

Entropy of Open System with Infinite Number of Conserved Links

A. Moldavanov*

2774 Sunnybridge Dr., Burnaby, BC Canada V5A 3V1
E-mail: trandrei8@gmail.com

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Abstract

Energy budget of open system is a critical aspect of its existence. Traditionally, at applying of energy continuity equation (ECE) for description of a system, ECE is considered as a declaration of local balance in the mathematical (infinitesimal) vicinity for the only point of interest and as such it does not contribute to entropy. In this paper, we consider transformation of ECE to account the effects in the physical (finite) vicinity with infinite number of energy links with environment. We define parameters of appropriate phase space and calculate Shannon's, differential, and thermodynamic entropy. Shannon's and differential entropies look sufficiently close while thermodynamic entropy demonstrates close character of variation in its functionality being different in its mathematical form. Physical applications to confirm contribution of a new concept to the real-world processes are also discussed.

Keywords: Information uncertainty; Shannon's entropy; thermodynamic entropy, continuity equation; energy exchange.

1. Introduction

1.1 Entropy

Information theory was established by Shannon in 1948 [1]. It allowed to introduce a remarkable measure of information – Shannon's (information) entropy [2]. Since that, entropy plays a central role in statistical mechanics, and, as a result, in physics.

A fundamental meaning of new concept was shortly confirmed by existence for a given probability distribution of notable complementary interpretation - quantity of information (after measurement) or uncertainty (before measurement) [3]. Within this way of thinking, Jaynes has seen a statistical mechanics as an application of informational theory, and thermodynamics as a special case of entropy maximization procedure [4].

In recent years, a concept of information entropy was being intensively developed within the framework of both, classic and quantum physics.

These days, we can think of an entropy as a key concept of quantum information theory [5]. In this sense, an entropy of a quantum system is a measure of its randomness and has many applications in quantum communication protocols, quantum coherence, and so on [6-8].

Important role in above development belongs to the so called Bialynicki-Birula and Mycielski (*BBM*) inequality

$$S_{nx} + S_{np} \geq d[1 + \ln(\pi)] \quad (1)$$

which can be considered as a new uncertainty relation in quantum mechanics, where S_x and S_p are entropy for position and momentum. This new relation has a clear interpretation in information theory as a formalism that relates the position and momentum uncertainties, where d denotes the dimension of the position and momentum space [9].

The study of Shannon entropy for a spinless non-Hermitian particle in the presence of a magnetic field was conducted in [10]. Numerical analysis demonstrates that Shannon's entropy satisfies the *BBM* relationship for ground and excited states independent of the value of the magnetic field. It was also shown that the magnetic field has an ability to modify the Shannon entropy which satisfies the *BBM* relationship of the model.

Modification of Shannon's entropy and thermodynamic properties under the linear potential action was studied in [11]. It was noted that Shannon's entropy of Majorana fermions satisfies *BBM* for fundamental and excited states. At this, an external force that acts on the Majorana fermions alters Shannon's entropy, however, this alteration still obeys *BBM* relation of the model.

Simulation of a Shannon entropy at abrupt heterojunctions in semiconductor materials in approximation of the soliton-like mass distribution (position-dependent mass) was investigated in [12]. It was shown that for the Hamiltonian operator to be Hermitian, Zhu-Kroemer ordering for the stationary Schrodinger equation can be employed.

Numerical calculation of the Shannon entropies for a rectangular asymmetric multiple quantum well system with a constant total length was fulfilled in [13]. It is demonstrated that the S_x and S_p do not always decrease or increase monotonically with the confined potential depth, but their sum always satisfies *BBM*.

A spherically confined hydrogen atom has been considered using two different confined potentials such as modified Kratzer and non-spherical oscillator potentials. *BBM* has been also tested. It was found that its validity depends on non-extensive parameter [14].

On the other hand, in classic physics, an entropy concept has taken important and prominently deserved place since

recognition of its remarkable meaning. However, the new results and fresh views to the well-known facts related to entropy are still being appeared regularly.

As an example, indicate to the recent research which demonstrates that information content and its uncertainty as measured from the file compression procedure can unexpectedly provide new insights like quantifying of hidden order in non-equilibrium physics [15].

Some uses of Shannon's entropy formula in information theory that have confirmed the functionality of this paradigm were considered in [16].

Advent of nanostructures that straddle the border between the molecular and the macroscopic levels of physical understanding, has opened new applications for informational entropy [17].

Analysis of entropy for obtaining of an uncertainty principle by utilizing of fundamental physical paradigm of continuity in the nanoscale level was conducted in [18-20].

New reading of the far from equilibrium thermodynamical concepts was recently achieved due to using of entropic relations [21,22].

Alternative approach to thermodynamic uncertainty relation as well as limitation to entropy variations for non-equilibrium thermodynamical states was considered in [23].

Above results confirm existence of the deep-laid connection between entropy and behavior of physical system. Further, we will be presenting transformation of energy continuity equation (*ECE*) and, on this basis, evaluation of entropy for open system with infinite number of conserved links with environment.

1.2 Extension of energy continuity equation

In this research, we will be using a physical model of the conserved link between system and its environment. By its definition, this link calls for the conserved quantities (*CQ*) that meet generic requirement of conservation [24]. This requirement in differential shape represents balance in the local form and in the non-relativistic approximation for energy is given by an *ECE*

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \mathbf{J} = 0 \quad (2.a)$$

where \mathbf{J} is flux of energy, ε is energy volume density, t is time, and ∇ is Nabra operator [25, 26].

So, considered approach contains such exchange scenarios that include an energy dimension. Hence, we only deal with the scenarios in which the change in system state can be described in energy terms irrelevant of the nature of the exchange processes themselves. Further discussion about employed approach can be found in [24].

By default, notation (2.a) appeals to a mathematical (infinitesimal) space-time vicinity (*STV*) for the only point of interest. As a result, (2.a) assumes a predetermined description of an energy exchange process in the only point and eliminates any chance for uncertainty in definition of parameters (2.a). Therefore, (2.a) brings no contribution to entropy.

However, validity of (2.a) becomes questionable if we do step aside from the mathematical to the physical (finite) *STV*, further *PSTV*. Obvious reason of that lies in breaking of the space-time predetermination which inevitably brings randomness, uncertainty, and missing information, *i.e.*, Shannon's entropy.

To reflect emergence of *PSTV* uncertainty, (2.a) can be extended to the system of infinite number of *ECE*

$$\left\{ \begin{array}{l} \frac{\partial \varepsilon_1}{\partial t} + \nabla \cdot \mathbf{J}_1 = 0 \\ \frac{\partial \varepsilon_2}{\partial t} + \nabla \cdot \mathbf{J}_2 = 0 \\ \dots \\ \frac{\partial \varepsilon_n}{\partial t} + \nabla \cdot \mathbf{J}_n = 0 \\ \dots \end{array} \right. \quad (2.b)$$

where $n \rightarrow \infty$ [25].

Below, it is assumed that *PSTV* is surrounded by a permeable boundary that supports the non-zero mass flow, then *PSTV* can be considered as an open thermodynamic system. For description of this system, we combine three kinds of energy flux under common symbol \mathbf{J} : (a) default heat transfer, (b) work transfer by the transport of *CQ* like charge, momentum, angular momentum, and mass, (c) enthalpy flow via the mass transfer across permeable boundary.

So, we make step from *STV* (2.a) to *PSTV* (2.b), and our aim is to estimate an appropriate increment in entropy that this step can cause.

2. Transformation of ECE

In *ECE* (2.a), conduct equivalent mathematical transformation.

So, let *STV* be the closed manifold oriented by inward-pointing normal \mathbf{n} at each point of the boundary S . Suppose the direction of $d\mathbf{J}$ is determined by the unit vector \mathbf{m} , $\mathbf{m} = (\cos \varphi_x, \cos \varphi_y, \cos \varphi_z)$, where $\varphi = \angle(d\mathbf{J}, \mathbf{n})$,

$$\cos \varphi_i = \frac{dJ_i}{dJ}, \quad (3)$$

dJ_i is i -th component of $d\mathbf{J}$, $d\mathbf{S}$ is a shorthand for $\mathbf{n}dS$, $i = \{x, y, z\}$ in the Cartesian system.

Multiply both sides of (2.a) by elementary volume dV and use (3), so we have

$$\frac{dU}{dt} = -dJ(\mathbf{m} \cdot d\mathbf{S}) = -dJ(\mathbf{m} \cdot \mathbf{n})dS \quad (4)$$

where $\mathbf{m} \cdot \mathbf{n} = \cos \varphi$, $dU = \varepsilon \cdot dV$.

Divide (4) by $J \cdot dS$ and observe $Q = J \cdot dS \, dt$, so

$$\frac{dU}{Q} = -d(\ln y) \, x \quad (5.a)$$

or, equivalently,

$$\frac{dU}{\delta Q} = -x \quad (5.b)$$

where $\delta Q = dJ \cdot dS \, dt$, random $x = \cos \varphi$, deterministic y (energy exchange rate) = J/J_0 , normalizing constant $J_0 > 0$.

Note that relations (5) explicitly include factor x . At variable nature of x , it naturally accounts an infinite n in $PSTV$ approximation (2.b).

3. Factor x as indicator of uncertainty

Physically, factor x determines the instantaneous status of an energy exchange pattern between $PSTV$ and its environment.

It should be noted that violation of (2.a) leads to widening of the uncertainty interval for quantity (dU/Q) in (5). In this sense, emergence of uncertainty in (5) could be considered as a natural adjustment to get to the higher confidence for the observed results.

Note that in alignment with above, generally, (5) cannot be considered as a *continuity* equation in its conventional meaning anymore.

So, at fixed x , we deal the mathematical STV with, and (5) is a regular ECE asserting the predefined energy transfer in dependence on y and certain match between the amount of energy brought to the STV boundary and that of finally acquired by STV , i.e., $dU = Q$.

In contrast to that, in $PSTV$ approximation, random x is taken from some range, hence uncertainty is being emerged, and it is no longer mandatory for dU and Q to be the same. In this sense, the set of x controls the set of possible scenarios of energy exchange at every given y , when the particular scenario is realized on the random basis.

We see from above that simple reformulation of x allows us to easily switch between the mathematical (2.a) and the physical (2.b) method of description. In turn, the latter provides a natural way to switch from the only possible scenario of energy exchange to many of them. This switching can be done by just changing of type and value of x .

4. Function Y as measure of phase volume

By definition, in this model variables x and y are independent, so from (5.a)

$$\int \frac{dU}{Q} dy = -\delta Y(x, y) = -x \cdot \ln y \quad (6)$$

where $\delta Y(x, y)$ is an instantaneous efficiency of energy exchange with suitable phase space $M \subseteq R^2$ for all possible states (Figure 1).

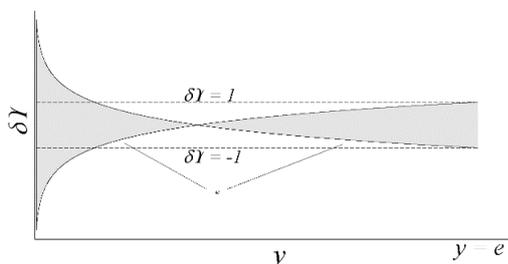


Figure 1. Phase space M for all possible microstates of instantaneous efficiency of energy exchange δY between $PSTV$ and its surroundings. In the plot, by an abscissa axis a energy rate $y = J/J_0$ is indicated, by an ordinate axis an instantaneous efficiency δY . Space M is marked by a light-grey area (taken from [24]).

Now, introduce function

$$Y = -\iint_M \delta Y(x, y) = -\int_{-1}^1 dx \cdot \int_0^y \ln y dy \quad (7)$$

which after integration can be expressed as

$$Y = y - y \ln y \quad (8)$$

By its appearance, Y describes the phase volume for random variations of δY .

Function Y is of maximum in the stationarity point $y = 1$, while its minimum is at the bounds of y -range for energy exchange (Figure 2). In the considered case, these bounds are $[0, e]$, where e is the base of natural logarithm.

Eq. (7) can be rewritten as an identity

$$\int_0^1 dy \int_{-1}^1 \delta Y(x, y) dx = \left| \int_1^e dy \int_{-1}^1 \delta Y(x, y) dx \right| = 1 \quad (9)$$

where $|a|$ denotes a modulus of a . Identity (9) can be also written as

$$\begin{cases} Y(1) - Y(0) = 1 \\ Y(1) - Y(e) = 1 \end{cases} \quad (10)$$

which assumes that the y -ranges $[0, 1]$ and $[1, e]$ mandatorily contain the full bunch of $PSTV$ exchange scenarios no matter which variations x (δY) happen. At this, the range $0 \leq y \leq 1$ deals with the preferable transportation of energy inwards $PSTV$, while the range $1 \leq y \leq e$ with the opposite transportation of energy outwards $PSTV$ [26].

In other words, (7) means that at arbitrary y , the existing phase volume Y does not guarantee $dU = Q$, however it can guarantee the maximum possible proximity of dU and Q at bidirectional transmission between $PSTV$ and environment on the confidence interval $[0, y]$. Generally, this transmission is not the error-free ($Y \neq 1$).

Remind that Shannon-Hartley theorem [27] states that theoretically it is possible to provide an error-free transmission through the noisy channel if channel capacity C exceeds the information transmission rate R , i.e., if

$$C \geq R \quad (11)$$

If (11) does not hold, then transmission should include the more or less percentage of errors.

In our case, function Y can be considered as equivalent of C while y as equivalent of R . Therefore, rewrite (11) as

$$Y \geq y \quad (12)$$

Using (8), it assumes that theoretically (12) holds in the range $0 \leq y \leq 1$, and violates in the range $1 < y \leq e$. As a result, in the real-world application the probability to observe the error-free energy exchange process is higher in the range $0 \leq y \leq 1$ compared the range $1 < y \leq e$.

In above way, (7,9) directly refers to the context of the theorem [27] as it determines the measure of error occurrence for energy exchange process in the noisy channel ($PSTV \leftrightarrow$ environment) in terms of volume Y and bandwidth y . At this, (9) provides conditions to guarantee the lossless ($dU = Q$) bidirectional transportation of energy through

PSTV boundary, whereas (7) indicates to the minimum portion of errors we should expect in the best case possible.

For example, given $y = 1/e$, then from (8) $\Upsilon = 2/e \approx 0.73$. As $1 - 0.73 = 0.27$, we should expect that about 27% of transmitted energy is dissipated as a useless heat.

All abovesaid prompts us to use the framework of information theory. So, now we are in a good position to calculate an entropy caused by the $STV \rightarrow PSTV$ jump.

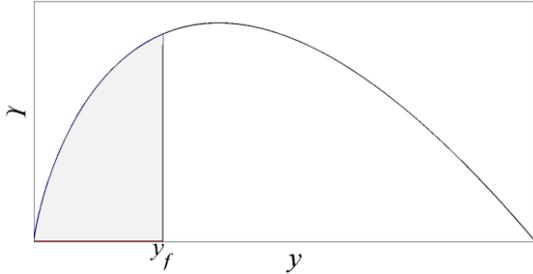


Figure 2. Phase volume Υ for all possible microstates of instantaneous efficiency of energy exchange δY . In the plot, designation of the horizontal axis is the same as in the Figure 1, by an ordinate axis the phase volume Υ is indicated. Phase volume at arbitrary $y = y_f$ is marked by a light-grey area.

5. Calculation of entropy

5.1 Shannon's entropy

As it was mentioned above, Υ can be interpreted as a phase volume for space M (Figure 2). Then in M , the maximum number of possible microstates W at given rate y is $(dY/dy)dy$ [28, 29]. Therefore, from (8) and using Gibbs' definition [28], Shannon's entropy up to a constant additive A_0 is

$$\Delta S = \ln W = \ln |\ln y| + A_0 \quad (13)$$

It is important that (13) fully coincides with the main part of differential entropy (16) discussed below.

5.2 Differential entropy

Although differential entropy cannot be considered as the mathematically rigorous extension of information entropy because of the known limitation $\lim_{\Delta \rightarrow 0} \ln(\Delta) \rightarrow -\infty$ [30], we consider dynamics of its main part yet believing that it may provide useful auxiliary information, where Δ is the size of discretizing for probability density function (PDF). Moreover, we are only interested in the difference of differential entropy ΔS^x between adjacent states which obviously lacks above shortcoming. Also, we will consider dynamics of ΔS^x , taking value of S^x at $y = 0$ as the anchor one.

So, let $g(x)$ be the PDF for random x , i.e.

$$g(x) > 0 \text{ for } x \in [-1, 1] \quad (14.a)$$

$$g(x) = 0 \text{ at } x \notin [-1, 1] \quad (14.b)$$

then from (6) at each y , PDF is

$$f^y(x) = \frac{g(x)}{|\ln y|}, \quad x \in [-1, 1] \quad (15)$$

[31], where $|\ln y|$ is taken to keep $f^y(x) \geq 0$, y is a parameter. Calculation of $f^y(x)$ is done in assumption that x is the random at each given deterministic y .

Now, introduce an entropy probability distribution for instantaneous random δY as

$$\Delta S^x = - \int_{-1}^1 f^y(x) \ln(f^y(x)) dx \quad (16)$$

Insert (15) to (16) and simplify, then Shannon's entropy is

$$\Delta S^x = \ln |\ln y| + H_x \quad (17)$$

with the plot shown in Figure 3, where H_x is an entropy probability distribution in the range $[0, \ln 2]$ for x on the compact support $[-1, 1]$

$$H_x = - \int_{-1}^1 g(x) \ln(g(x)) dx \quad (18)$$

Now, we can observe meaning of the constant A_0 in (13), i.e., $A_0 = H_x$.

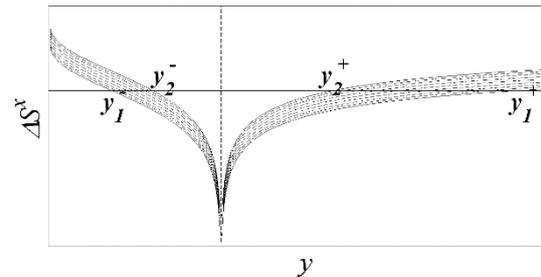


Figure 3. Shannon's entropy ΔS^x for PSTV. In the plot, designation of the horizontal axis is the same as in the Figure 1, by an ordinate axis Shannon's entropy ΔS^x is indicated. The spectrum nodes y_1^\pm and y_2^\pm match the roots of entropy ΔS^x . Allowable ΔS^x is located within two dashed area (taken from [24]).

6. Physical applications of calculated entropy

6.1 Bunch of evolutionary scenarios

As shown in [24], spectrum of Υ at $1/e \leq y \leq e$ becomes discrete

$$y_n = \exp\left[\pm \frac{1}{n}\right] \quad (19)$$

where $n = 1, 2, \dots$.

Then, from (17), using (19)

$$\Delta S_n = H_x - \ln n \quad (20)$$

and solution for entropy is localized within the area restricted by the roots of ΔS_n (20) for bounds of H_x that, at the same time, are the first and second harmonic of the spectrum (19) as shown in Figure 3 [24].

As the peak of ΔS^x fits to the peak of H_x (18), then according to the principle of maximum entropy production [32], such scenario deals with the most probable and the fastest path of $PSTV$ evolution. In Figure 3 appropriate curve

crosses the points of the first harmonic of the discrete spectrum, *i.e.*, y_1^- and y_1^+ (Figure 3).

In the same way, minimum ΔS^x fits to the minimum H_x . Then, using [32] one more time, it accommodates requirements for the least probable and the slowest path of evolution. In Figure 3, curve addressing the least probable evolutionary scenario crosses the points of the second harmonic *i.e.*, y_2^- and y_2^+ .

The other scenarios fall in the y -range $[y_1, y_2]$ so that the probability of realization decreases from y_1 to y_2 .

The more thorough investigation [24] shows that at $y = y_2^+$, the probability of evolutionary scenario (assumes quality changes in energy structure of *PSTV*) matches the probability of non-evolutionary scenario (plain mode of receiving and losing of energy). At $|\ln y_1| \geq |\ln y| \geq |\ln y_2|$, probability of the evolutionary scenario is higher, at all other y the non-evolutionary scenario predominates (Figure 3).

6.2 Thermodynamic uncertainty relation

Ratio

$$\Delta E \cdot \Delta\left(\frac{1}{T}\right) \geq k_B \quad (21)$$

is known as a thermodynamic uncertainty relation (*TUR*), where k_B denotes the Boltzmann constant, T is temperature, E is energy, and arguments ΔE and $\Delta(1/T)$ could be, generally, replaced with some functions of these arguments [33].

Write $\Delta U = (\Delta U/\Delta T)\Delta T$, then (5.b) can be expressed as

$$\frac{(\Delta U / \Delta T)\Delta T}{Q} = -x \quad (22)$$

Apply to (22) Clausius inequality for entropy [34]

$$\delta Q \leq T\Delta S \quad (23)$$

then it is possible to determine the physical conditions when *TUR* is valid.

6.3 Lower limit for thermodynamic entropy

Recently, the new limiting condition was shaped in nonequilibrium thermodynamics for total entropy rate in Markov jump processes [17,18] dealing with the state arbitrary far from an equilibrium, which could be written as

$$\frac{\dot{S}_t}{2k_B} \geq \frac{\langle J \rangle^2}{\langle \delta J \rangle^2} \quad (24)$$

where \dot{S}_t is total entropy rate, $\langle J \rangle$ is an average flux, $\langle \delta J \rangle$ is variance of flux fluctuations.

Show that (18) can be stemmed from (2.a,b). So, combine (5.b) with (23), then we obtain

$$\frac{dS}{k_B} \geq \frac{J^2}{2\Delta J^2} \quad (25)$$

Having (25) averaged on the time interval $\tau \sim \Delta t$, and denoting $\dot{S}_t = \Delta S/\Delta t$, we have solution that up to a constant multiple coincides with (24).

So, we see that presented approach (2.b) allows to predict possible way of *PSTV* energy development (section 6.1), provide useful information for working conditions of *TUR* (section 6.2), derive lower entropy constraint in the non-equilibrium thermodynamics (section 6.3). Hence, (2.b) can be considered as a common basis for several physical applications.

7. Discussion

Generalization of physical uncertainties was considered in a number of articles. As shown in [35], in approximation of the highest energies it is possible to bring in to the classic *TUR* an extra term related to the internal energy that causes appearance of the lower boundary for inverse temperature. Technically, eq. (2.b) could be also thought as the consequence of applying to (2.a) some additional uncertainty (energy) which transforms (2.a) to (2.b) and, ultimately, emerges as constraint for Shannon's entropy.

In [36], authors examine collection in which energy E , temperature T and multiplicity N can vary. Then, with the support of non-extensive statistics they suggest interconnection for all varying factors that formalizes the known Lindhard's *TUR* [37]. As it is known, the non-extensive statistics does not use conventional Boltzmann-Gibbs statistical mechanics. The latter seems interesting first of all for study of the objects with complicate structure like nanostructures.

Results [38] presume that an indefinity in the fundamental pattern allows use of the framework of information concept. In this way, it seems acceptable to seek confirmation of uncertainty links using the methods of information concept. We think that it aligned with our analysis in the sections 1.2, 2 where we discussed the "uncertainty" value of (2.b) unlike quite deterministic (2.a).

Presence of resembling entropy limitation was discussed in [17-19,39]. Existence of an uncertainty bound for the small-scale fluctuations in equilibrium thermodynamics, and for the large-scale fluctuations arbitrary far from equilibrium for Markovian processes in non-equilibrium thermodynamics was demonstrated in [17]. In [18], at the nonequilibrium steady states of Markovian processes, a few universal bounds valid beyond the Gaussian regime was derived. Authors [39] declared existence of a new class of thermodynamic uncertainty inequalities, which have revealed that dissipation constrains fluctuations in steady states arbitrarily far from equilibrium. A possible way to come to the identical constraint for the thermodynamic entropy based on (2.b) and Clausius inequality for *PSTV* was demonstrated in [19].

Generalizing the said above in [17-19,39], an entropy constraint for *PSTV* could be given as

$$dS \geq \frac{k_B}{2} \frac{1}{y^2} \quad (26)$$

where $y = \langle \Delta J \rangle / \langle J \rangle$.

Integrating (26) on y , we obtain

$$\Delta S \geq -\frac{k_B}{2} \frac{1}{|y|} + C_S \quad (27)$$

where C_S is an integration constant.

Assuming C_S is bounded like H_x in (18), we obtain that solution (27) could also have the quasi-continuous y -

spectrum that in its form (shown in Figure 4) is close to the depicted in Figure 3.

Of course, (17) and (27) are parametrically different equations, however, our purpose is to demonstrate similarity in behavior of these two dissimilar methods.

Novelty of considered approach, primarily, lies in analytic solution of (2.b) and finding of reasonable physical applications for the found solution. Discovered γ -solution deals with average measure for uncertainty of energy exchange process in open system with infinite number of conserved energy channels with environment, and as such, has natural connection with an entropy. This foundation permits to calculate an increment in Shannon's and differential entropy, as well as study conditions to constrain thermodynamic entropy. Follow this way, it is possible to forecast possible scenarios of energy development in open system, to draw existence of the lower threshold of entropy in the non-equilibrium thermodynamics, and obtain conditions for validity of *TUR*, i.e., describe sufficiently unrelated physical phenomena.

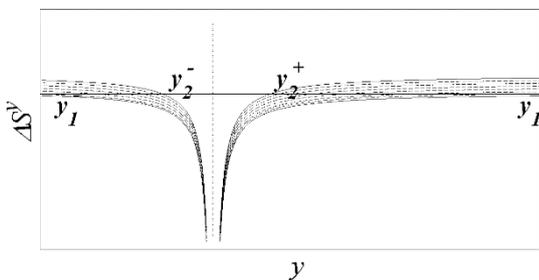


Figure 4. Lower threshold for thermodynamic entropy ΔS^v in PSTV. In the plot, designation of the horizontal axis is the same as in the Figure 1, by the ordinate axis the lower threshold for thermodynamic entropy ΔS^v is indicated. Meaning of the points y_1^\pm and y_2^\pm is identical to the y -points in the Figure 3.

8. Conclusions

This report presents a nontraditional formalism to Estimate alteration of Shannon's, differential, and thermodynamic entropy in *PSTV* approximation. Found entropy provides a new look at the process of energy exchange in open system with unlimited number of conserved energy links. Generalizing, *PSTV* approximation (2.b) acts as a common basis that demonstrates its value in several dissimilar physical applications.

Nomenclature

ε : volume energy density [J/m]³

J : energy flux [J/m²·s]

k_B : Boltzmann constant [J/K]

Q : energy transfer [J]

t : time [s]

T : absolute temperature [K]

U : internal energy [J]

All other variables are dimensionless.

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