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In a 2015 paper, Mohr and Phillips point out practical ambiguities associated with the treatment of dimensionless units in the SI, with an eye toward helping scientists to address these in the future. In particular the two fundamental constants "related to counting", namely Avogadro's number N_A and Boltzmann's constant k_B, in the proposed new SI will serve primarily as scaling relations between dimensionless quantities. We show here that the role of molar heat capacity as a multiplicity exponent gives to the numerical value chosen for k_B a natural connection to information units, like bits. At the same time, the promise of graphene (e.g. in nanotube form) as a portable molar *and* mass standard (thanks to its small intersheet-bonding mass deficit) suggests a natural connection between the numerical value chosen for N_A and well-defined graphene structures, including a particular graphite arm-chair hex-prism.

CONTENTS

I. INTRODUCTION

The recent paper by Mohr and Phillips[1] raises important issues about the explicit specification of "dimensionless" units, and has helped to broaden the discussion of strategies[2,3] for considering such units in the upcoming revision of the international system of units[4]. For example, measures of spatial frequency (like wavenumber, reciprocal lattice vector magnitude, etc.) implicitly vary with discipline[5] (e.g. as $2\pi/\lambda$ or $1/d_{hkl}$) when (as is often done) they are listed only as "reciprocal distance". The explicit specification of angle units (like radians or cycles) would remove this ambiguity, and make the conventions cross-consistent as well.

This note focuses instead on the two fundamental constants that involve counting[1], and on the possiblity that along with "dimensionless" units for angles and counting the proposed new SI might also want to consider dimensionless units for information. Following Taylor[6], one might define unit $[A]$ in terms of an implicitly-physical, as e.g. in Taylor's equation 3b, "invariant-quantity" A divided by a numerical reference constant $\{A\}_{[A]}$ that we are free to choose in context of both existing practice and future needs. Here we make the case that Avogadro's number N_A and Boltzmann's constant k_B don't have physical invariants associated with them, but that they are instead scale-factors which connect physically-dimensionless size scales (N_A) or information units (k_B). As a result it might make sense to choose the unit-defining numerical constant for N_A to a physical structure with potential for replicating standards downstream, and to link the numerical constant for k_B to an information-unit convention. Specific possibilities are suggested as well.

II. AVOGADRO AND SIZE SCALES

In the proposed new SI, the second [s] may be defined in terms of the ground-state hyperfine splitting transition-frequency of Cs-133, the meter [m] then in terms of the lightspeed constant, the kilogram [kg] and joule [J] then in terms of Planck's constant, the coulomb [C] and ampere [A] in terms of the fundamental charge, and the lumen [lm] and candela [cd] in terms of the luminous/radiant intensity-ratio for 540[THz] light.

The new SI may also decouple the definition of Avogadro's number from the number of Daltons (defined *not by the SI* e.g. as one twelfth the mass of an isolated C-12 atom) per gram[7]. This is perhaps reasonable given the fact that, when molecular binding energies are considered, mass is not simply proportional to the number of atoms in an object.

Hence Avogadro's number N_A would not be linked to an experimental invariant, like the number of isolated C-12 atoms needed to make up a kilogram of mass. Without a physical invariant, this makes Avogadro's number a scale-factor for the dimensionless quantity "number of entities' in moving from the size-scale of atoms and molecules to the human-specific "macroscopic" size scale of the laboratory.

Hence the mole [mol] may be defined by picking any number consistent with prior practice, or by "in additon" asking that the numeric value of N_A be associated with a physical object for which precise molar standards (with a specified number of atoms/molecules) may be possible to generate in the days ahead. One such standard might be a well-defined 3-dimensional graphite structure. This is because graphite is quite stable (in the absence of hot oxygen & molten iron), and is made of graphene sheets which might be generated e.g. with well-defined chirality

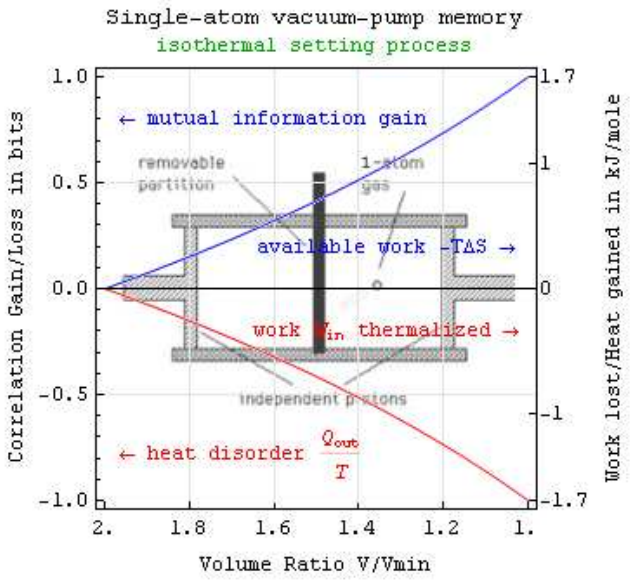

FIG. 1. Single-atom isothermal-setting process schematic.

by future nanotube generators to create portable molar standards. These in turn, thanks to the weak binding between graphene sheets, could also serve as relatively precise mass standards independent of the layering-configuration of the graphene sheets themselves.

For example, imagine that Avogadro's number N_A was defined as the number of atoms in an arm-chair graphite hex-prism with m hexagonal graphene sheets each with m atoms on a side, using:

$$\left[\frac{\text{entities}}{\text{mol}}\right] \equiv \frac{\text{N}_\text{A}}{6.022\ 141... \times 10^{23}} \simeq \frac{\text{N}_\text{A}}{3m^2 + 9m^3/2}. \quad (1)$$

We specifically propose[8] using $m = 51,150,060$ carbon atoms along the sides and height of an armchair-graphite hex-prism, as a value which perhaps provides the closest match to the experimental value at present.

III. BOLTZMANN AND INFORMATION UNITS

The statistical approach to thermal physics, pioneered by Ed Jaynes[9,10] in the 1950's to include the information-theory connection between Gibb's work and statistical inference[11], in the second half of the 20th century has pretty much found its way into all senior undergraduate thermal physics texts[12–15] even if it is not familiar across all disciplines. It includes the recognition that reciprocal-temperature has natural (as distinct from historical) units as energy's uncertainty slope ($1/T = dS/dE$), which stem from its role as a Lagrange multiplier in the uncertainty maximization for "taking the best guess" about where energy (when shared randomly) will go.

More recently, a strong connection between the 2nd law of thermodynamics, these uncertainty measures, and subsystem correlations in general has been established. For example, Seth Lloyd has discussed the role of the multi-moment correlation-measure mutual information in the context of quantum computing[16]. This is a special case (namely that for an uncorrelated reference probability set) of an even more general correlation measure called Kullback-Liebler divergence[17] or relative/cross-entropy[18], which e.g. is behind engineering measures (like "exergy") for available work in a given setting[19,20]. Work on applying KL-divergence, in turn, to layered complex systems[21] (e.g. behind life's dependence on thermodynamic availability) as well as to model selection (with separate converging threads in both the behavioral[22] and physical[18] sciences) are active areas of applied research.

Stepping back to the mathematics of statistical inference[23], just as cycle and angle "units" arise when we mark a unitless interval-fraction (e.g. in units of the repeat-period) along the path of a periodic function, so information "units" of base-b arise when we take the log to the base-b of a unitless reciprocal-probability. Hence the surprisal[24] $s \equiv k\ln[1/p] \geq 0$ associated with *any* probability $0 \leq p \leq 1$ has "dimensionless" units of [bits] if $k = 1/\ln 2$, [nats] if $k = 1$, or [J/K] if $k = k_B$ in units of [J/K] is taken as dimensionless. Uncertainties and entropies are generally defined as "average surprisals", while KL-divergence based measures of (delocalized) correlation between subsystems, as well as of *available information* on deviations from ambient, define a kind of "net-surprisal" that may also be expressed in energy units (e.g. as available work) if multiplied by ambient temperature in [K].

It is natural in this context to ask "What specific correlations are being linked to the 2nd law?". The answer might be "correlations between the state of *any* two separate physical systems or subsystems". A classic example[25–28] is the Szilard "vacuum-pump memory", which in simplest form (Fig. 1) is a two-chamber structure with a removable partition and one gas atom bouncing around inside. Imagine that there is no record in the outside world as to which side the atom is on. By using e.g. a piston to reversibly push the "gas" into say the left chamber we thermalize (at constant T) an available work of $W = (k_BT)[\text{J/nat}]\ln(V_o/V)[\text{nat}] = k_BT\ln 2[\text{J}]$, but we also lessen our total uncertainty about the state of the "structure plus outside world" by $\Delta S/k_B = Q[\text{J}]/(k_BT)[\text{J/nat}] = \ln 2[\text{nat}] = 1[\text{bit}]$ of mutual information (correlation between *our idea* of which side the atom is on, and the position of the atom itself). Here as usual W is work done to compress and Q is heat lost to hold T constant, both in [J], and S is the entropy of our 1-atom gas in [J/K]. The second law of course allows us to irreversibly forget which side we put it on, but makes it less likely that we'll unforget something we never knew.

In this context, therefore, the kelvin [K] may be defined by expressing the thermodynamic information unit [J/K] for measuring subsystem correlations, expressed in terms of everyday measures of energy and temperature

(the reciprocal of energy's uncertainty-slope dS/dE), as a certain number of [bits] (the smallest standard unit of information) via the relationship which connects e.g. molar heat capacity[29] in [J/K] to the number of molecular degrees-freedom in a gas:

$$\left[\frac{\text{Joule}}{\text{nat Kelvin}}\right] \equiv \frac{k_B}{1.380\ 648... \times 10^{-23}} \simeq nk_B \ln 2 \quad (2)$$

where k_B is Boltzmann's constant and $n \simeq 1.0449378 \times 10^{23}$ is an integer, so that 1[J/K] is about 13.0617[ZB] $\simeq$ 11.0637[ZiB], where [ZiB] is a possible binary-multiple unit symbol for 1[zebibyte] $\equiv 2^{73}$[bits].

This integer may be selected to match the current value of Boltzmann's constant to any precision, or as a binary multiple times a prime number. A 6-figure match is e.g. provided by k_B as $1/(2^{61}45317 \ln 2)$[J/nat K]. Unfortunately the large size of that prime number (45,317) limits its the mnemonic value of this choice, over e.g. simple truncation of a decimal.

IV. DISCUSSION

In this comment we reinforce the case made by Mohr and Phillips[1] that dimensionless units are an important element of future work with fundamental constants. We suggest adding "standards generation" into the choice of a numerical constant for Avodagro's number, and adding information units into the discussion of a specific value for Boltzmann's constant. One possible example of each is also provided.

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