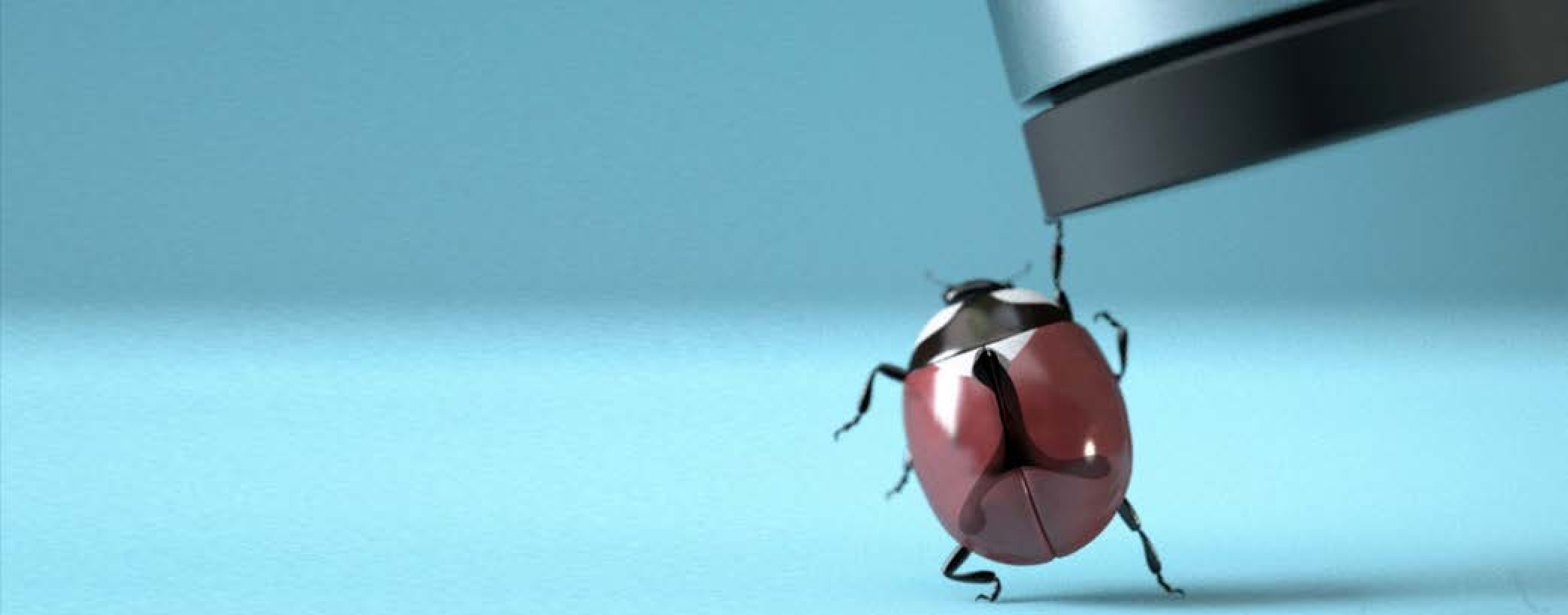

Entropy and Geometric Objects

4th International Electronic Conference on
Entropy and Its Applications
21st November - 1st December 2017

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MICRESS® group at ACCESS e.V.

Introduction

There are different senses of entropy*:

- Thermodynamic Sense
- Information Sense
- Statistical Sense
- Disorder Sense
- Homogeneity Sense

Especially the „disorder" and „homogeneity" senses are related to *and even require* the notion/specification/definition of space

Only few formulas for Entropy comprise spatial aspects/entities

*Haglund, J.; Jeppsson, F.; Strömdahl, H.:
"Different Senses of Entropy—Implications for Education."
Entropy 2010, 12, 490-515.

Objective

One example for an entropy formula comprising spatial entities is the Bekenstein-Hawking entropy S_{BH} which in its dimensionless form* reads:

S_{BH}: dimensionless Bekenstein-Hawking entropy

A: area of the event horizon/ surface area of the black hole

$$S_{BH} = \frac{A}{4L_p^2}$$

L_p: Planck length/ a small positive number having the dimension of a length

1/4: important factor

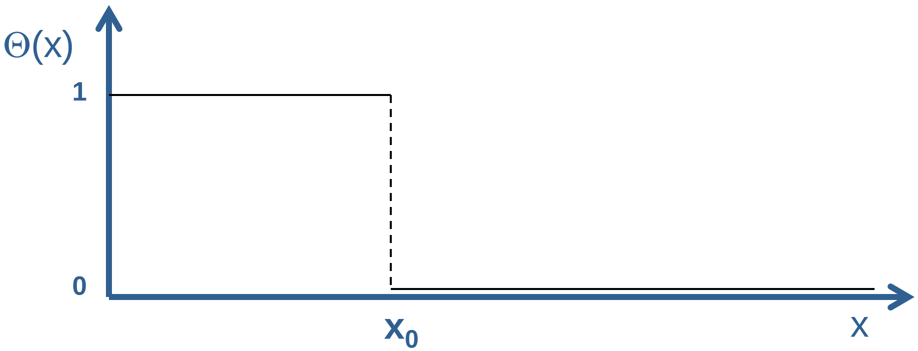
In spite of describing a physics object – a black hole - having mass, charge spin etc. this formula only contains geometric entities

Objective of the presentation is to derive the structure of this formula based on geometric considerations.

* Bekenstein, J. D. (2008): Scholarpedia, 3(10):7375. doi:10.4249/scholarpedia.7375

The Heaviside function

The approach starts from the Heaviside function* $\Theta(x_0)$:



which can be used to describe a sphere or any other geometric object.

The volume V of a sphere with radius r_0 in spherical coordinates is then given by:

$$V = \iiint \Theta(r - r_0) r^2 dr d\Omega = \frac{4}{3}\pi r_0^3$$

with dΩ being the differential solid angle: $sin\Theta d\Theta d\varphi = d\Omega$

The δ function

The Dirac δ function actually is defined* as the distributional derivative of the Heaviside function Θ(x) as

$$\delta(x) := \frac{d\Theta(x)}{dx}$$

Using the δ function the surface A of the sphere – and also the surface of more complex geometric objects - can easily be calculated :

$$A = \iiint \delta(r - r_0) r^2 dr d\Omega = 4\pi r_0^2$$

see e.g.: https://en.wikipedia.org/wiki/Heaviside_step_function

Intermediate summary : the „A“

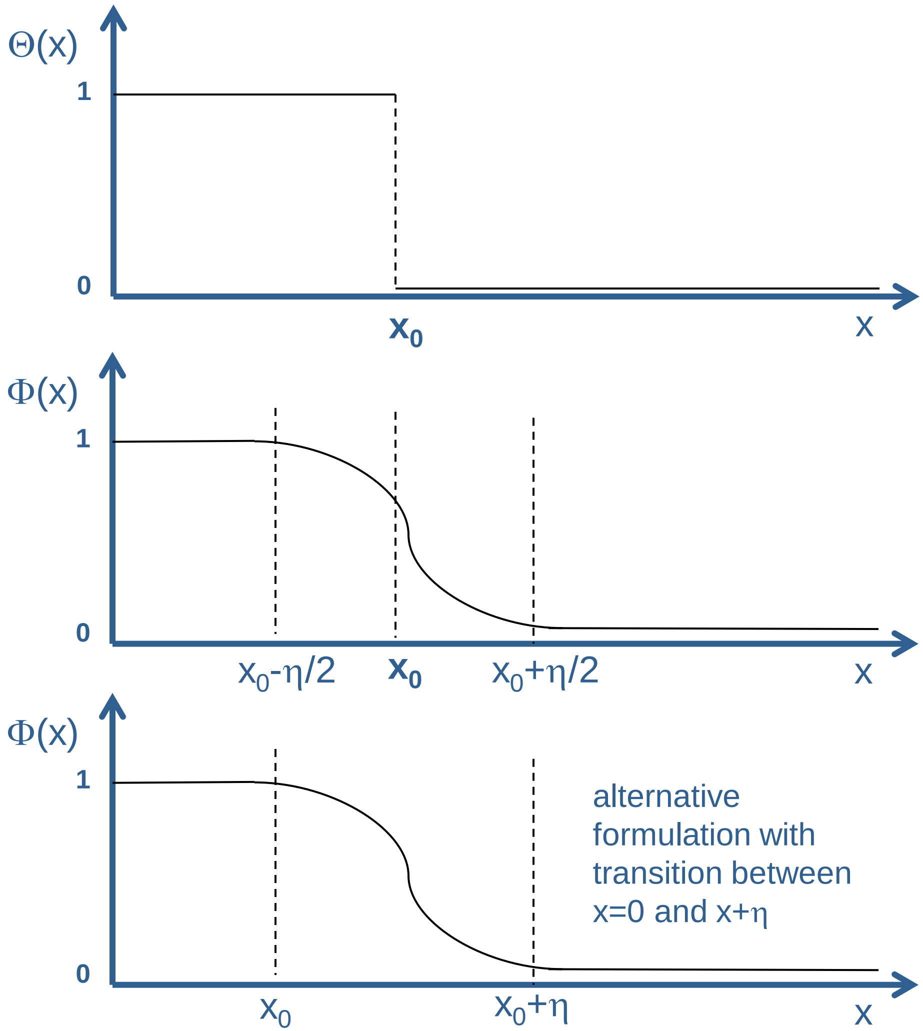
This approach thus has allowed to calculate the area „A“ as the first step towards deriving the entropy of a geometric sphere

$$S_{GS} = \frac{A}{4l_p^2}$$

In fact, however, nothing has been said by now about entropy.

The next steps will have a closer look at the transition region of the Heaviside function and introduce the phase-field function

The phase field description of a transition



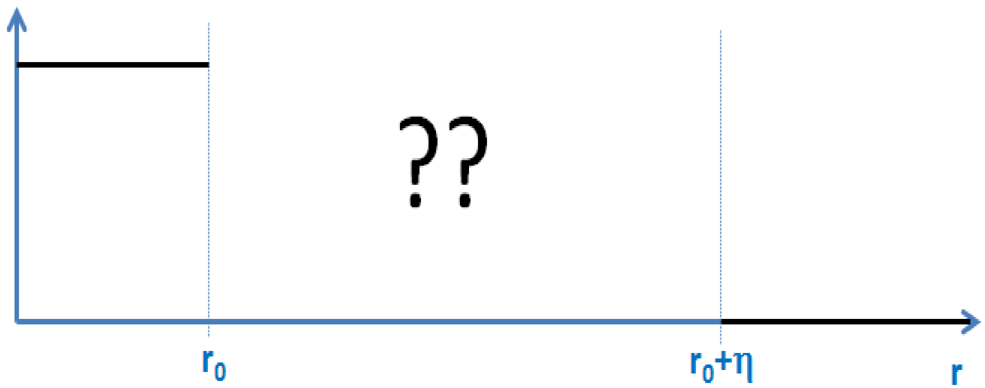
The Heaviside function varies discontinuously from 1 to 0 in an infinitesimally small transition region. Nothing is thus known about the shape of this function in the transition region.

The phase- field variable Φ in contrast varies *continuously* from 1 to 0 in the transition region with finite width η

The shape of the transition in phase-field models depends on the choice of the potential. A double-well potential e.g. leads to a hyperbolic- tangent profile while a double obstacle potential leads to a cosine profile of the Φ function

However, nothing is a priori known about the shape of this function in the transition region also in phase-field models.

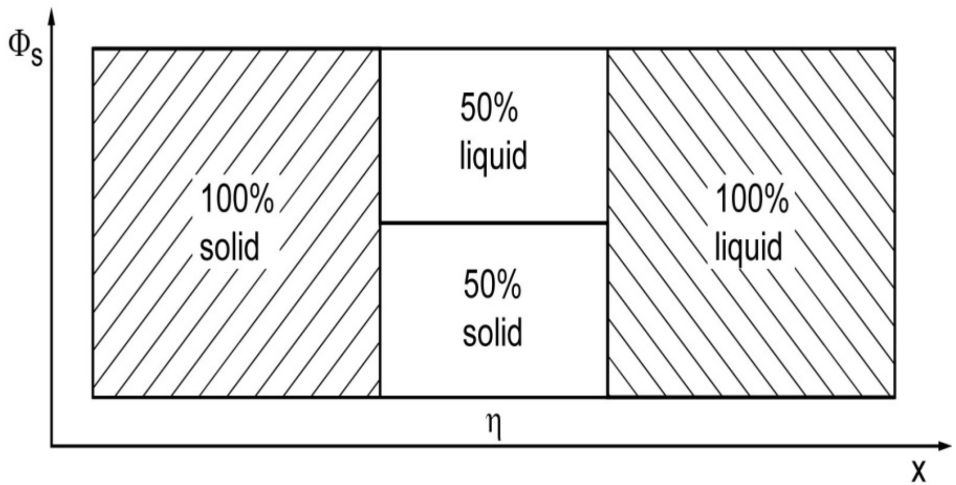
Can we learn more about the interface region?



The Phase-field function Φ can be considered as a contineous formulation of the Heaviside function Θ if the interface thickness η becomes infinitesimally small.

Is there a rationale for the shape of both the Heaviside and the phase-field functions in the transition region?

Entropy of a single interface layer: the Jackson Model



The Jackson model*:

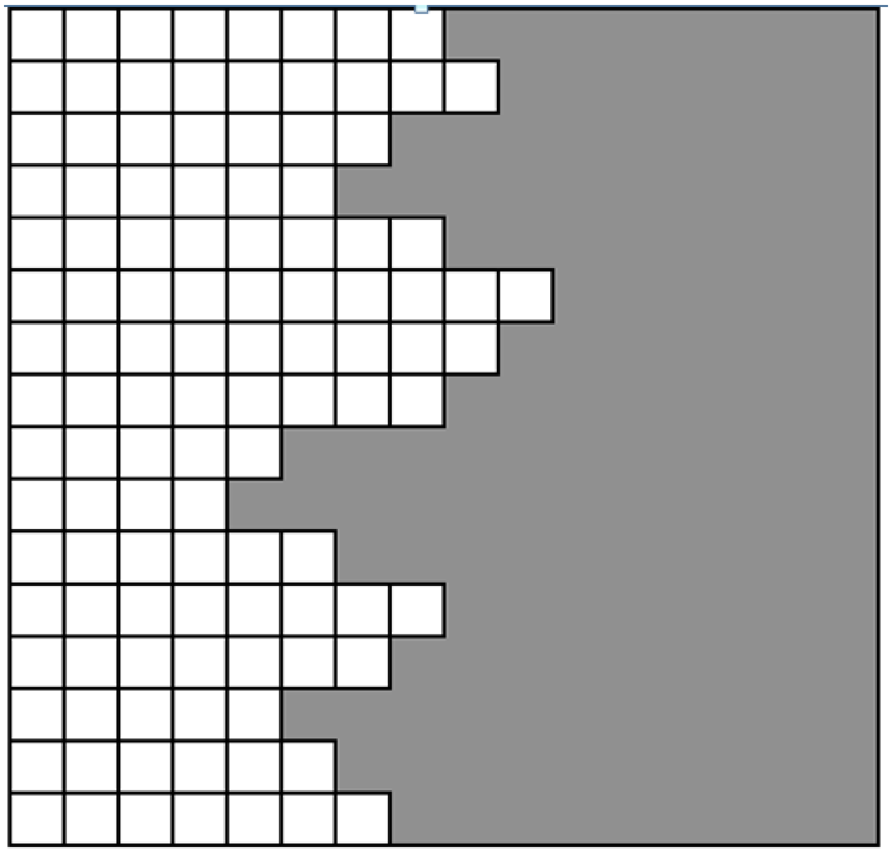
- is used to describe facetted growth of crystals
- assumes ideal mixing of the two states (solid/liquid) in a single interface layer between the bulk states
- describes the entropy of the interface as:

$$S = \Phi ln \Phi + (1 - \Phi) ln(1 - \Phi)$$

- which generates $\Phi = 0.5$ as the most probable value

*Jackson, K.A. Liquid Metals and Solidification; ASM: Cleveland, OH, USA, 1958
cited in :
Woodruff, D. The Solid Liquid Interface; Cambridge University Press: Cambridge, UK, 1973

Describing a diffuse interface: the Kossel Model

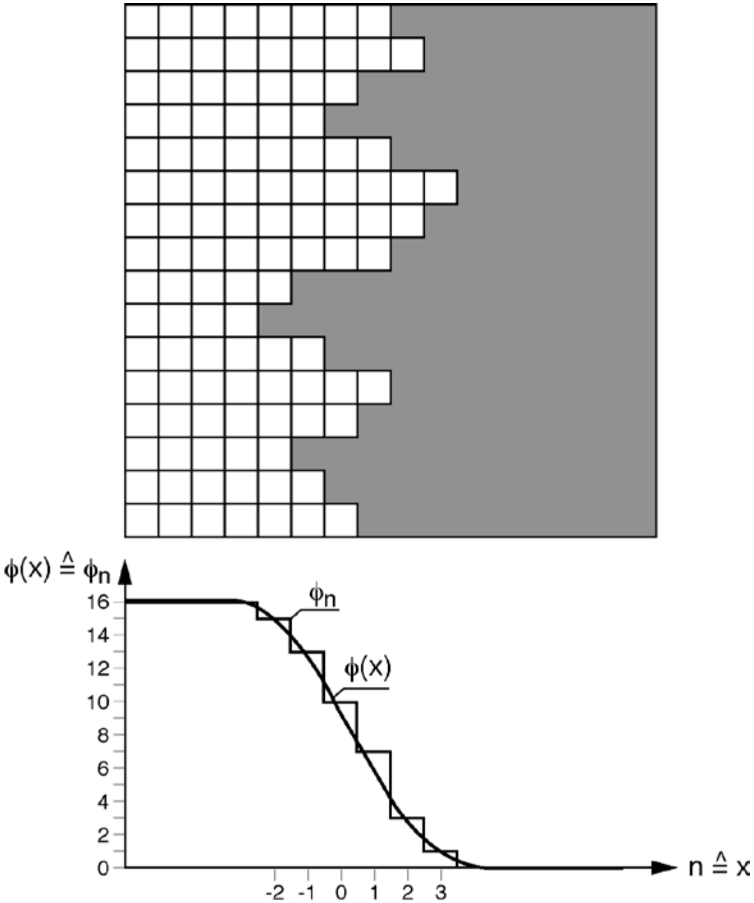


The Kossel model*:

- is a discrete model
- is used to describe the growth of crystals with diffuse interfaces
- assumes attachment of solid on existing solid only (no overhang)
- describes a stepwise transition from 100% solid (the 4 left layers) to 100% liquid (from layer 11 to the right)
- provides the basis for Temkin‘s discrete formulation of the entropy of a diffuse interface

*see e.g. :
Woodruff, D. The Solid Liquid Interface; Cambridge University Press: Cambridge, UK, 1973

Entropy of a diffuse interface: the Temkin Model



The Temkin model*:

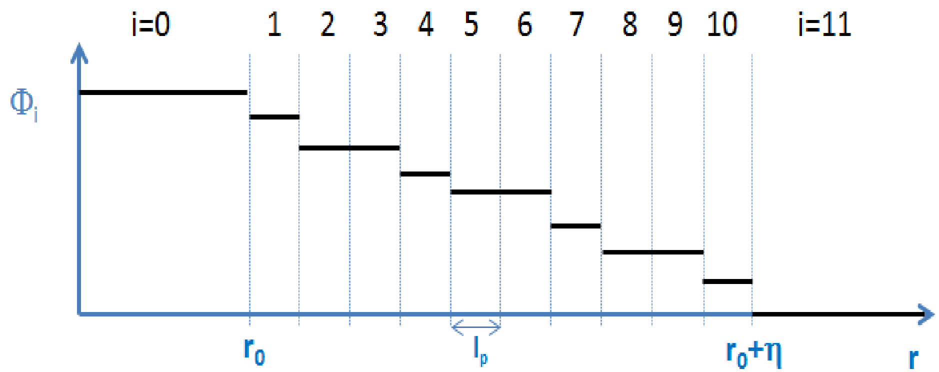
- is used to describe growth of crystals with diffuse interfaces
- assumes ideal mixing between two adjacent states/layers in a multilayer interface
- describes the entropy of the diffuse interface as:

$$S = -\sum_{n=-\infty}^{\infty} (\Phi_{n-1} - \Phi_n) ln(\Phi_{n-1} - \Phi_n)$$

- recovers the Jackson model as a limiting case for a single interface layer

*Temkin, D.E. Crystallization Processes; Sirota, N.N., Gorskii, F.K., Varikash, V.M., Eds.; English Translation; Consultants Bureau: New York, NY, USA, 1966.
cited in : Woodruff, D. The Solid Liquid Interface; Cambridge University Press: Cambridge, UK, 1973

Highlighting the importance of the Temkin model



The Temkin model:

- introduces neighborhood relations between adjacent layers and thus an „order“ resp. „disorder“ sense
- **introduces a** gradient and thus a **length scale into** the formulation of **entropy**
- can be extended to a continuous formulation
- can be extended to 3 dimensions

The gradient in the Temkin model is identified as follows:

$$d\Phi_n = \Phi_{n-1} - \Phi_n = \int_{nl}^{(n-1)l} \frac{d\Phi}{dr} dr = \frac{d\Phi_n}{dr} \int_{nl}^{(n-1)l} dr = l \frac{d\Phi_n}{dr}$$

with „l“ being the distance between two adjacent layers and the gradient being assumed as constant between these two layers

*Temkin, D.E. Crystallization Processes; Sirota, N.N., Gorskii, F.K., Varikash, V.M., Eds.; English Translation; Consultants Bureau: New York, NY, USA, 1966.
cited in : Woodruff, D. The Solid Liquid Interface; Cambridge University Press: Cambridge, UK, 1973

From discrete to continuous*

$$r(n) = r_0 + nl \quad and \quad dn = \frac{dr}{l}$$

$$S = -\sum_{n=-\infty}^{\infty} (\Phi_{n-1} - \Phi_n) ln(\Phi_{n-1} - \Phi_n) = -\sum_{n=-\infty}^{\infty} \left\{ l \frac{d\Phi}{dr}(nl) \right\} ln \left\{ l \frac{d\Phi}{dr}(nl) \right\}$$

Making the transition from discrete to continuous:

$$-\sum_{n=-\infty}^{\infty} \left\{ l \frac{d\Phi}{dr}(nl) \right\} ln \left\{ l \frac{d\Phi}{dr}(nl) \right\} \rightarrow -\int_{-\infty}^{\infty} \left\{ l \frac{d\Phi}{dr}(nl) \right\} ln \left\{ l \frac{d\Phi_n}{dr}(nl) \right\} dn$$

and substituting: $$nl = r - r_0 \quad and \quad dn = \frac{dr}{l}$$

in 1 dimension yields: $$S = -\int_{-\infty}^{\infty} \{ l \nabla_r \Phi(r - r_0) \} ln \{ l \nabla_r \Phi(r - r_0) \} \frac{dr}{l}$$

see also:**Schmitz, G.J. Thermodynamics of diffuse interfaces. In *Interface and Transport Dynamics*; Emmerich, H., Nestler, B., Schreckenberg, M., Eds.; Springer Lecture Notes in Computational Science and Engineering; Springer: Berlin/Heidelberg, Germany, 2003; pp. 47–64**

Extending to 3D

extending the formulation to 3 dimensions in cartesian coordinates reads:

$$S = -\iiint_{-\infty}^{\infty} (\vec{l}\vec{\nabla}\phi)\ln(\vec{l}\vec{\nabla}\phi)\frac{dx}{l_x}\frac{dy}{l_y}\frac{dz}{l_z}$$

Assuming isotropy of space resp. of the discretization i.e. $l_x = l_y = l_z = l_p$ eventually leads to

$$S = -\iiint_{-\infty}^{\infty} \frac{(\vec{l}\vec{\nabla}\phi)\ln(\vec{l}\vec{\nabla}\phi)}{l_p^3} dxdydz$$

The term

$$s = \frac{(\vec{l}\vec{\nabla}\phi)\ln(\vec{l}\vec{\nabla}\phi)}{l_p^3}$$

can be interpreted as an entropy density.

Extending to 3D in spherical coordinates

$$S = -\iiint_{-\infty}^{\infty} (\vec{l}\vec{\nabla}\phi)\ln(\vec{l}\vec{\nabla}\phi)\frac{dx}{l_x}\frac{dy}{l_y}\frac{dz}{l_z}$$

Switching to spherical coordinates yields:

$$\frac{dx}{l_p}\frac{dy}{l_p}\frac{dz}{l_p} = \frac{1}{l_p^3} r^2 dr sin\Theta d\Theta d\varphi = \frac{r^2}{l_p^2}\frac{dr}{l_p} d\boldsymbol{\Omega}$$

$$S = -\iiint (\vec{l}\vec{\nabla}\phi(\mathrm{r}))\ln(\vec{l}\vec{\nabla}\phi(\mathrm{r}))r^2\frac{dr}{l_p}\frac{d\Omega}{l_p^2}$$

Assuming isotropy (i.e. no dependence on angular coordinates) allows for integration over the solid angle $d\Omega$:

$$S = -\frac{4\pi}{l_p^2}\int_0^{\infty} (\vec{l}\vec{\nabla}\phi(\mathrm{r}-\mathrm{r}_0))\ln(\vec{l}\vec{\nabla}\phi(\mathrm{r}-\mathrm{r}_0))r^2\frac{dr}{l_p}$$

Intermediate summary: the „lp2“ term

The integral

$$S = -\frac{4\pi}{l_p^2}\int_0^\infty (\vec{\mathrm{l}}\vec{\nabla}\phi(\mathrm{r}-\mathrm{r}_0))\ln(\vec{\mathrm{l}}\vec{\nabla}\phi(\mathrm{r}-\mathrm{r}_0))r^2\frac{dr}{l_p}$$

will only deliver contributions at the interface $r = r_0$ as only at interfaces there is a finite gradient. The integrand can thus be considered being proportional to the δ function:

$$\frac{1}{l_p}\left(\vec{\mathrm{l}}\vec{\nabla}\Phi(\mathrm{r}-\mathrm{r}_0)\right)\ln\left(\vec{\mathrm{l}}\vec{\nabla}\Phi(\mathrm{r}-\mathrm{r}_0)\right) = constant * \delta(\mathrm{r}-\mathrm{r}_0)$$

$$S = -\frac{4\pi}{l_p^2}\int_0^\infty constant * \delta(\mathrm{r}-\mathrm{r}_0)r^2dr = -constant * \frac{4\pi r_0^2}{l_p^2} = -constant * \frac{A}{l_p^2}$$

The entropy of a geometric sphere S_{GS} thus gets closer to the formulation known for the Bekenstein-Hawking entropy S_{BH} of a black hole:

$$S_{GS} = -constant * \frac{A}{l_p^2} = \frac{A}{4l_p^2}$$

How to get further?

Can we learn more about the shape of the transition ?

Can we learn more from exploiting the term:

?

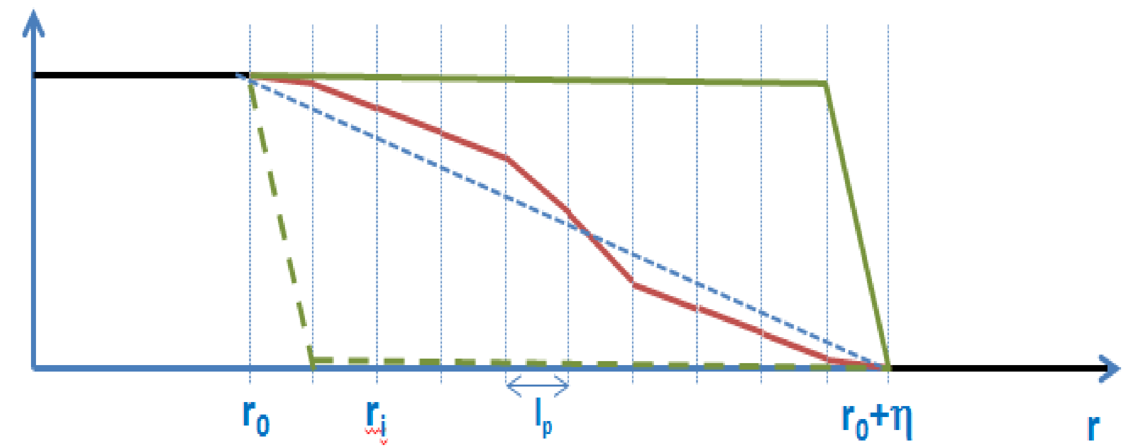
$$\frac{1}{l_p}\left(\vec{\mathrm{l}}\vec{\nabla}\Phi(\mathrm{r}-\mathrm{r}_0)\right)\ln\left(\vec{\mathrm{l}}\overrightarrow{\nabla\Phi}(\mathrm{r}-\mathrm{r}_0)\right)$$

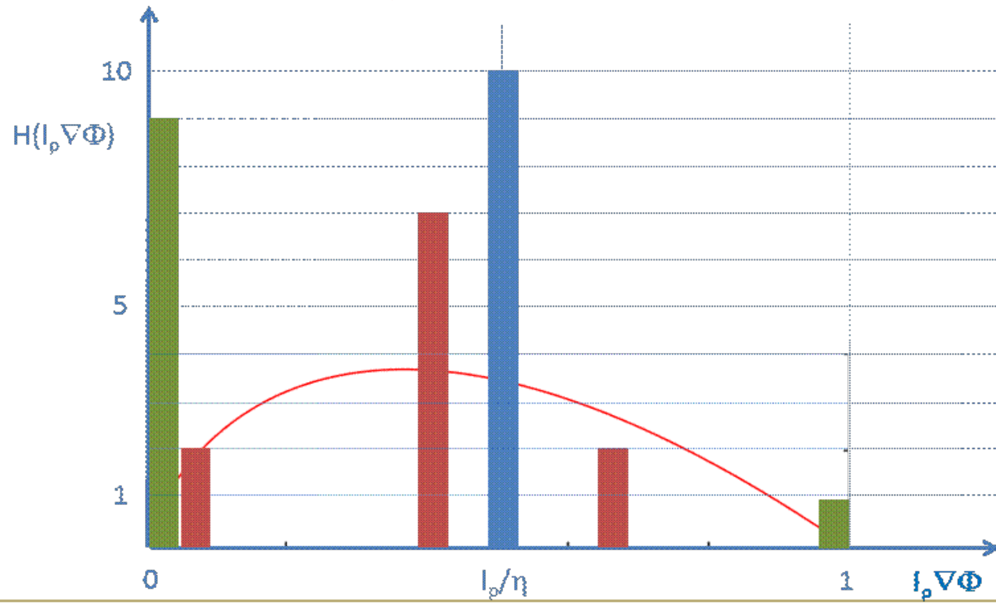
Is there a way to explain the factor ¼?

Statistics of „contrast“ might help
with „contrast“ being defined as….

$$contrast := \vec{\mathrm{l}}\vec{\nabla}\Phi$$

From average gradients to distribution of gradients (resp. contrast)





Possible shapes of the Φ function in the transition region:

A constant average gradient (blue) leads to an extremely narrow distribution of contrast being centered around l_p/η

The green shapes lead to high counts for small contrast

The red shape leads to a broader distribution of small and high contrast values

An entropy type distribution of contrast x_i (i=10) :

$$H(x)= -10*x*\ln(x)$$

is indicated as the red-line overlay

Averaging the distribution of contrast

The average of the contrast distribution can be calculated as follows

$$\langle l_p\,\nabla\Phi\rangle = \frac{\int_{l_p\,\nabla\Phi_{min}}^{l_p\,\nabla\Phi_{max}} (l_p\,\nabla\Phi)\ln(l_p\,\nabla\Phi)\,d(l_p\,\nabla\Phi)}{\int_{l_p\,\nabla\Phi_{min}}^{l_p\,\nabla\Phi_{max}} d(l_p\,\nabla\Phi)}$$

The minimum contrast in the distribution has the value 0 while the maximum contrast is 1 with the maximum gradient then being1/l_p. This allows to fix the boundaries of the integral to 0 resp. 1. For these boundaries the integral in the denominator yields a value of 1. The remaining integral

$$\langle l_p\,\nabla\Phi\rangle = \int_0^1 (l_p\,\nabla\Phi)\ln(l_p\,\nabla\Phi)\,d(l_p\,\nabla\Phi)$$

according to a standard formula* interestingly yields

$$\int_0^1 x ln(x) dx = 1\left[\frac{ln1}{2} - \frac{1}{4}\right] - 0\left[\frac{ln0}{2} - \frac{1}{4}\right] = -\frac{1}{4}$$

* See : Ilja N. Bronstein, Heiner Mühlig, Gerhard Musiol, Konstantin A. Semendjajew: Taschenbuch der Mathematik (Bronstein): Edition Harry Deutsch (2016)

Intermediate summary : the „1/4“

Replacing the contrast distribution in the integral

$$S = -\frac{4\pi}{l_p^2}\int_0^\infty (\vec{\mathrm{l}}\vec{\nabla}\phi(\mathrm{r}-\mathrm{r}_0))\ln(\vec{\mathrm{l}}\vec{\nabla}\phi(\mathrm{r}-\mathrm{r}_0))r^2\frac{dr}{l_p}$$

by its average

$$\langle l_p\,\nabla\Phi\rangle = -\frac{1}{4}\ \ resp.\ \ \langle\,\nabla\Phi\rangle = -\frac{1}{4l_p} = -\frac{1}{4}\frac{1}{l_p} = -\frac{1}{4}\nabla\Phi_{max}$$

leads to

$$S = \frac{4\pi}{l_p^2}\int_0^\infty \frac{1}{4}r^2\left|\overrightarrow{\nabla_{max}}\phi(\mathrm{r}-\mathrm{r}_0)\right|dr$$

and thus eventually to

$$S \sim \frac{4\pi}{l_p^2}\int_0^\infty \frac{1}{4}r^2\delta(\mathrm{r}-\mathrm{r}_0)dr = \frac{4\pi r_0^2}{4l_p^2} = \frac{A}{4l_p^2}$$

Summary

The structure of the Bekenstein- Hawking formula for the dimensionless entropy of a black hole has been derived for a geometric sphere

The derivation is based only on geometric considerations

Key ingredient to the approach is a statistical description of the transition region in a Heaviside resp. phase-field function.

Based on the Temkin entropy of a diffuse interface gradients are introduced in form of scalar products into the formulation of entropy for this purpose.

This introduces a length scale into entropy and provides a link between the world of entropy type models and the world of Laplacian type models (see following slides)

Most interesting physics and new insights – e.g. on entropic gravity - may emerge when applying and exploiting the „contrast- concept“ in more depth (see final slide).

„Contrast“ may also be considered as the contrast between two quantummechanical states

Entropy type equations

$$S = k_B \ln W$$

Boltzmann entropy

$$S = -k_B \sum p_i \ln p_i$$

Gibbs-Boltzmann entropy

$$\mathrm{H} = -p \cdot \log_2 p - (1-p) \cdot \log_2 (1-p)$$

Shannon entropy (binary)

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log p(x_i).$$

Shannon entropy (general)

$$S = -k_B \mathrm{Tr}\left(\hat{\rho} \log(\hat{\rho})\right).$$

von Neumann entropy

$$H_\alpha(X) = \frac{1}{1-\alpha} \log \left(\sum_{i=1}^{n} p_i^\alpha \right)$$

Rényi entropy

$$S_q(p_i) = \frac{k}{q-1} \left(1 - \sum_i p_i^q \right)$$

Tsallis entropy

Incomplete list of models for a **statistical/entropic description** of entities in physics and in information theory

Most of these models have a logarithmic term as a common ingredient.

None of these expression comprises gradients and/or Laplacian operators

Laplacian type equations

$$-\Delta u = f$$ Poisson Equation

$$\Delta\Phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon}$$ Coulomb Equation

$$\Delta\Phi(\mathbf{r}) = 4\pi \cdot G \cdot \rho(\mathbf{r})$$ Newton Equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

Schrödinger Equation

$$\frac{\partial\phi(\mathbf{r},t)}{\partial t} = D\nabla^2\phi(\mathbf{r},t)$$ Diffusion Equation

$$\Box = \frac{\partial^2}{c^2\partial t^2} - \Delta$$ Wave Equation (operator)

$$\alpha\varepsilon^2\partial_t\phi = \varepsilon^2\nabla^2\phi - f'(\phi) - \frac{e_0}{h_0}h'(\phi)u + \tilde{\eta}(\mathbf{r},t)$$

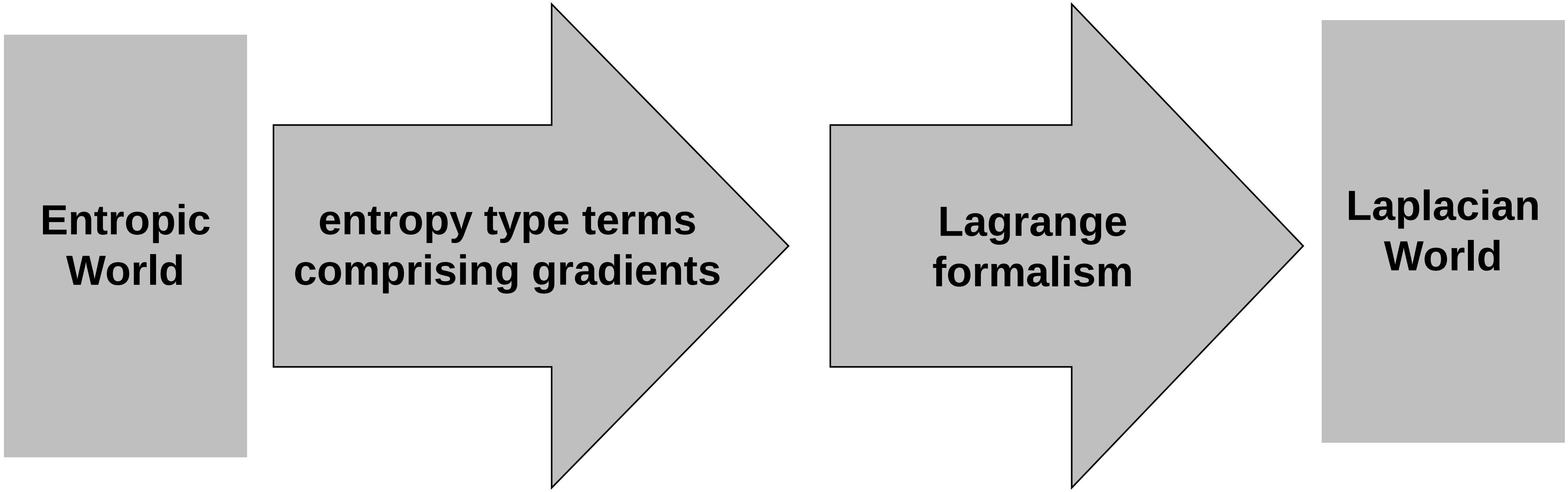
Phase-field Equation

$$\frac{\partial c}{\partial t} = D\nabla^2\left(c^3 - c - \gamma\nabla^2 c\right)$$ Cahn-Hilliard Equation

Incomplete list of models for a **spatio-temporal description** of stationary solutions or for the evolution in physics systems

Many of these models have a Laplacian operator as a common ingredient.

Combining statistical and spatially resolved models



Bridging the gap between statistics/entropy type models and spatio-temporal models of the Laplacian world

Benefits

First application of this concept:

Entropy **2017**, *19*(4), 151; doi:10.3390/e19040151 Open Access Article

A Combined Entropy/Phase-Field Approach to Gravity

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Academic Editor: Remo Garattini

Received: 9 March 2017 / Revised: 28 March 2017 / Accepted: 29 March 2017 / Published: 31 March 2017

(This article belongs to the Section Astrophysics and Cosmology)

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resulted in :

- **Poisson equation/Newtons law**
- **terms related to curvature of space,**
- **terms possibly explaining modified Newtonian dynamics**