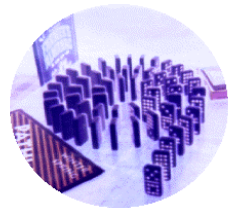
Heat Capacity in Bits

P. Fraundorf
UM-StL: Physics&Astronomy/CME
Washington U: Physics/MCSS



The developing awareness of entropy as *lack of correlation* between system and environment can be used by intro-physics teachers to deepen student insight into widening applications of information physics e.g. in molecular biology and computer science.

Today I’d like to talk a bit about how and why the intro-physics classroom might be a good place to define natural as well as historical units for thermal physics quantities, like temperature and heat capacity.

Acknowledgements

Direct: Inspiration by Mike Kraus and fellow students at UM-StL, by E. T. Jaynes, and by AAPT colleagues committed to never-ending work on the details of content-modernization. Feedback and clarifying reviews from Keith Stine at UM-StL and AJP.

Indirect: U. S. Dept of Energy, Missouri Research Board, Monsanto and MEMC Electronic Materials Companies.

Lots of my time is spent studying materials with sub-nanometer-resolution electron and scanning force microscopes. Thanks to inspiration *and some fantastic notes* by the late E. T. Jaynes at Washington University, I can also offer some perspective on ways that the statistical approach to thermal physics (having pretty much taken over the senior undergraduate textbook market) has even better things in store for the introductory physics class.

Deep simplifications offered by Minkowski, Feynman, and Shannon are only beginning to have the impact they will have in the introductory science classroom.

cf. recent work by E. F. Taylor and T. A. Moore.

Gambling Theory connects…
The Logic of Science with *The Physics of Information*

cf. E. T. Jaynes, and senior undergrad texts since.

Key Concepts:

- Multiplicity and it's Logarithm
- Uncertainty Slopes & Best Guesses
- Multiplicity Exponents
- Net Surprisals: Deviations from Expected

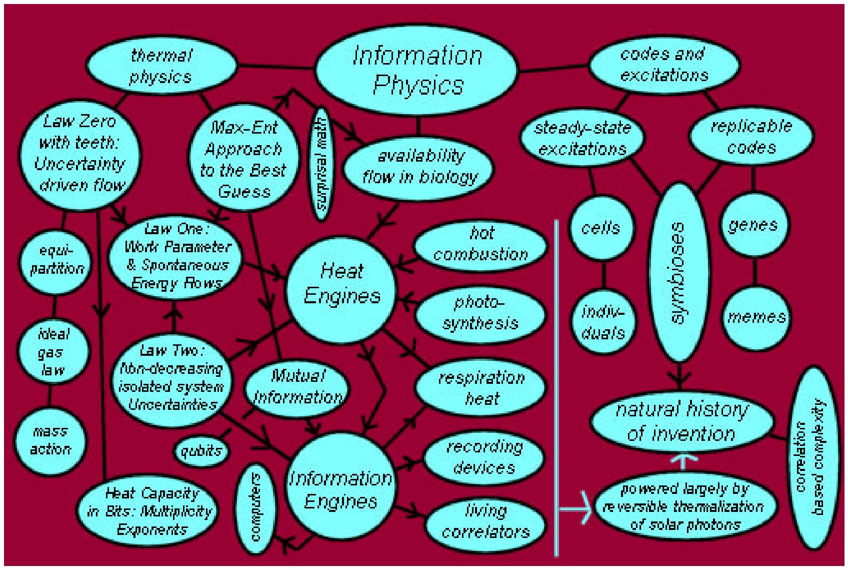
This Talk

(i) The metric equation (Minkowski), least action (Feynman & others), and information physics (Shannon) all offer ways to significantly improve intro-student capabilities, while clearing up dissonance between traditional pedagogy and forefront research. There are folks at this conference who know a lot about the challenges.

(ii) In this talk we focus on the power of statistical inference to give shape to the laws of thermal physics, and to extend them to complex systems as well as to the study of replicable codes.

(iii) Key concepts of gambling theory as applied to physical systems are multiplicities and it's logarithm entropy, and max-ent tools for deriving state equations from information on physical constraints that apply to a system. Over the past 5 decades these have become ubiquitous in senior undergraduate and graduate treatments of thermal physics, and are slowly working their way into the introductory classroom. Tom Moore's Six Ideas book is one example. We'll go over some math underlying these, as well as the last two items in the list above, shortly.

Relevance in the Introductory Class…



In addition to giving form to the laws of thermal physics, gambling theory shows how these laws have implications for available-work flow in biological systems. It provides ways to compress data, as well as tools for understanding symbioses between replicable codes and steady-state excitations that underlie the natural history of invention. The recent Sci Am article on chain letter and mitochondrial DNA trees is an example. These processes impact the everyday life of the majority of consumers and taxpayers. If folks get only one physics course, it is better they learn about the physics of information there rather than from the tabloids.

Gambling Theory (MaxEnt) Review

Multiplicity and it's log:	$S = k \ln \Omega$ in [nats, bits, or J/K] if $k \equiv [1, \frac{1}{\ln 2}, k_B]$
Uncertainty Slopes and Best-Guess Eqns of State:	X equilibrated $\Rightarrow S_{tot}$maxmized $\Rightarrow$ all $\frac{\partial S_i}{\partial X}$ equal $\Omega \propto U^{\frac{\nu N}{2}} \Rightarrow U = \frac{\nu N}{2} kT$ where $\frac{\partial S}{\partial U} \equiv \frac{1}{kT}$ $\Omega \propto V^N \Rightarrow PV = NkT = nRT$ where $\frac{\partial S}{\partial V} \equiv \frac{P}{kT}$
Multiplicity Exponents:	$\xi_U \equiv \frac{U}{kT} = U \frac{\partial S}{\partial U}$ and $C_U/k \equiv \frac{1}{k}\frac{\partial U}{\partial T} = T \frac{\partial S}{\partial T}$
Net Surprisal & dev. from expected (e.g. free energy over kT & mutual information):	$I_{net} \equiv -k \sum_{i=1}^{\Omega} p_i \ln(\frac{p_{oi}}{p_i}) \geq 0,$ $\frac{I_{net}}{k} = \frac{\nu}{2} N \Theta[\frac{T}{T_o}] + \sum_j N_j \Theta[\frac{N_{jo}}{N_j}]$ where $\Theta[x] \equiv x - 1 - \ln x \geq 0$

future links: story #1, #2, #3; puzzler #1, #2, #3; faq; read more about it

For each row, note the relationship discussed, and it's units.

(i) Defining surprisal as the log of probability's reciprocal for each accessible state, average surprisal (entropy, uncertainty) has information units (how many are familiar with this?);

(ii) Max-ent best guesses yield intensive Lagrange multipliers, often derivatives that involve entropy and an extensive conserved quantity X, which "equilibrate as initial conditions fade" making temperature an energy derivative that's not always proportional to total energy, much as acceleration is not always proportional to velocity, in spite of occasional textbook allusions to the contrary (how many have seen this?);

(iii) Dimensionless integral and differential capacities (elaborate here) then have units of what? (Answer: bits per 2-fold increase in X or one of it's multipliers); and

(iv) Net-surprisals in information units measure finite deviations from expected, and reduce near equilibrium to availabilities (free energy over kT) and in the case of correlated subsystems to mutual information now so fashionable in the study of evolving codes, nonlinear dynamics, and quantum computing.

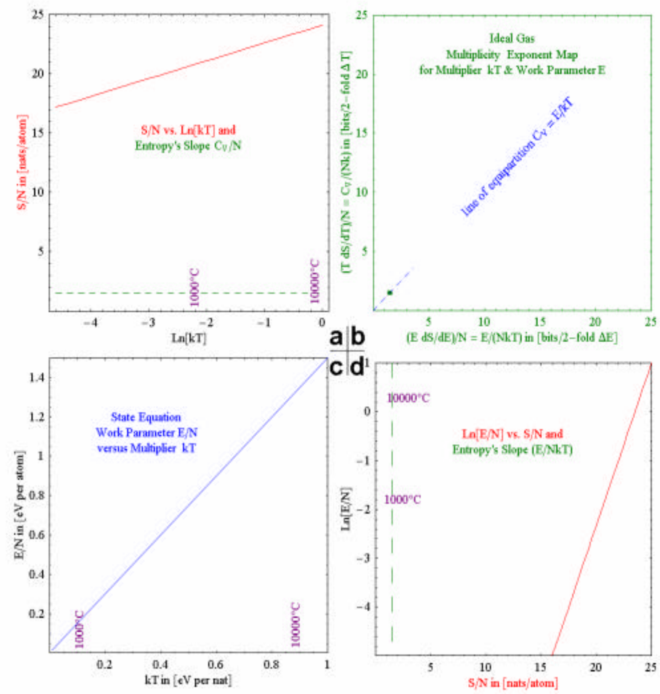
Note on multiplicity exponent partials: dS/dU, dU/dT and dS/dT may be no-work partials, and might also be defined with ensemble constraints e.g. if an appropriate enthalpy is allowed to substitute for U. This slide, by the way, is example of one kind of visual sound-byte (or light-meme) that might have a variety of auxiliary classroom uses, if linked to suitable supporting materials on the web.

Argon’s
Multiplicity
Map

Ideal gas
model
Argon: a
simple
quadratic
system

key:

(a) S/N vs. ln[kT]
(b) exponent map
(c) Energy/N vs. kT
(d) ln[E/N] vs. S/N



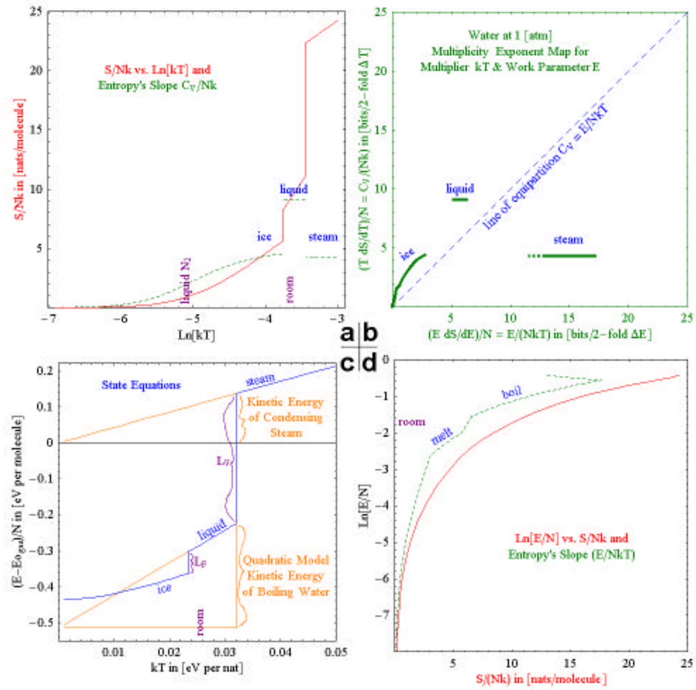
A simple quadratic system: Given multiplicity proportional to E^(3N/2), one can show that E = (3/2)NkT in the lower left, S/N versus Ln[kT} and S/N versus Ln[E/N] are both straight lines of slope 3/2, and hence both E/kT and Cv/Nk in the upper right plot to a single point on the “line of equipartition”. In other words, each molecule on average really does get kT/2 units of thermal energy for each of 3 degrees of freedom. In natural as distinct from historical units, entropy is in [nats of uncertainty per molecule], temperature in [energy per nat of mutual information lost between system and environment], and heat capacity is in [bits of mutual information lost per 2-fold increase in energy per molecule] OR in [molar heat capacity divided by the gas constant R]. Some texts (HRW?) already list heat capacity in this latter way, so as to offer insight into “degrees freedom per molecule” if defined as equal to temperature’s multiplicity exponent times 2.

Water's Multiplicity Map

from a steam, water, and Debye model ice system where, for simplicity, we've ignored the effect of volume changes on energy.

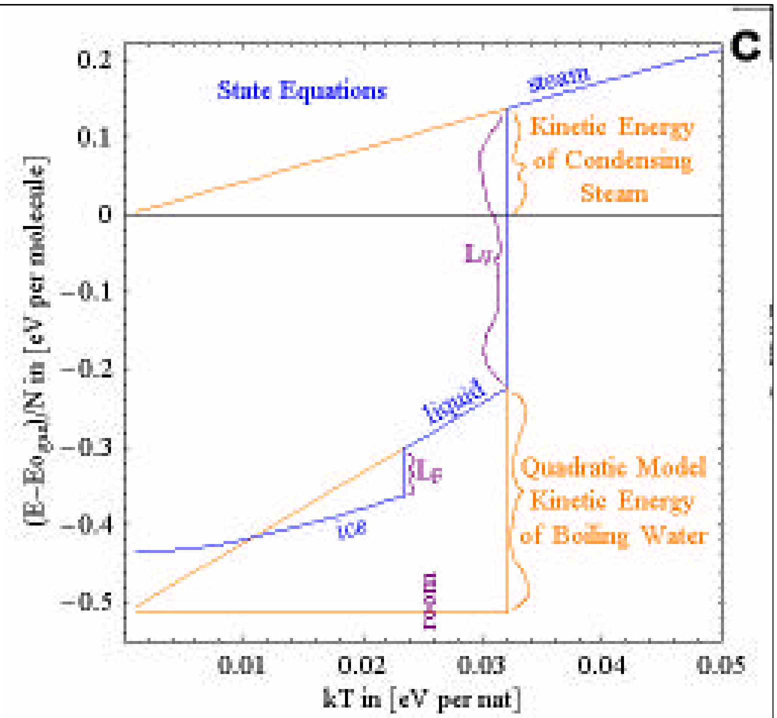
Key:

(a) S/N vs. ln[kT]
(b) exponent map
(c) Energy/N vs. kT
(d) ln[E/N] vs. S/N



The same multiplicity map in natural units is here provided for a steam, water and Debye model ice system. As you can see, the multiplicity map is quite complex (more like spaghetti or a patchwork quilt). Note for example that the map of multiplicity exponents in the upper right corner bounces around, and never does intersect the "line of equipartition". Let's take a closer look at the state equation plot on the lower left…

Closeup of Water’s Energy vs. Multiplier Plot



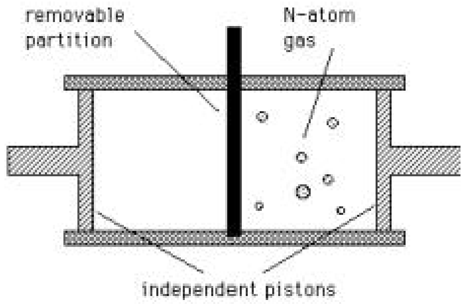
This is the state equation plot (c) from the lower left of water’s multiplicity map.

As you can see, the concept of “energy per molecule” is itself hard to define as one cools steam, while the concept of temperature remains quite well-defined. Note also that the “quadratic model” thermal energy of water at 100C is actually greater than the “quadratic model” thermal energy of steam at the same temperature. You’ll find some more examples in a paper coming out in AJP later this year.

Action items possible today…

• Discuss the meaning of molar heat capacity divided by the gas constant for the microscopic insight it provides on how a given system accommodates thermal energy
• Show a slide or two at the beginning of the thermochapter section discussing how equations of state follow from multiplicities, and uncertainties can be measured in information units.
• Mention that information physics approaches are opening the door to new studies of quantum computing and living systems.

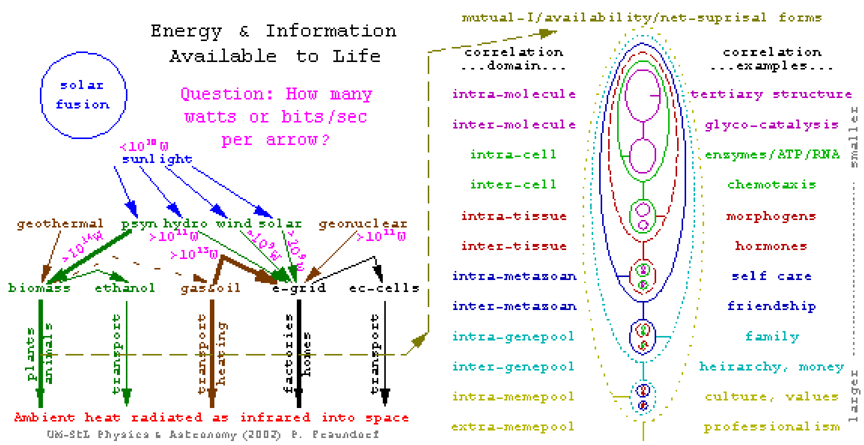
Natural units *will* facilitate the application of thermal physics to information engines…



The price of correlating two subsystems (e.g. a code and and excitation) is for Szilard's vacuum-pump memory and in general: $Work/I = kT_{ambient} \ln(2)$ [e.g. in joules/bit].

For example, information engines which reversibly thermalize work to create correlated subsystems are quite topical in modern day studies of code replication (cf. Tom Schneider at NIH), of code origins (cf. the recent Scientific American article by Bennett and others on chain letters), and of quantum computing (cf. articles in the past decade on mutual information and it's applications by Seth Lloyd).

Life’s power stream / correlation-based complexity



Refs: cf. http://www.umsl.edu/~fraundor/hcapbits.html

Thus thermal physics in natural units provides clues to the role of reversible thermalization in the natural history of invention. This will continue to impact our day to day life much as each of us on this planet can have an impact on all. Information physics could therefore inject very timely new life into an old subject: a subject we might as well modernize before the chemists and engineers and biologists and programmers most directly impacted are forced to figure out how to do it themselves.