Entropy fluctuations reveal microscopic structures

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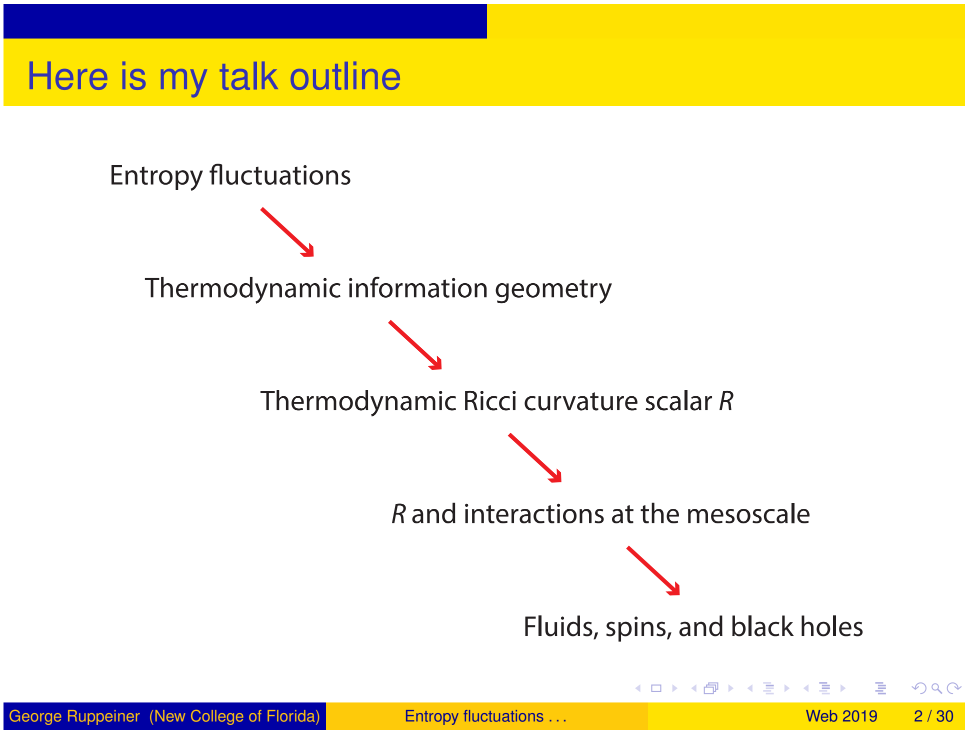
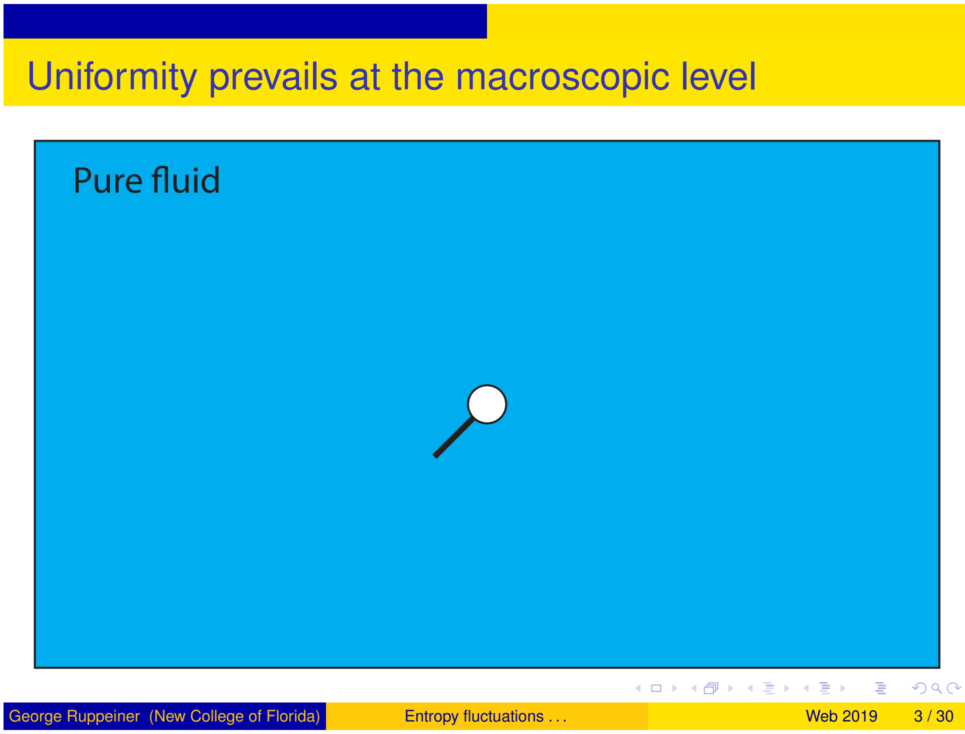
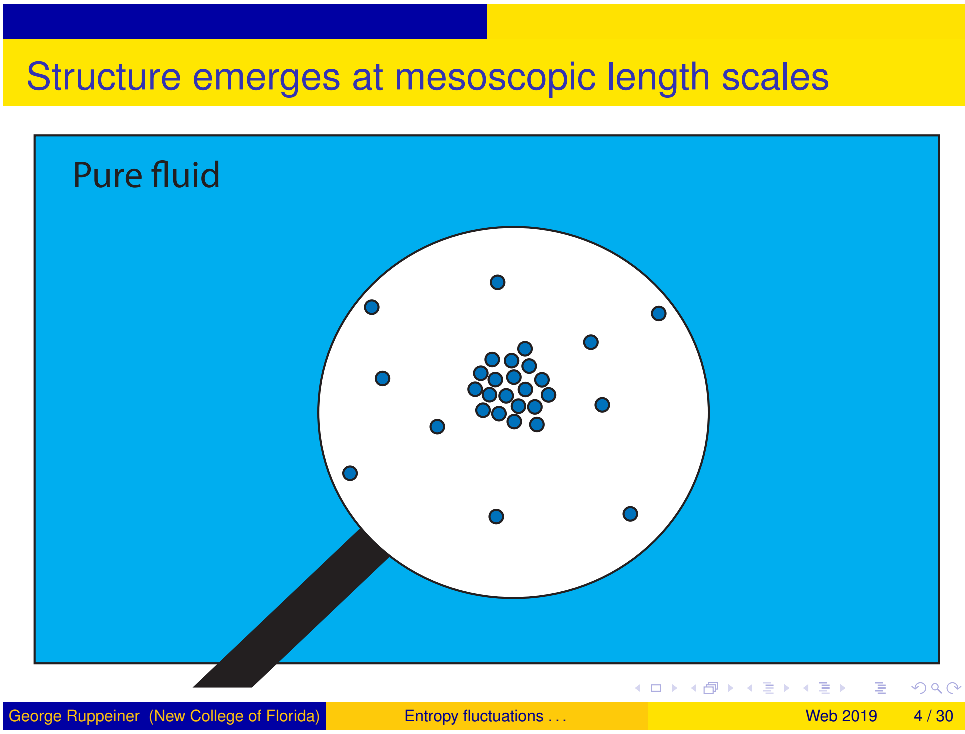
Welcome to my talk on thermodynamic information geometry. My basic theme is that spontaneous fluctuations that decrease the local entropy within some system indicate the formation of organized temporary structures at the mesoscopic length scale. I hope to persuade you that the Ricci curvature scalar R of this geometry provides information about the character of these structures, and that R is an essential feature of thermodynamics.



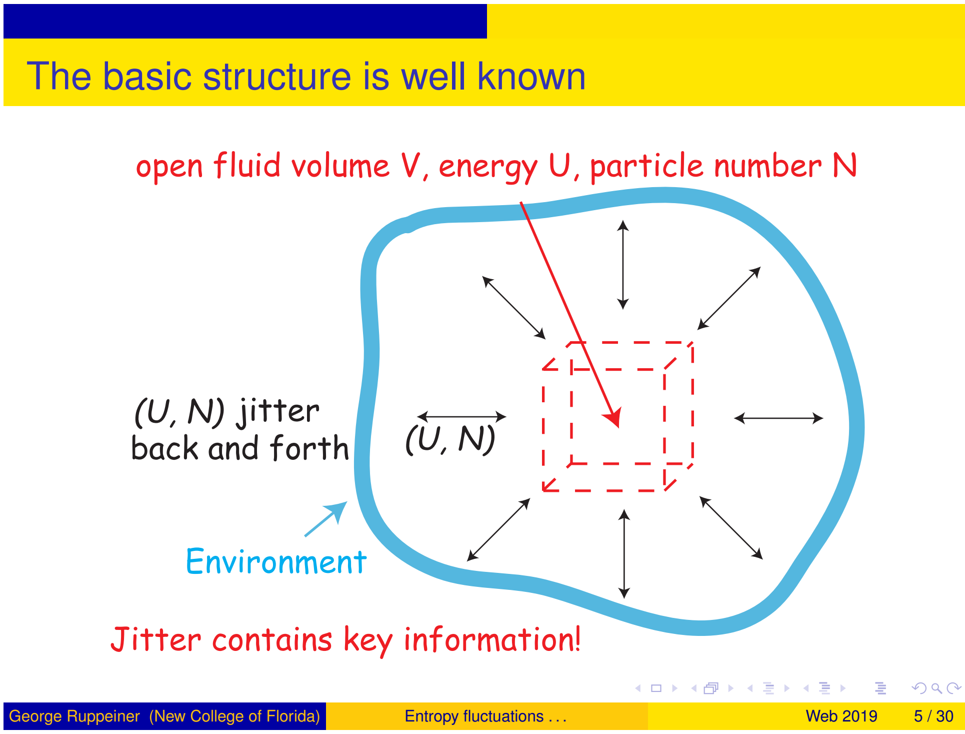
Here is how my talk organizes. I start by discussing entropy fluctuations, and the natural role they play in forming internal system structures. This discussion leads naturally to the information geometry of thermodynamics, and the indispensable thermodynamic curvature R. R connects to the formation of fluctuating structures at the mesoscopic length scales. I conclude with a list of some mesoscopic structures and their thermodynamic signatures. The list spans encompass fluids, magnetic systems, and ends with black holes.



Here is a sketch of a fluid at the macroscopic length scale. Uniformity prevails here. But look through a magnifying glass, and the situation looks quite different.



This magnified mesoscopic image shows a group of atoms that have banded together under the influence of their attractive interatomic interactions, such as prevail near a critical point. Such groupings of atoms always reduce the local entropy, an entropy reduction predicted by thermodynamic fluctuation theory. However, we need some mathematical apparatus to bring this out.



Here is the foundation of the mathematical set-up. In this magnified view, the blue surroundings represent the uniform environment of the previous slide. We zoom in on an open sub volume within the fluid, and we imagine keeping track of the number of particles and the energy present inside it. These quantities jitter back and forth as particles in the fluid flow in and out of the sub volume from the larger environment. This jitter contains key information.

Thermodynamic fluctuation theory gives the probability

- Einstein (1904) $(k_B = 1)$

$$probability \propto \exp\left(S_{universe}\right).$$

- Expand entropy $S_{universe}$ about its maximum:

$$probability \propto \exp\left(-\tfrac{1}{2} g_{\mu\nu} \Delta x^\mu \Delta x^\nu\right),$$

where $(x^1, x^2) = (U, N)$,

$$g_{\mu\nu} = -\frac{\partial^2 S}{\partial x^\mu \partial x^\nu}, \text{ heat capacities, etc.}$$

and S is the thermodynamic entropy.

Thermodynamic fluctuation theory is given in all the books on statistical mechanics; for example, Landau and Lifshitz. The fluctuation probability is given by the exponential of the entropy of the universe, Einstein's famous formula. Fluctuations take place about the state of maximum entropy, about which we can expand to second-order. The Hessian of the entropy function in this expansion consists of thermodynamic quantities like heat capacity and compressibility.

A thermodynamic information metric results

- $\Delta\ell^2 = g_{\mu\nu}\Delta x^\mu \Delta x^\nu$ is a probability "distance."
- *Greater distance has a less probable fluctuation.*
- This is the entropy metric.
  Weinhold (1975), Ruppeiner (1979)
- Related to Fisher-Rao metric (1945).
  Brody, Diósi, Dolan, Ingarden, Janyszek, Johnston, Mrugała, Salamon

This mathematical apparatus can be pitched as a metric information geometry giving probability. The less the probability of a fluctuation between two thermodynamic states, the further apart they are. This metric was originally envisioned as a thermodynamic metric, but a number of authors connected it to the broader context of information geometry in the form of the Fisher-Rao information geometry metric.

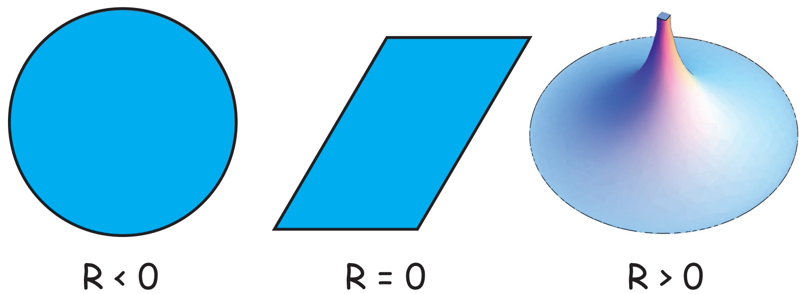
The Ricci curvature scalar R follows

- Metric leads to the curvature scalar R.
- Thermodynamic R has units of volume.
- R is always a feature of a Fisher-Rao metric.
- Physical interpretation requires additional theory.

Ruppeiner (1983), Diósi and Lukáks(1985)

The metric leads directly to the invariant thermodynamic Ricci curvature scalar *R*. The units of *R* are those of volume. *R* gives the size scale of mesoscopic fluctuations. Let me add that a Ricci curvature scalar is always a feature of the Fisher-Rao metric. However, the interpretation of *R* is not generally clear, a priori. The interpretation requires additional theory, and this is offered by the thermodynamic formalism. Unfortunately, I will not have time in this talk to go into this theory.

R is a signed quantity



R can be negative, zero, or positive.

I use Weinberg's (1972) sign convention.

The Riemannian curvature scalar is a signed quantity. I use the curvature sign convention of Weinberg, in which the two-sphere has negative curvature *R*.

R has been calculated in many models

Model	n	d	R sign	$\lvert R\rvert$ divergence
Ideal Bose gas	2	3	$-$	$T \to 0$
Ising ferromagnet	2	1	$-$	$T \to 0$
Critical regime	2	$\cdots$	$-$	critical point
Mean-field theory	2	$\cdots$	$-$	critical point
van der Waals (critical regime)	2	3	$-$	critical point
Spherical model	2	3	$-$	critical point
Ising on Bethe lattice	2	$\cdots$	$-$	critical point
Ising on random graph	2	2	$-$	critical point
q-deformed bosons	2	3	$-$	critical line
Tonks gas	2	1	$-$	$\lvert R\rvert$ small
Ising antiferromagnet	2	1	$-$	$\lvert R\rvert$ small
Ideal paramagnet	2	$\cdots$	0	$\lvert R\rvert$ small
Ideal gas	2	3	0	$\lvert R\rvert$ small
Multicomponent ideal gas	> 2	3	$+$	$\lvert R\rvert$ small
Ideal gas paramagnet	3	3	$+$	$\lvert R\rvert$ small
Kagome Ising lattice	2	2	$\pm$	critical line
Takahashi gas	2	1	$\pm$	$T \to 0$
Gentile's statistics	2	3	$\pm$	$T \to 0$
M-statistics	2	2, 3	$\pm$	$T \to 0$
Anyons	2	2	$\pm$	$T \to 0$
Potts model ($q > 2$)	2	1	$\pm$	$T \to 0$
Finite Ising ferromagnet	2	1	$\pm$	$T \to 0$
Ising-Heisenberg	2	1	$\pm$	$T \to 0$
q-deformed fermions	2	3	$+$	$T \to 0$
Ideal Fermi gas	2	2, 3	$+$	$T \to 0$
Ideal gas Fermi paramagnet	3	3	$+$	$T \to 0$
Unitary thermodynamics	2	3	$+$	$T \to 0$

n = number of independent thermodynamic variables, and d = spatial dimension

Here is a table of R in many models. Patterns are clearly evident. For models where interactions between molecules are attractive, the curvature is negative. Prominent here is the Bose gas, as well as all of the typical critical point models. If interactions between molecules are repulsive, the curvature is mostly positive. Prominent here is the Fermi gas, where the atoms repel due to quantum statistics. For models with weak interactions, the absolute value of the curvature is zero or small. For example, the ideal gas has curvature zero. R diverges in a number of models, either at critical points or at absolute zero.

A number of authors made model calculations . . .

S. Bellucci	D. Brody
J. Chance	A. Dalafi-Rezaie
B. P. Dolan	H. Hara
D. W. Hook	W. Janke
H. Janyszek	D. A. Johnston
K. Kaviani	R. Kenna
R. P. K. C. Malmini	P. Mausbach
H.-O. May	B. Mirza
H. Mohammadzadeh	R. Mrugała
J. Nulton	T. Obata
H. Oshima	A. Ritz
N. Rivier	G. Ruppeiner
A. Sahay	P. Salamon
T. Sarkar	G. Sengupta
Z. Talaei	M. R. Ubriaco

A number of authors contributed to the model calculations on the previous slide. This model evaluation was a group project done over a number of years.

The sign of R characterizes interactions . . .

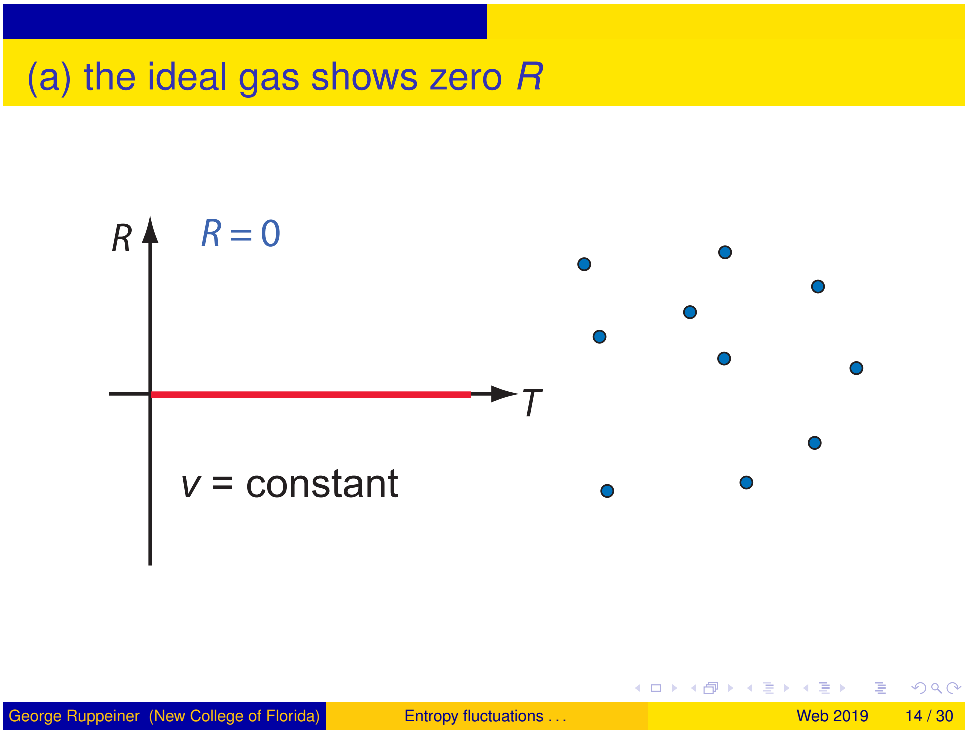
- $R < 0$ for attractive interactions.
- $R > 0$ for repulsive interactions.
- $R = 0$ for the ideal gas (noninteracting).

To repeat, the central point is that R measures interactions between microscopic elements, atoms, molecules, or spins. The sign of R is negative, positive, or zero depending on the character of the interactions.

. . . and $|R|$ measures mesoscopic cluster size

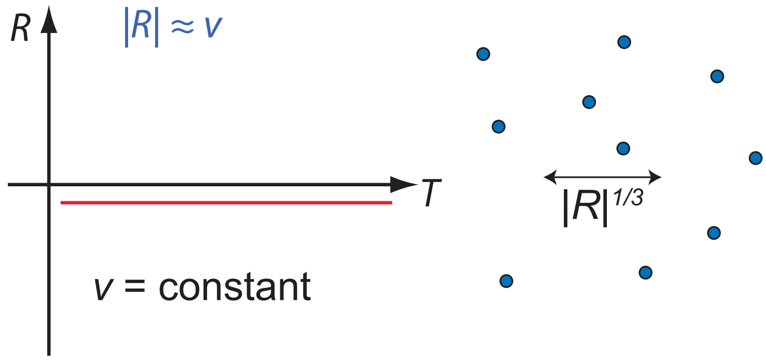
- R diverges at critical points ($R \to -\infty$).
- $|R| \propto \xi^d$, with correlation length ξ.
- $R = -2\,\xi^d$, asymptotically.

Calculations in a number of cases have shown that *R* diverges to negative infinity at the critical point. Near the critical point, *R* is proportional to the correlation length ξ raised to the power of the spatial dimensionality. Asymptotically, the proportionality constant between *R* and the correlation volume has been found to be exactly negative two, a value obtained regardless of the spatial dimensionality, or even whether we compute in a fluid or in a spin system.



I now start a sequence of brief slides sketching results that have been obtained in the literature for R. When possible, I also indicate the corresponding mesoscopic structures in play in each scenario. The first example is the ideal gas, which has identically zero R. My slide indicates this with a path along a line of constant molar volume v. To the right, I indicate a collection of randomly placed atoms devoid of any organized structure.

(b) the rare-field gas shows small negative R



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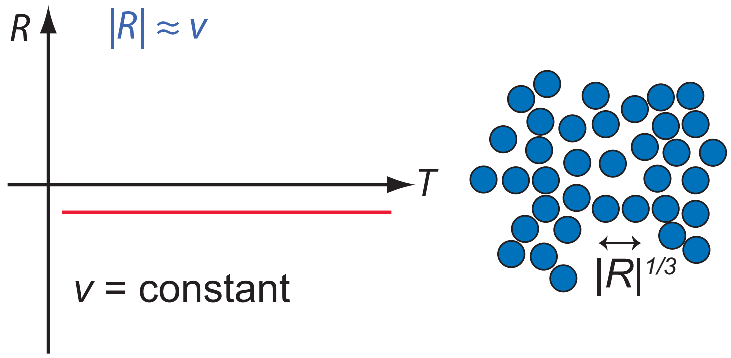
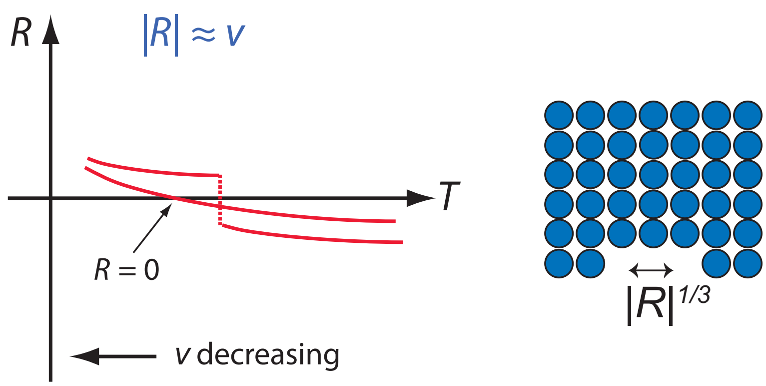
The rare-field gas, in which the long-range attractive tail of the intermolecular force dominates, shows negative R. $|R|^{1/3}$ is on the order of the spacing between molecules. This volume marks the lower limit of thermodynamic validity. Such results are evident particularly on calculating R with fit fluid equations of state.

(c) the liquid shows small negative R



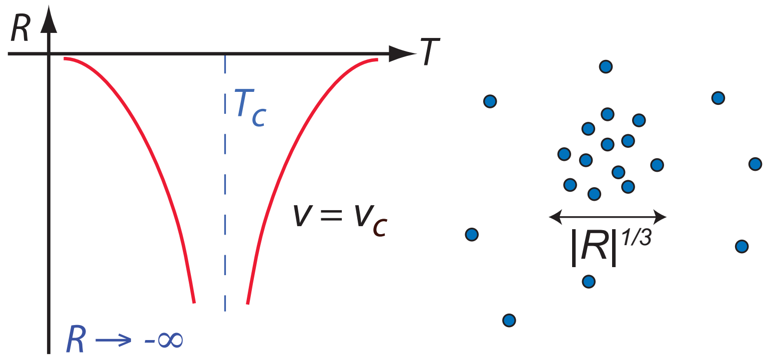
A liquid could result from compressing a gas to a condensed, disorganized state. It has negative R, with $|R|$ roughly the volume v occupied by a single molecule.

(d) the solid phase shows small positive R

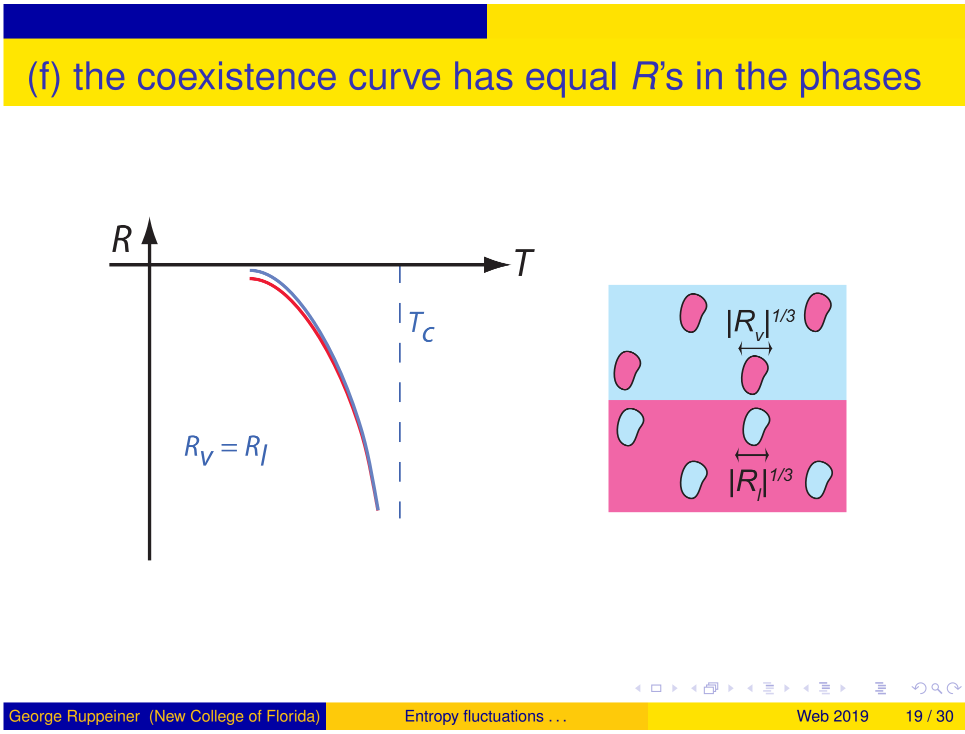


Compress the liquid further, and we transition into a solid. The solid has positive R, roughly the volume v occupied by a single molecule. Is the transition gradual or is there a jump between R's with opposite sign? Not enough work has been done here to give any general conclusion.

(e) the critical point shows $R \to -\infty$

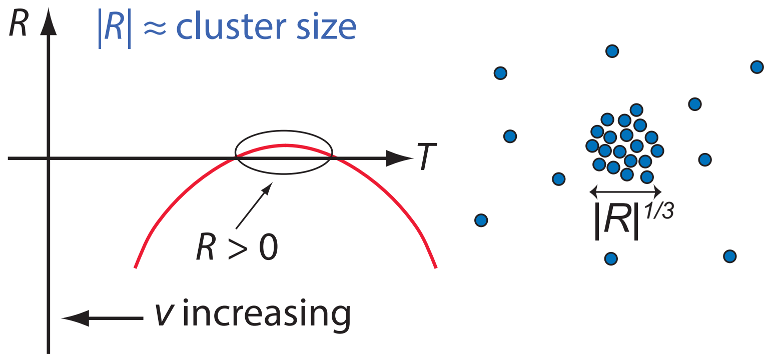


The critical point has the molecules aggregating to large correlated groups of size the correlation length, which is given directly by R. R diverges to minus infinity on approaching the critical point from any direction, shown here on the critical isochore ($T>T_c$) and along both branches of the coexistence curve ($T<T_c$).



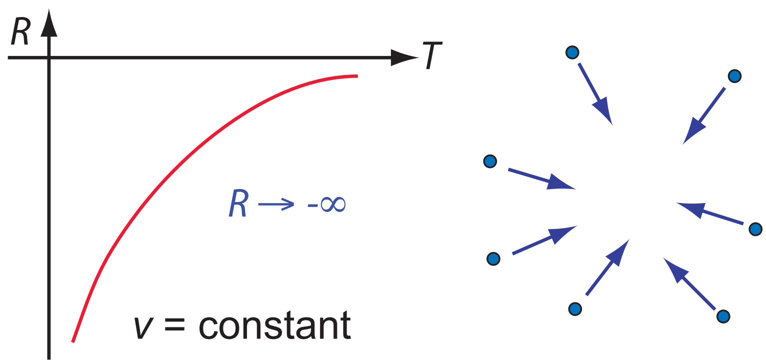
The coexisting vapor and liquid phases have the same values of *R*. The fluctuating droplets, liquid droplets in the vapor, and vapor droplets in the liquid, are the same sizes. This striking principle persists even a long way from the critical point.

(g) the repulsive cluster, with $R > 0$, is logical



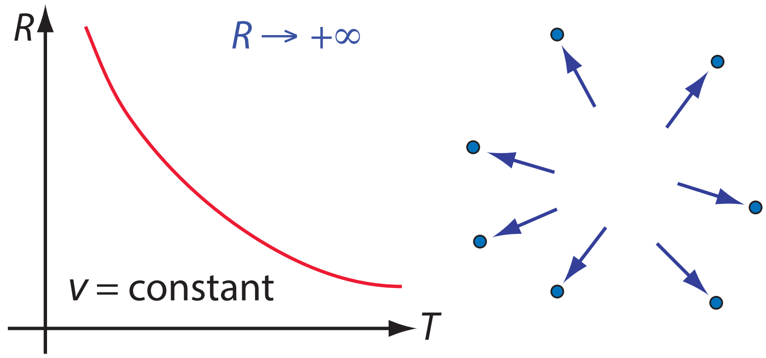
One can envision organized solid-like structures with $R > 0$, held up by repulsive forces between the molecules, and held together by pressure from collisions with outside molecules. Such structures have been proposed in the vapor phase near the critical point.

(h) the ideal Bose gas attracts



The ideal Bose gas has effectively attractive interactions due to quantum statistics. These interactions become quite dramatic at absolute zero, where *R* diverges to negative infinity.

(i) the ideal Fermi gas repels



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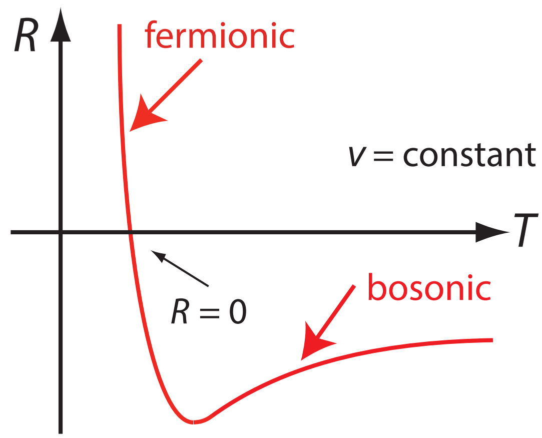
The ideal Fermi gas has effectively repulsive interactions due to quantum statistics. These interactions become quite dramatic at absolute zero where R diverges to positive infinity.

(j) the anyon transition from Bose to Fermi



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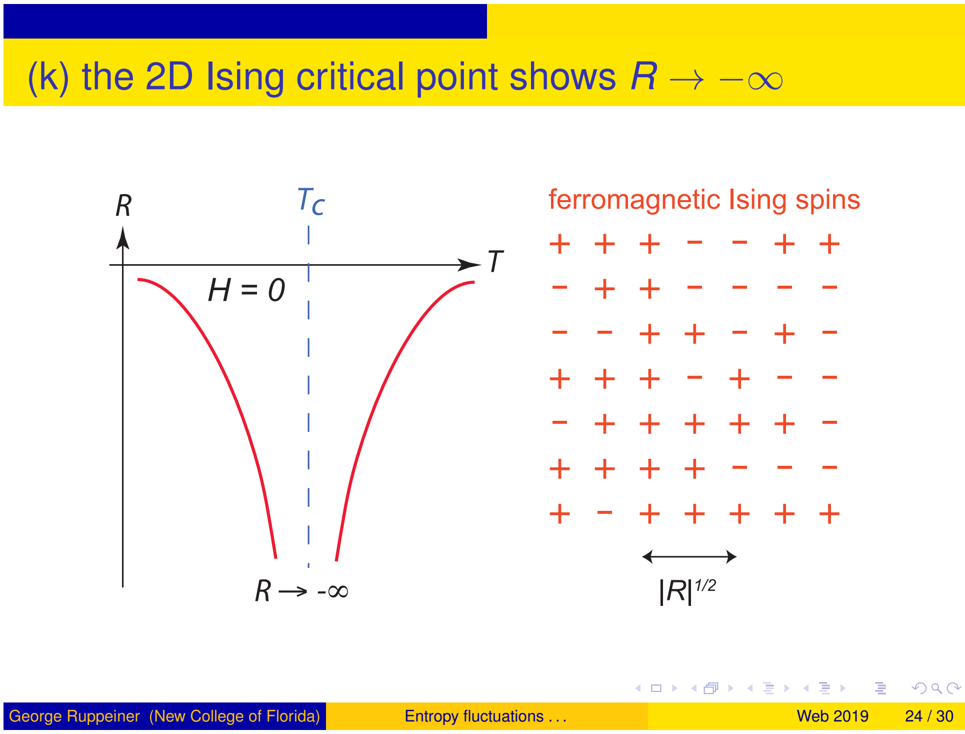
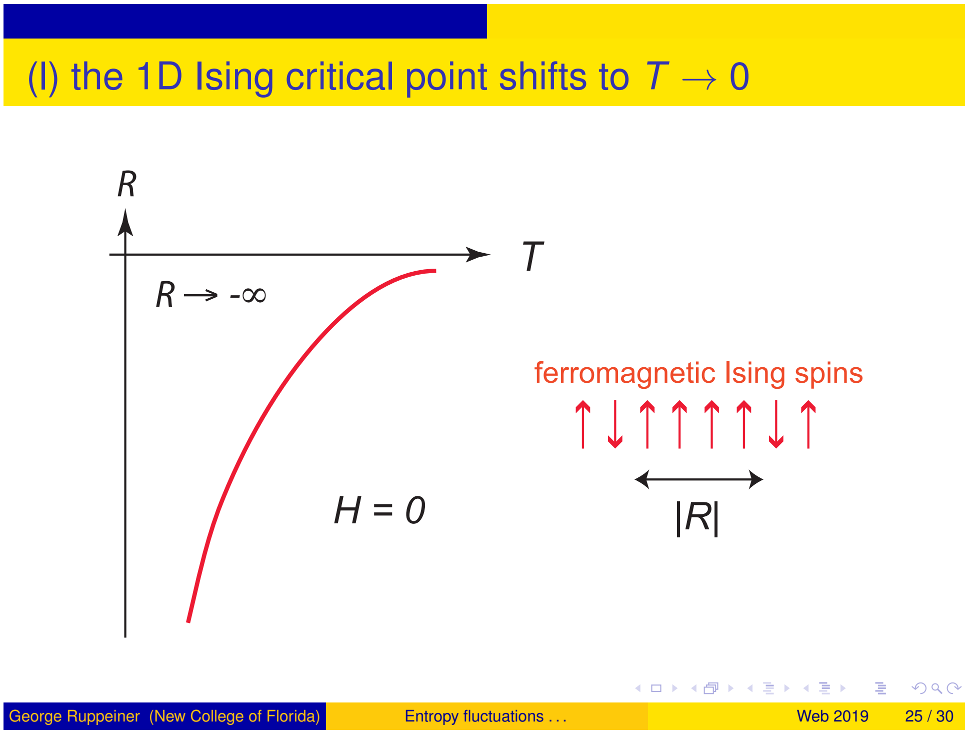
The anyon is a theoretical particle that transitions continuously from Bose to Fermi. *R* likewise transitions from negative to positive.

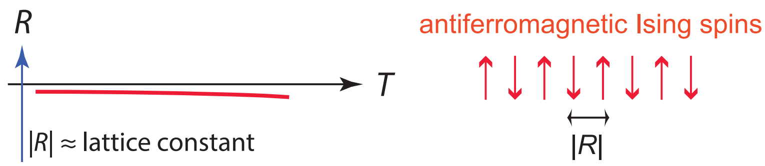


The two-dimensional ferromagnetic Ising model has R going to negative infinity at the critical temperature, fitting the general pattern of divergences of R to negative infinity at critical points.

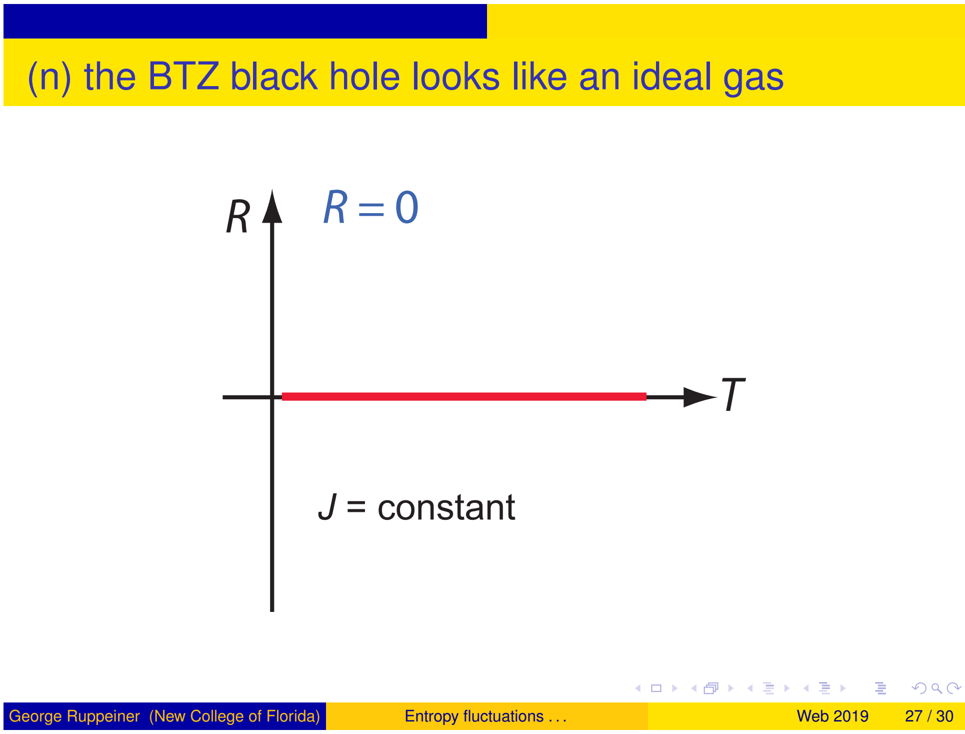


The one-dimensional ferromagnetic Ising model has R going to negative infinity at absolute zero, which is the critical temperature in one dimension.

(m) the 1D Ising antiferromagnet looks liquid-like

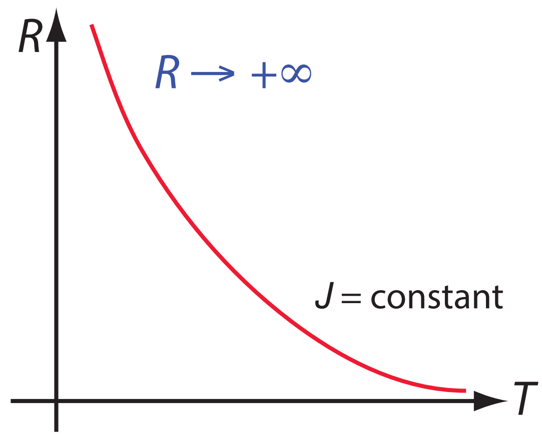


The one-dimensional antiferromagnetic Ising chain has negative R of rough order of the lattice constant. It thus resembles the liquid in sketch (c). One might have expected more the solid phase in sketch (d), but this did not obtain. Maybe there is not that much difference between these cases. Perhaps one might even have expected the critical point behavior in sketch (l), but this is definitely not in play.



Turn now to some black hole thermodynamic cases. Unlike the fluid and spin cases presented above, there is absolutely no consensus in the Physics community what the microscopic and mesoscopic structures might be, or whether this question even has meaning. But my opinion is that if there is thermodynamics, then there must be fluctuations, and, hence, microscopic fluctuating entities. My first black hole example is the two-dimensional BTZ black hole. It has identically zero R, and thus appears to be composed of noninteracting microscopic constituents, as is the ideal gas in sketch (a).

(o) the Kerr black hole resembles Fermi gas as $T \to 0$



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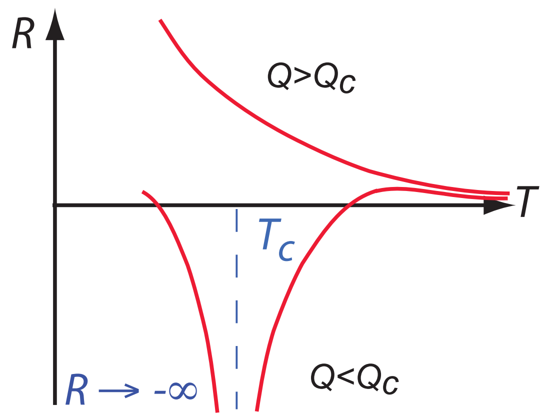
The rotating Kerr black hole, with angular momentum *J*, has an extremal situation where the spin rate is maximized. At that maximum spin, the black hole temperature *T* is zero. In the extremal limit, *R* goes to plus infinity in a similar way as for the ideal Fermi gas in sketch (i). This suggests that the fundamental microscopic constituents of these black holes are some type of Fermi particles.

(p) the RN-AdS black hole has a critical point



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The RN-AdS black hole is charged but not spinning. It sits in a background space with constant negative Einstein curvature scalar. This black hole has a phase transition at a non-zero temperature qualitatively similar to that in sketch (e).

Conclusion: calculate R whenever you can!

- R measures mesoscopic structures naturally.
- Other thermodynamic functions can be useful, but which "are right"?
- R is invariant and universal.
- R is always available!

In conclusion, the thermodynamic curvature would appear to be an important thermodynamic property, one connecting macroscopic thermodynamics directly to interactions between microscopic constituents. This talk is based on too many references to cite here. Some of these references are in "Thermodynamic curvature and black holes," G. Ruppeiner, in "Breaking of Supersymmetry and Ultraviolet Divergences in Extended Supergravity," Springer Proceedings in Physics **153**, 179-203 (2014). (arXiv:1309.0901). Email me if you have questions.