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About continuity and discreteness of quantities: examples from physics and metrology

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Abstract

The VIM3 defines a quantity as a "property of a phenomenon, body, or substance", leaving the characteristics of the term 'quantity', related to the chosen characteristics of the relevant properties. The question is: does necessarily a property also necessarily refer to the possible granularity of a phenomenon, body, or substance?

Take, for example, for the quantity "mass": it does not always have to take into account whether or not a phenomenon, body, or substance is subdivided into discrete entities? It depends of the frame of the analysis and also on the chosen measurement unit. In other cases, like temperature, the macroscopic properties are related to the statistical properties of granular substances like atoms and molecules are, so the present meaning of 'temperature' is generally lost at the numerical level where the entity's statistics become meaningless. Yet another case is quantum physics. The paper illustrates the issue and possible solutions under development.

Keywords: continuous; granular; quantity; magnitude; quanta; integer number; real number; counting; function.

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1. Introduction

Several experts claim that the SI measurement unit mole and the quantity 'amount of substance', $n(X)$, are *continuous* concepts, inappropriate for substances that, according to the atomic theory, are clearly made up of a collection of *discrete* entities, [1, 2] where the critical comment is that every "phenomenon, body, or substance" [3] is a collection of discrete entities.

The present VIM3 [3] defines a "quantity" as a "property of a phenomenon, body, or substance", leaving the characteristics of the term 'quantity' related to the chosen characteristics of the relevant properties. Therefore, the question is: does necessarily a quantity also necessarily refer to the possible granularity of a phenomenon, body, or substance?

Take, for example, for the quantity "mass": does one always to take whether or not a phenomenon, body, or substance is subdivided into discrete entities? It depends of the frame of the analysis and also on the chosen measurement unit. If the appropriate unit is the atomic mass, one should *count* the number of atoms in the amount being measured, like, indirectly, is done for a silicon sphere of the Avogadro Project, [4] or when measuring a very small amount of mass. However, the appropriate unit is most often determined by the used measuring apparatus: if a two-pan scale is used, one compares two macroscopic entities, and in that case the composition of the body or substance does not need to be taken into consideration, at least only at the level of a collection of discrete entities.

In other cases, like temperature, the macroscopic properties are related to the statistical properties of granular substances like atoms and molecules, are, so the present meaning of 'temperature' is generally lost at the numerical level (numerosity) where the entity's statistics become meaningless, at least from an experimental viewpoint. In another case, radiation, the current model units are quanta, leading to the development of quantum physics.

2. Distinction between continuous and discrete in physics

The distinction between continuous (treated by differential maths) and discrete (treated by counts) is real: "everyone is used to consider a quantity as a continuous function, so the perception of the 'granular' nature of the substance, relevant when only its colligative properties are considered, is lost", ... "in other fields of science the granular nature is recognised but taken into account only from a statistical viewpoint". [5] This could be the case when, in fact, not a count is performed, but the measurement of a related quantity – i.e., the mass, with an hypothetical resolution, say, $d = 30\times10^{15}\ m_0$, where m_0 is the mass of one entity. Instead, this is not appropriate in the case of the amount of substance, since the only property considered for the entities is their 'numerosity', not their kind.

(**Note**: However, in the paper a clear distinction should be taken into account between the uses in physics which require continuous functions and real numbers but no differential math – e.g. the gas law and Coulomb's law – and those that also require differential math – e.g. Newton's second law of motion.)

Some relevance has also the fact that in English the term "quantity" is used for a property of a phenomenon, body, or substance that has a "magnitude", and the term "amount" is used for a portion of that phenomenon, body, or substance.

In another group of languages, including French (and Italian), the same term is instead "grandeur" ("grandezza") for a "propriété ... que l'on peut exprimer quantitativement" for the first, and "quantité" ("quantità") for the second. "Magnitude" is "ampleur" but also "(ordre de) grandeur" for order of magnitude. For this reason, in these languages the expression "amount of substance", becoming "quantité de substance" (quantità di sostanza), does not raise the irritation that it apparently does in the English world [6, 7] – apart the limitation inherent in the term "substance".

In the above respect, can in English "amount" be considered a "quantity"? i.e., a property of a phenomenon, body, or substance? Maybe not: 'amount' is a property of something only in the sense that, and if, the 'thing' can be partitioned, so that an amount can be *separated from the rest*: this is the property; or, maybe, only when considering the aggregate 'thing' as a mass of substance in the everyday meaning.

The magnitude of the chosen amount can, in itself, not be a property of the 'thing' in itself. Should this be true, "amount of substance" is not a quantity. The chemist determines the amount needed for a specific process through other properties, like mass. Then, through the Avogadro number, the chemist can compute how many entities are approximately involved in the process, and compute its evolution and outcome. However, that seems to be difficult or even impossible for something that cannot be partitioned, for example a "phenomenon" like, e.g., a field: what is the amount of a field? Or of vacuum? In the opposite situation of "quantum physics", can one consider a mass as continuous or discrete? [8]

3. Tools for processing discreteness

Discreteness suffers from a lack of efficient tools for treating complex cases. Though it is the original foundation of the concept of *number* as an *integer*, their ratios initially in common use as fractions (a popular tool in several old civilisations – from Greece to China), soon lead in mathematics to a different tool, the concept of 'real number', considered to be "exact" by having *infinite* decimal digits.

(**Note:** Mathematics, differently from experimental physics, admits – even requires – exactness. Pythagoras based his authority, also political, on that, and when it was demonstrated that the diagonal of a rectangular triangle cannot be expressed by any finite method (discovery of irrational numbers), there was in Agrigento popular violence and killing of pythagoreans, and Pythagoras had to hide himself! Today, the dispute among mathematicians about the concept of infinity is still open. [9]).

The infinitesimal calculus was developed since the Greek times, but was consolidated only since the XVII Century thanks to Newton and Leibniz [10], and continuous functions with it.

For discrete counting (not making use of real numbers), some development can be found in recent times, especially concerning the simplest, the binary one (or ternary one now in today quantum physics, also involving time [11]). Some additional fields are informatics and nominal scales, or space.

Actually, one striking example of granularity is available long since, that of the fractals. Their coherent patterns are obtained only by sparse points, defeating any coherence among them (be an infinite set of unconnected points, like, e.g., a Cantor dust, referring to a space of fractional dimensions), by means of a deterministic equation whose computation leads to chaos when plugging hordes of random numbers in it [12–14].

It is meaningless, in principle, to talk about discrete 'functions' because discreteness seems to lack a basic properties that a function can be considered to need, autocorrelation underlying its trend, at least as long the differentiability property stands.

(**Note:** However, also a discrete mathematics exists, and the above definition of continuous functions also applies in mathematics to a special kind of set, that is fully connected but discontinuous everywhere, like the Weierstrass function. It also exists in 3D and it has also been used for the treatment of properties of molecular ensembles, a granular type. [15, 16]).

There is an urgent need for more mathematics of the discrete to develop. Even the recent quantum model of physics is still formalised and treated by means of continuous mathematical functions, a patent contradiction not really resolved by the mathematical concept of "states" and the lack of the need of the physical concept of "space" – a concept that looks useless also in counting, contrarily to moving. The massive use of the concept of "informatics" in quantum physics, limited to the binary – or tri-logic – frame, does not seem to be able to surrogate a true mathematics of the discrete.

4. Infinity in a discrete world and exactness

Discreteness also puts a question mark on the possibility of the assumption of an infinite number of entities, material or mathematical, e.g. on the 'reality of real numbers', a concept still popular also in quantum physics. This would also require a change in the concept of exactness, and probably a limit on the 'maximum possible exactness' [17, 18].

(**Note:** There is a singular case about discreteness. In commerce, a popular "*para*-drug" (homeopathic) exists that is stated to be obtained by a specific method of many subsequent dilutions of a substance of given concentration of the active molecule, with so many dilutions indicated that it is simple to compute that not a single molecule of that substance can exist in the final "solution" sold!)

The latter argument leads to the domain of metro-logy, where exactness is a basic issue. In 2007 R. Fox and T. Hill published a short article [19] about the mole where an "exact" value for the Avogadro *number* was indicated – an *integer* number, which differs from the Avogadro *constant* requiring *stipulation* in the definition of the mole, but whose value is considered to be anyway a real number: $(N_A)_{FH}$ = 602 214 141 070 409 084 099 072.

(**Note:** In experimental science, only a *stipulated value* can be exact. In a computation of the number of entities like in this case, on the contrary, where the result is an *integer* number, it can be considered exact under the specified assumptions of the count).

This was not the first time to happen. In 1999 Williams [20] had introduced a different "exact" numerical value, a "binary mole", as 2^{79} = 604 462 909 107 318 607 353 088, which is seemingly found useful in nuclear physics because it differs only by 0.37 % from the experimental value. A third attempt, based on the number of entities in a cube of some 84 millions of entities per side lead in 2010 to the number 602 214 162 464 240 016 093 369 [21].

This prompted me to look, with similar approaches, at the possible intrinsic limits to the exactness of a granular unit mass, here reported in the **Appendix**.

5. A final remark

A continuous quantity can be quantitatively expressed by a numerical value *depending on* the chosen measurement *unit* (note, also in the case of a theoretical reasoning): the resulting *function* is a *property* of such a quantity.

(**Note:** The 'shape' of the continuous function does *not* depend, instead, on the chosen unit. In a nominal scale too numerical values can be attributed to each level (or groups of them), and also in this case a "graphical shape" of the trend can be obtained, as points, "stairs" or by means of an continuous interpolating function).

For a discrete function, on the other hand, a nominal scale can be constructed, and a discrete function requires a *ratio scale with only integers*, each item be named one of its *levels*. In a generic sense, the "value" and the "level" can be taken as an indication of – be called – the "magnitude" of the quantity, continuous and discrete respectively. The use of this term allows a qualitative comparison of quantity conditions, and is useful also in measurement science because it does not need further specifications.

(**Note:** The term "magnitude" has been *cancelled* in the most recent draft of VIM4 [22], now under examination of the International Scientific Community and of Organisations like ISO. See author's opinion above. The change in the VIM4 draft comes from the proposed new formulation of the term "quantity": "property whose instances can be compared by ratio or only by order", where the addition to the VIM4 of also the nominal quantity, requires the addition in this definition of a non-quantitative result of measurement, an "order" in the nominal scale).

The revised SI eventually based the unit of mass on the Planck constant *h*, measured with two basic methods and the results from the Kibble balance and the Avogadro Project. However, studies are now continuing toward obtaining the mass amount also (and possible only, in future) directly via counting of ^{28}Si atoms [23–25].

Finally, this paper does not pretend to indicate ways to perform advancements in the treatment of discreteness and counts, its only intention is to contribute to foster studies in this field.

Appendix

The Fox and Hill exercise considers the entities ideally packed into a cube of some 84 millions of entities per side, to reproduce a numerical value metrologically compatible with the experimental ones. This is shedding light on some interesting aspects of the issue.

First, it recalls us that the Avogadro number is an integer one property (and so is the Avogadro constant). This is not evident from the normal 'scientific notation' used for representing real numbers [26]. The number in question comes, in its essence, from counting entities, no fraction of any of them being meaningful. Therefore, it can only increase by one entity at a time, in discrete steps of one unit on the real-number continuous line.

Secondly, the Fox and Hill exercise is invariant with respect to the shape and size of each entity, to the (varied) distance in space between them and to their distribution (homogeneity) in the 3 dimensions, except for a single condition: in the Euclidean 3-dimensional space where the (non-interacting) entities are deployed, one should count the same number of them for each of the 3 Cartesian axes.

Third, the immense number of entities indicated by N_A has to be considered deployed in the above space (except in the case of a macroscopically-extended monolayer of them), and thus be as small as the cubic root of 10^{24}, i.e. 10^{8}, for each dimension of it, a number much closer to the precision obtainable today.

Fourth, for its validity, the present mole definition does not explicitly place for its validity a lower limiting value for the number of entities (as implicitly happens, e.g. for temperature, where the statistics of kinetic temperature must hold), so that, in principle, a single entity is an amount of substance of 1.66... yocto moles – dots indicating a *rational* number.

I see consequences from some of these facts.

While the cube representation is restrictive, in the vast majority of the cases where the entities are indubitably scattered in a tridimensional space, the simple requirement of an equal number of entities per each of the three dimensions of space is quite more general. For example, in the case of fluids I do not see specific reasons why this condition should not hold.

However, numbers I, with $I = I_1, ..., I_N$ that are consecutive integers, will produce a sequence of I^3 that are discontinuous values equally spaced. Therefore, experimental values expressed as real numbers cannot exactly match this sequence, but only fall in between two consecutive proxies.

Let us consider the most precise present value obtained from measurements on the monoisotopic silicon in the Avogadro Project, N_A = 6.022 140 76(12)×10^{23} mol^{-1} [27]. Thus u = 1.2×10^{-30} mol^{-1}, or 2.0×10^{-8} relative. (The last (2017) CODATA recommended value had a relative uncertainty of 1×10^{-8}, while the 2018 new-SI *stipulated* value (6.022 140 76×10^{23} mol^{-1}) has an implicit relative uncertainty corresponding to 0.17×10^{-8}, better than obtained by the atom count!)

In the (adjourned) case of Fox and Hill, [22] I = 84 446 884 to 84 446 886 entities per perfect-cube dimension is the range of integers generating values of I^3 that correspond to the above observed N_A best value, [27] and the spacing is 0.000 000 213 938 29(1)×10^{23} (for a computer providing a 15 digits accuracy). Let us call it the unitary spacing (*US*). This spacing value is the change in the value of $(N_A)_{FH}$ for 1 atom difference per dimension.

The above fact means, in metrology, that the uncertainty of any assigned numerical value representing N_A could not be lower than the *US*, so the latter will be the minimum uncertainty ($US = u_{min}$) to be associate with any measured amount of substance.

Then, let us now compare the *US* for $(N_A)_{FH}$ with the current uncertainty associated to experimental numerical values of N_A.

By using the *US*, one finds $(N_A)_{FH}$ = 6.022 140 55$_5$–6.022 140 98$_3$×10^{23} as the proxies in that experimental uncertainty interval, for a cube of 84 446 884 to 84 446 886 entities per dimension, respectively. There are *approximately* 602 214 076 888 919 0×10^9 entities for 84 446 885 entities per dimension, or $(N_A)_{FH}$ ≈ ≈ 6.022 140 76(8 88 919)×10^{23} mol^{-1}.

(**Note:** The approximation holds because of the use of a 15-digits computer. By using the fourth initial consideration, one might consider to obtain the 15-digit result *exactly* for nanomoles (10^{-9} mol). In this case, one should use a 5-digit number of entities per dimension, e.g. 84 446: the result is that one gets an exact 15-digits value for the total number of entities, but the *US* is now 1000 times larger, so that one is unable to get a sufficient approximation of the measured values of N_A (the closest proxy being 84 446^3 = 602 195 143 548 536). Computations made using up to 100 digits can be found possible in the Appendix of [28].)

Therefore, according to this model, the reported measurement has an *uncertainty range of 1 entity*. Notice also that the *US* corresponds to a range (21) while for the Avogadro Project experimental value of N_A, where the indicated experimental uncertainty u is ±12 = (24).

Different entity-packing geometries might possibly allow for a higher resolution, but I am unsure that any of them could lead to resolutions higher by orders of magnitude.

In author's view this means that, under certain circumstances – not necessarily applicable to [23] using a solid sample – we are looking to be already (but for an *ideal lattice*), and we will soon reach experimentally, at a limit resolution for the determination of N_A, at least unless the above considerations are weighted in respect to each specific experimental conditions, and their possible influence on the results can be taken in due account and circumvented [24].

Про неперервність та дискретність величин: приклади з фізики та метрології

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Анотація

У 3-му виданні Міжнародного словника з метрології (VIM3) величина визначається як "властивість явища, тіла або речовини", залишаючи характеристики терміну "величина" (англ. "quantity") пов'язаними із вибраними характеристиками відповідних властивостей. Виникає питання: чи повинна властивість також обов'язково мати відношення до можливої гранулярності явища, тіла або речовини?

Візьмемо, наприклад, величину "маса": чи повинна вона завжди враховувати те, чи ділиться явище, тіло або речовина на окремі елементи? Це залежить від системи аналізу, а також від вибраної одиниці вимірювання. В інших випадках, таких як температура, макроскопічні властивості пов'язані зі статистичними властивостями гранулярних речовин, таких як атоми і молекули, тому нинішнє значення "температури" зазвичай втрачається на числовому рівні, де статистика елемента стає беззмістовною принаймні з експериментальної точки зору.

У статті розглядаються відмінності між неперервним та дискретним у фізиці, наводяться розбіжності тлумачення терміну "величина" у різних мовах. Висвітлено проблему вибору інструментів для обробки дискретності у складних випадках у математиці, квантовій фізиці та метрології.

Досліджено питання нескінченності у дискретному світі та точності. Зокрема, дискретність ставить під сумнів можливість допущення нескінченного числа елементів, матеріальних або математичних, наприклад "реальності дійсних чисел", концепції, що досі є популярною у квантовій фізиці. Обгрунтовано необхідність зміни концепції точності та можливого обмеження "максимально можливої точності".

У Додатку розглянуто підходи щодо можливих внутрішніх границь точності гранулярної одиниці маси.

Ключові слова: безперервний; гранулярний; величина (англ. "quantity"); величина (англ. "magnitude"); кванти; ціле число; дійсне число; рахунок; функція.

О непрерывности и дискретности величин: примеры из физики и метрологии

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Аннотация

VIM3 определяет величину как "свойство явления, тела или вещества", оставляя характеристики термина "величина" (англ. "quantity") связанными с выбранными характеристиками соответствующих свойств. Возникает вопрос: должно ли свойство также обязательно иметь отношение к возможной гранулярности явления, тела или вещества?

Возьмем, например, величину "масса": должна ли она всегда учитывать то, делится ли явление, тело или вещество на отдельные элементы? Это зависит от системы анализа, а также от выбранной единицы измерения. В других случаях, таких как температура, макроскопические свойства связаны со статистическими свойствами гранулярных веществ, таких как атомы и молекулы, поэтому нынешнее значение "температуры" обычно теряется на числовом уровне, где статистика элемента становится бессмысленной. Еще один случай – квантовая физика. В статье показана проблема и возможные решения, находящиеся на стадии разработки.

Ключевые слова: непрерывный; гранулярный; величина (англ. "quantity"); величина (англ. "magnitude"); кванты; целое число; вещественное число; счет; функция.

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