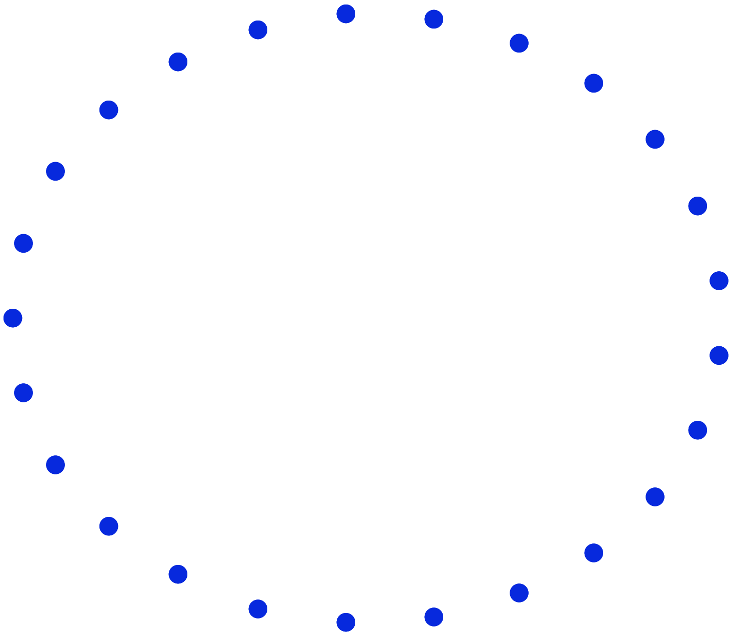
three phases of matter are described by an
asymptotic analysis

Theory Connections: Different Kinds of Theories

Finite N/ Critical Behavior/ Thermodynamic Phases
are also asymptotically connected

Another example: Grainy Charges

Now think about a grainy problem: n changes with strength 1/n all arranged on a conductor. For simplicity let the conductor be a circle.



the charges are at

$z_j=x+iy=\cos \Box_j +i \sin \Box_j =\exp(i \Box_j) =\exp(2 \pi i j/n)$

j^{th} root of unity. The complex potential is

$$\Box_n(z) = \Box(1/n) \Box_j \ln(z-z_j) = \Box(1/n) \ln \Box_j (z-z_j)$$

$$=\Box(1/n) \ln (z^n-1)$$

Homework: derive the “theories” which describe this potential asymptotically in its 3 regions. Extra credit: Do the same for the equilibrium distribution of equal line charges on a square 2d conductor.

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Credits

The coulomb problem has been mostly solved by

Maciej Nicewicz, Marko Kleine Berkenbusch, Isabelle Claus, Shankar Venkataramani, Paul Wiegmann, Katherine Dunn and LeoKadanoff.

Graphs here by Marko Kleine Berkenbusch

I had useful discussions with Robert Batterman and earlier with Michael Berry.

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The Amistad:

Even more than most academics, J. Willard Gibbs, Jr. led an uneventful life, far from the great events of his day. (Of course, as Muriel Rukeyser pointed out his ideas were in themselves a great event of his era, but that's different) . His father J. Willard Gibbs, Sr. also a Yale academic, a philologist, also spent almost all of his life far from the press of real life.

The senior Gibbs had one notable real-world achievement, connected with the arrival of the rebellion-torn slave ship Amistad from Cuba. President Van Buren wanted the mutineers to be considered, in modern terms, terrorists and sent back-- without trial-- to Cuba. Since nobody seemed to know their language, a return without a real hearing appeared inevitable. But Gibbs used gestures to found out how they counted and called out the number-words thus garnered at the port of New York. In this way, he found two translators. The translators gave voice to these captives and enabled them to convince the courts of their innocence. Thus, the senior J. Willard Gibbs gave a trial and justice to these accused terrorists.

Nobody, in our day, has equalled this achievement for our prisoners now being held in Cuba.