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The Energy probability distribution of quantum levels of a particle imprisoned in a three dimensional box

T Yarman,[1] B Akkus,[2] M Arık,[3] C Marchal, S Cokcoskun,[5]
A Kholmetskii,[6] O Yarman,[2] N Zaim,[7] A A Altıntas,[2] F Özaydın[8]

[1] Okan University, Istanbul, Turkey
[2] Istanbul University, Istanbul, Turkey
[3] Bogazici University, Istanbul, Turkey
[4] ONERA, Cedex, Paris, France
[5] Yildiz Technical University, Istanbul, Turkey
[6] Belarus State University, Minsk, Belarus
[7] Trakya University, Edirne, Turkey
[8] Tokyo International University, Saitama, Japan

 E-mail: tolgayarman@gmail.com

Abstract. This work was trigerred by the earlier achivements of Yarman et al, aiming to bridge themordynamics and quantum mechanics, whence, Planck constant came to replace Boltzmann constant, and "average quantum level number" came to replace "temperature". This evoked that the classical Maxwell energy probability distribution $p(E)$ with respect to energy E of gas molecules might be taken care of, by the *"energy probability distribution of the quantum levels"* of a particle imprisoned in a given volume, assuming that in the case we have many particles, following Pauli exclusion principle, no pair of particles can sit at the same level. Thereby, the energy probability distribution of the quantum levels of a particle imprisoned in three dimensions, will be the subject of this essay. Such an outlook becomes interesting from several angles: i) It looks indeed very much like a classical Maxwellian distribution. ii) In the case we have as many free particles in the box as the number of levels depicted by the number of quantum levels in between the predetermined lower bound energy level and the upperbound energy level, all the while assuming that the Pauli principle holds, the distribution we disclose becomes the energy probability distribution of the ensemble of particles imprisoned in the given box. iii) It can even be guessed that, if elastic collisions between the free particles were allowed, and still assuming quantization and the Pauli principle, the outcome we disclose should be about the same as that of the energy probability distribution, molecules in a room would display in *equilibrium.* iv) The *quantized energy* being proportional to the sum of three squared integers associated with respectively, each of the spatial dimensions; the property we reveal certainly becomes remarkable from the point of view of mathematics of integer numbers. All the more, we further disclose that, to the probability distribution outlook remains the same, be this qualitatively for higher dimensions than 3.

1. Introduction
This work is trigerred by the precedent work of Yarman et al, aiming to bridge thermodynamics and quantum mechanics [1-5].

This way, it is important to sketch the energy probability distribution of the quantum levels of a particle imprisoned, say, in a cube in the accustomed archetype of the Schrödinger equation, where the minimum energy E_{min} and the maximum energy E_{max} of the particle is fixed a priori.

2. Different quantum states, but bearing the same energy value

The solution, i.e., the energy eigenvalue E of the Schrödinger equation written for a particle of mass m in a cubic box of size L, and situated at the energy level characterized by the quantum numbers n_x, n_y, n_z, which are associated with, respectively, the three spatial dimensions of concern, is given via the familiar notation by [6]

$$E = \frac{h^2 \left(n_x^2 + n_y^2 + n_z^2 \right)}{8mL^2}. \tag{1}$$

A brief reflexion on this relationship shows that, there can be many equal values of E for different sets of $[n_x, n_y, n_z]$.

Let us for the simplest case choose the quantum numbers 1 and 2, allowed in all thereee directions. So we have 1 and 2 along each of x, y and z directions. Our setup of *allowed quantized energy levels* will thus point to $N=2^3=8$ different quantum locations, in the space represented by the coordinate system [Ox, Oy, Oz], bearing the quantum numbers 1 and 2 in the given directions.

Let us write down all of them: (1,1,1), (1,1,2), (1,2,1), (2,1,1), (2,1,2), (2,2,1), (1,2,2), (2,2,2).

Let us next, i) consider each set, ii) square all three coordinates and, iii) sum the three squared quantum numbers of concern to obtain:

$(1,1,1) \rightarrow (1^2 + 1^2 + 1^2) = 3$
$(1,1,2) \rightarrow (1^2 + 1^2 + 2^2) = 6$
$(1,2,1) \rightarrow (1^2 + 2^2 + 1^2) = 6$
$(2,1,1) \rightarrow (2^2 + 2^2 + 1^2) = 6$
$(2,1,2) \rightarrow (2^2 + 1^2 + 2^2) = 9$
$(2,2,1) \rightarrow (2^2 + 2^2 + 1^2) = 9$
$(1,2,2) \rightarrow (1^2 + 2^2 + 2^2) = 9$
$(2,2,2) \rightarrow (2^2 + 2^2 + 2^2) = 12$

This mere exercise shows that, although we have different sets of three quanutm numbers, for all of our 8 quantum locations; we land at the same output as the sum of the squares of the given quantum numbers.

Since energy E to be associated with the locations displayed above is proportional to the final output numbers, i.e. 3, 6, 9, and 12 (see equation (1)), we have out of 8 energy values, for 8 states,

1 *of them proportional to the number* 3,
1 *of them proportional to the number* 12,
3 *of them proportional to the number* 6, *and*,
3 *of them proportional to the number* 9,

with the proportionality constant $h^2 / 8mL^2$ according to Eq. (1).

3. Energy probability distribution function

We now define the *energy probability distribution (or densıty) function $p(E_i)$* versus E_i, as

$$p(E_i) = \frac{f(E_i)}{N}; \qquad\qquad (2)$$

$f(E_i)$ is the frequency of occurrence of the energy value E_i out of N possible energy values.

Note that, as mentioned, no any pair $[n_{xp}, n_{yp}, n_{zp}]$ and $[n_{xq}, n_{yq}, n_{zq}]$ associated with two different quantum locations p and q in the space $[Ox, Oy, Oz]$ are, in the present approach, allowed to be identical.

The outcome we frame herein, is interesting from many perspectives:

i) The higher the number of states; the more the probability distribution function $p(E)$ versus E looks very much like a Maxwellian distribution [7,8,9].

ii) Presuming we have as many free particles in the box as the number of energy levels depicted by the number of quantum levels in between the lowerbound and upperbound energies that one determines beforehand; all the while, supposing that the Pauli exclusion principle remains in force, insofar as assuring that *"no pair of particles can occupy the same level represented by the corresponding set of quantum numbers";* the distribution we disclose becomes the energy probability distribution of the ensemble of particles imprisoned in the given box.

iii) It can even be guessed that, if elastic collisions between the free particles were allowed, and still assuming quantization and relatedly the Pauli principle, the outcome we disclose should be about the same as that of the energy probability distribution, molecules in a room would display in equilibrium, i.e. Maxwellian distribution.

iv) The energy of concern being proportional to the sum of three squared integers associated respectively with each of the three spatial dimensions, the property we reveal becomes exceptionally interesting from the viewpoint of mathematics of integer numbers; so much so that, one may further disclose that, the setup pertaining to the probability distribution output holds the same for higher dimensions than 3, i.e., the sum of, say, four squared integers yields qualitatively the *same output* for all intents and purposes.

It is clear that equation (2) may lead to zero probability for *energy numbers* in between those proportional to the numbers output from the precedent exercise of summing the squares of quantum integers for each of the given quantum locations. Indeed, there we had the final integer numbers 3, 6, 9, 12, and thusly no 2, 4, 5, 7, 8, 10 and 11. While this characteristic becomes less important, in the case we pick very many integers along each direction, we can still improve the definition of the *energy probability distribution function,* and define $p(E)dE$, as the probability of finding a *quantum energy level* bearing the energy value E within the enegy interval dE, placed around E. Thereby $p(E)$ becomes the probability of finding a quantum energy level bearing the energy value E, within the unit energy interval placed around E:

$$p(E) = \frac{f(E)}{N}, \qquad\qquad (3)$$

$f(E)$, is then the *frequency* of occurrence of an energy falling within the unit interval of energy around E, the full energy range in question being, $E_{max} - E_{min}$.

It is evident that we can further write the following relationships, out of Eqs. (2) and (3):

$$\sum_{i=1}^{I} p(E_i) = 1 = \sum_{i=1}^{I} \frac{f(E_i)}{N} = \frac{1}{N} \sum_{i=1}^{I} f(E_i) = \frac{N}{N} = 1 \quad , \tag{4}$$

$$\int_{E_{min}}^{E_{max}} p(E)dE = 1 = \int_{E_{min}}^{E_{max}} \frac{f(E)}{N}dE = \frac{1}{N} \int_{E_{min}}^{E_{max}} f(E)dE = \frac{N}{N} = 1 \;. \tag{5}$$

In any case, the energy *probability distribution function p(E)* with respect to energy *E,* comes out to look very similar to Maxwelian energy distribution. One thing is clear from our plots that we will present below; it is that the energy E_{peak} corresponding to the peak of *p(E),* lies at the left of the *average energy* $\overline{E}$, i.e.

$$\overline{E} = \int_{E_{min}}^{E_{max}} E \, p(E)dE \qquad . \tag{6}$$

4. Graphical representation of the energy probability density p(E) distribution

We now plot *p(E)* with respect to *E* in accordance with the definition provided via equation (3), for the cases, where the same set of integers, were picked in all three dimensions: 100-200, 300-400, 900-1000 (Figures 1, 2, 3 and 4, correspondingly). This means, we have already 100×100×100=10^6 locations in our space of quantum numbers, defined by a set of 100 integers picked along each axis of our coordinate system.

5. Higher and lower dimensions

Further on, we can notice that, whereas quantum mechanically, the summation $n_x^2 + n_y^2 + n_z^2$ is indeed *special* (see equation (1)); one can generalize it to the form,

$$\zeta = n_1^{\,m} + n_2^{\,m} + n_3^{\,m} + ..., + n_I^{\,m} = \sum_{i=1}^{I} n_i^{\,m} \,, \tag{7}$$

where the subscript "*i*", points to the *ith* dimension, and the superscript "*m*" points to any exponent, be this equal to 2, greater than 2 or smaller than 2. We have done a few simulations, in 4 and 5D, along with an exponent *m* just above 2, and below 2, and, even for *m*=1/2, and so forth within similar ranges as those considered in Figures 1-4. The outputs interestingly enough turns out to be about same as those sketched in the mentioned Figures, though the problem remains to be thoroughly investigated. All the same, it falls outside of the scope of the present paper; the entire problem seeming to be rooted to the number theory, and in particular to Ramanujan's work [10-15].

The special case pops out immediately, where *m* = 0:

$$\zeta_{0I} = n_1^{\,0} + n_2^{\,0} + n_3^{\,0} + ..., + n_I^{\,0} = I\,. \tag{8}$$

Let us, as an example reconsider the 3D case:

$$\zeta_{03} = 1 + 1 + 1 = 3. \tag{9}$$

Then within any given range, made of N locations along each axis, pointing to a total of N^3 locations, in our *quantum mechancial integers space of the coordinate system,* we will just have the sum 3, and the probability distribution function will be same, and equal to unity, everywhere.

6. Discussion

First of all, we discuss the relationship between our results obtained in the basis of equation (1) and the framework of statistical quantum mechanics [16]. We remind that the latter theory, the momentum $p_n = nh/2L$ of the particle in a box of length L is also considered – where, in a stationary gas regime, it can be interpreted as the mean free path of molecules of the gas. At a large n, the common practice implies the limit $\sum_n \rightarrow \int dn = \int 2L dp_n / h$, and with $L = \int dx$, we have $\int dn = \iint 2 dx dp_n / h$.

Furthemore, it is widely affrimed that Maxwell-Boltzmann distribution is compatible with quantum mechanics. But, why the energy (1) of the particle in a 3D box, more precisely, the sum of the squares of three integers, $n_x^2 + n_y^2 + n_z^2$, in a domain of integers tending to infinity, must delienate a Maxwellian distribution, in conformity with Eqs. (3) and (5)? This is not trivial at all…

This mathematical problem appears to no have been rigorously solved up to date.

All the more, we remind that the Boltzmann transport equation in a stationary regime (where there is no leakage, no abosorption, and no source), leading to Maxwell distribution, i.e.

$$\Sigma_s(E)\phi(E) = \int_0^\infty \Sigma_s(E' \rightarrow E)\phi(E')dE', \tag{10}$$

does not constitute an *eigenvalue – eigenstate* equation.

Here, $\Sigma_s(E)$ is the scattering macroscopic cross section of target entities, that scatter the striking objects of flux $\phi(E)$, and bearing energies within *a unit energy interval around the energy E,* and $\Sigma_s(E' \rightarrow E)$ represents the scattering macroscopic cross section of target entities of energy E', lying within the infinitely small energy interval dE around the energy E.

The quantity on the lhs of equation (10) points to the number of scatterings taking place in a unit volume per second, for the energies of the colliding objects lying within a unit energy interval around the energy E.

The rhs of the above equation, on the other hand, points to the number objects that bear originally all possible energies other than the energy E, and collides the targets, but come out of the collisions in consideration with an *energy lying within the unit energy interval taking place around the energy E,* within the same unit volume and per second.

Thereby, in a stationary situation, within the given volume, we have at any time *momen* the same number of objects bearing an energy within a unit energy interval around a given energy E.

Therefore, the number of objects in the given volume within the energy interval dE depicted around E, which collide with the targets during a unit time interval and leaving this energy interval, is equal to the number of objects bearing energies comprised in any other interval dE', around E', which after collisions with the given targets present in the given volume per second, land at the energy interval dE of concern, depicted around E.

Note that equation (10) has the general character, and describes, for example, neutrons' energy distribution in a nuclear reactor, when we have no leakage, no absorption, no source [17].

Let us recall that the solution of equation (10) has the form of

$$\phi(E) \sim E \exp(-E/kT) ; \tag{11}$$

where k is Boltzmann Constant, and T is the average absolute temperature of the medium. We further recall that the *flux $\phi(E)$* is defined as the integral of the directional flux $\psi(E,\underline{\Omega})$ over the solid angle $d\Omega$, i.e.

$$\phi(E) = \int_{\Omega} \psi(E, \underline{\Omega}) d\Omega, \tag{12}$$

and the *directional flux* is expressed as

$$\psi(E, \underline{\Omega}) = n(E, \underline{\Omega}) v(E), \tag{13}$$

where $n(E, \underline{\Omega})$ is the number of objects per unit volume with energy lying in a unit energy interval around the energy E at any time t in a stationary regime, and moving in a direction comprised in a unit solid angle drawn around the direction represented by the unit vector $\underline{\Omega}$; $v(E)$ stands for velocity directed within the direction $\underline{\Omega}$.

Thence, in order to be able to affirm that quantum statistical mechanics will lead to a Maxwellian distribution of the sum of the squares of three integers

$n_x^2 + n_y^2 + n_z^2$ at n_x, n_y, n_z tending to infinity, one has to show based on equation (10), how this can

be done, if not, directly based on the theory of integer numbers, which, in general, represents a non-trivil mathematical problem.

We would like to note that Yarman et al. have already shown that Boltzmann expression for entropy, written based on the binomial distribution, does not hold valid within the framework of quantum mechanics [5].

Thus, the approach undertaken in this work, does not appear to have any similarity with what is done within the framework of quantum statistical mechanics. It is not even sure, whether the value of

the sum of the squares of three integers $n_x^2 + n_y^2 + n_z^2$ at n_x, n_y, n_z tending to infinity, will delineate a

Maxwellian distribution. If so, this seems to promise to be a great challenge with respect to the properties of integer numbers, thus to be led to by quantum statistical mechanics.

7. Conclusion

This work is trigerred by the precedent work of Yarman et al, aiming to bridge thermodynamics and quantum mechanics [1-5], whence, Planck constant came to replace Boltzmann constant, and "average quantum level number" came to replace "temperature".

This evoked that the classical Maxwell energy probability distribution $p(E)$ with respect to energy E, of gas molecules, might be taken care of, by the *"energy probability distribution of the quantum levels"* of a particle imprisoned in a given volume, assuming that in the case no pair of particles can sit at the same level due to Pauli exclusion principle.

In the present paper, we considered energy probability distribution of the quantum levels of a particle imprisoned in three dimensions in the manner of Schrödinger's common setup engenders, as contingent upon a fixed energy range.

The result we disclosed; if elastic collisions between the free particles in question, were allowed, just like is the case for molecules in the room, and still assuming quantization and the Pauli Principle; should be expected to be about the same as that of the energy probability distribution, molecules, in the room would display, in equilibrium.

All the same, it appeared mathematically appealing, to go beyond the three dimensions, we have adopted, thusly, along with the "sum of three squared integers". It appeared furthermore appealing to play with the exponent 2, we applied to the integer numbers in consideration, as originally implied by quantum mechanics.

Thusly; we have done a few simulations, i) in 4 and 5D, as well, along with an exponent m picked to be 2, in the foregoing text, also ii) with an exponent m above 2, and below 2, and even iii) with an exponent $m=1/2$, and so forth, within similar ranges as those considered in Figures 1-4. The outputs, interestingly enough, turn out to be about nearly the same as those sketched in the mentioned Figures, though the problem remains to be thoroughly investigated.

The main reason for shape similarities we come across to, for different type of applications, we mentioned, is that the *frequency of occurrence of a given value* picked in our space of quntum numbers for a given combination, say in 3D, in the form of $\zeta = n_x{}^m + n_y{}^m + n_z{}^m$, remains the same, no matter what *m* is. Therefore, the same frequencies corresponds to lower energies, if *m*<2, and to higher energies if *m* < 2.

All the same, the related quest falls totally outside of the scope of the present paper, seemingly being rooted to the number theory, and in particular to Ramanujan's work [10-15].
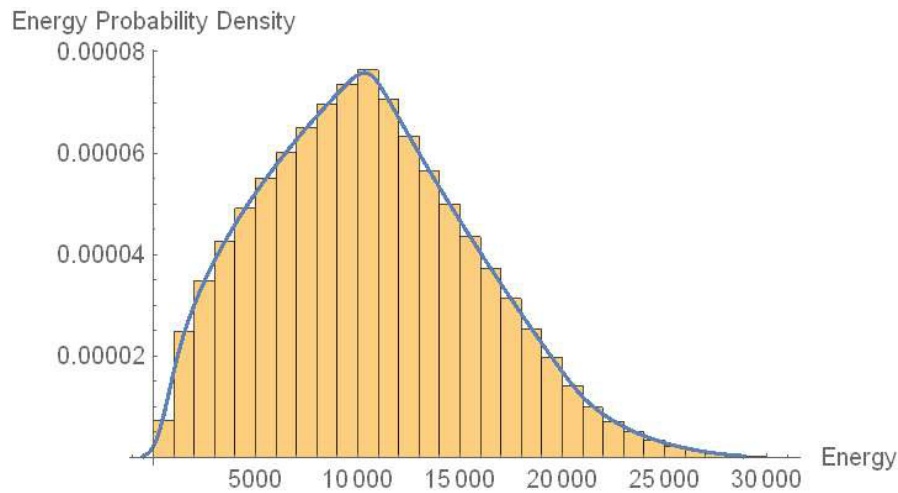
1-100

Figure 1. Energy probability distribution versus energy, where the same set of integers 1-100, were picked in all three dimensions
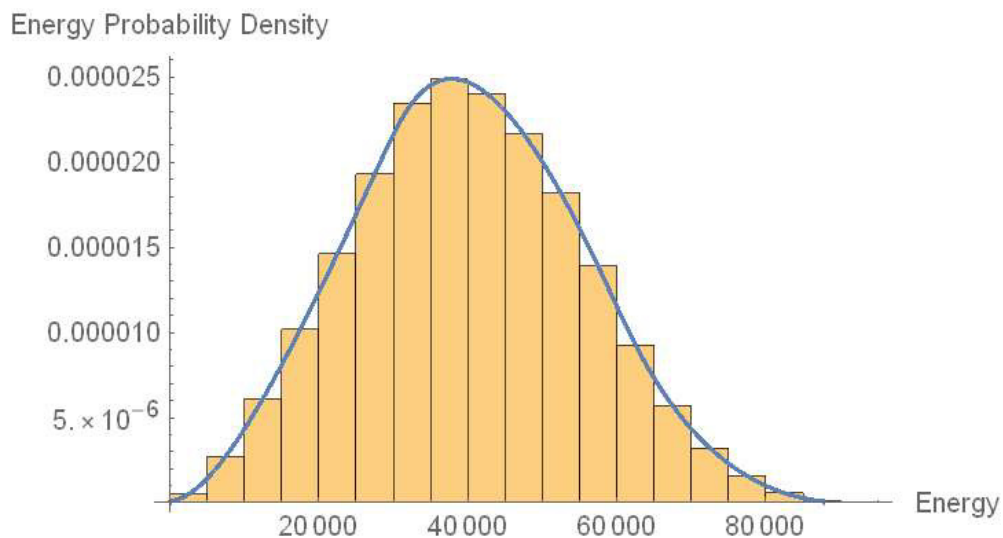
100-200

Figure 2. Energy probability distribution versus energy, where the same set of integers 100-200, were picked in all three dimensions
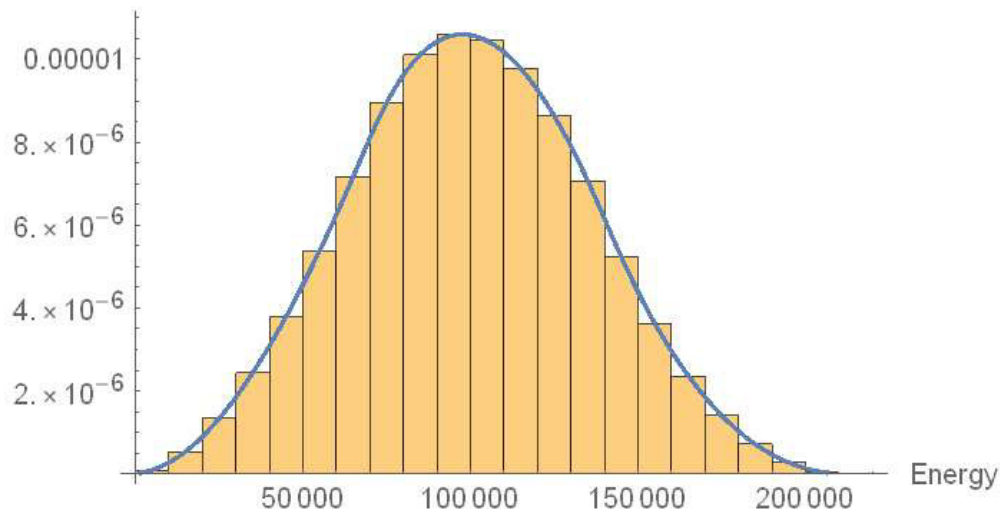
300-400

Figure 3. Energy probability distribution versus energy, where the same set of integers 300-400, were picked in all three dimensions
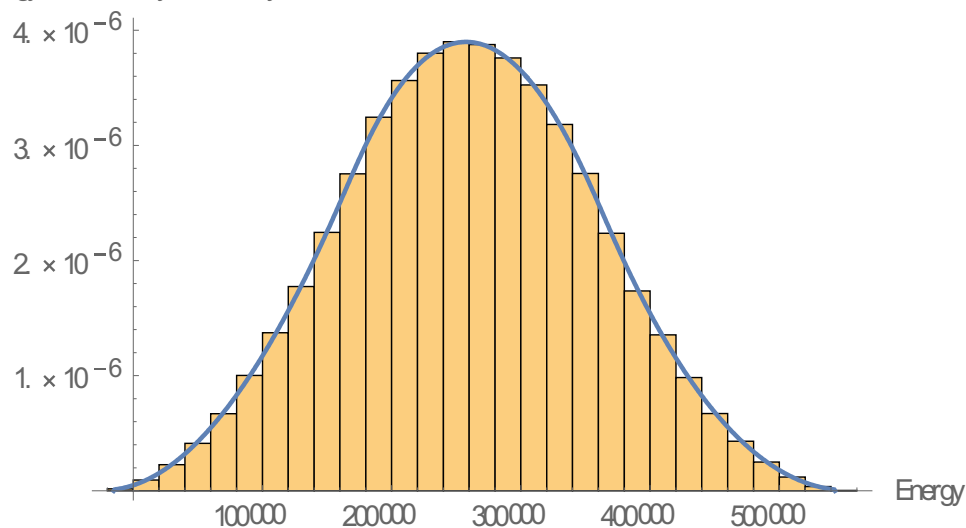
900-1000

Figure 4. Energy probability distribution versus energy, where the same set of integers 900-1000, were picked in all three dimensions

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