

ABOUT DEFINING THE REFERENT THERMAL SCALE POINTS

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ABSTRACT

The absolute temperature T has a recognized physical meaning in equilibrium thermodynamics. The scale realized by the closely related Lagrange coefficient β usually figures as an auxiliary scale. In this article, the scale spanned by β is a proper intensive thermal quantity for equilibrium and, suitably generalized, for stationary non-equilibrium state description. The coefficient β measures a relative deviation of a system state from the state of uniform distribution function. The cause of deviation is coupling to environment, which is realized as a net energy transfer and which ceases in the $\beta = 0$ state. A canonical ensemble of two level atoms coupled to electromagnetic quasi-continuum is considered as an example. The proposed and the usual interpretations of β are applied to stationary states of the same system, in which case the notion of the generalized absolute temperature is introduced. The generalized absolute temperature is a measure of a deviation of a system state from a state of infinitely intense external influence.

KEY WORDS

non-equilibrium thermodynamics, equilibrium, Lagrange coefficient

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INTRODUCTION

The absolute temperature, T , connects the differential changes of system energy and its entropy in isochoric processes. In description of a system of classical particles with translational degrees of freedom, it is a measure of the difference between the average and the minimal system energy. Within statistical physics it is introduced through a distribution function determination. In that determination the auxiliary quantities, the Lagrange coefficients, occur [1] and are, for the sake of simplicity, often used throughout the calculations. In the case of a system with known spectrum and energy, the Lagrange coefficient β is a quantity sufficient to determine the equilibrium distribution. Coefficient β is related to the absolute temperature usually as $\beta = T^{-1}$.

In cases of stationary non-equilibrium states, β is not sufficient to determine the distribution function [2, 3] as it does not include the effects of the fluxes between the system and its environment. One of the quantities encountered in stationary non-equilibrium state description is the non-equilibrium absolute temperature θ [2-5]. Its limit when the system approaches equilibrium is the absolute temperature T . In cases of relatively small non-equilibrium effects θ is expressible as the absolute temperature modified by a flux-dependent part [2, 4, 6, 7]. A number of thermally related quantities have been introduced in order to provide an intensive quantity for description of out of equilibrium states [5]. However, at the present moment, there is no such generally applicable quantity recognized.

Exchange of energy with the environment is an environment influence, realized with the opening of channels for delocalization of system energy. The system state obtained asymptotically the alignment of the environment and the system state occurs [8]. Cases of environments parameterized through several influences with the corresponding limiting, stationary system states, are straightforwardly included. Regarding the system state evolution, the referent state is introduced. It is the origin of a scale spanned by the system state variable. Generally, when the system state is close to some limiting state, the limiting and referent state coincide. The absolute temperature T is an example of a state variable the zero of which is both a referent state and a limiting state of system coupled with environment in the minimal energy state. However, there are several objections to equating the limiting and referent state. Operationally, the thermodynamic description based on one limiting state becomes rather complex when states close to another limiting state are considered. Substantially, such a reference emphasizes one particular environment influence, and that may screen some of the underlying system evolutionary characteristics (one example is discussed in the last paragraph of Section 3). Furthermore, in stationary non-equilibrium states the influence of the environment on the system is not fully developed, hence a reference to some intrinsically system quantity is more aligned with that fact. This is emphasized in systems with slow relaxation or with intensive environment dynamics. Regarding that, the intrinsic system state is introduced as the state with the uniform level population function.

In this article the referent state is the system's intrinsic state, unlike the case in which the referent state is one of its limiting states.

The central point of this article is to contribute to the recognition of the intrinsic state. The specific cases are considered for illustration purposes. Because in equilibrium statistical mechanics the approaches based on T and β are formally equivalent, the article largely deals with the case of stationary non-equilibrium.

The first case considered is an ensemble of two level atoms in equilibrium with an electromagnetic field, the state of which is described using β . As the second case, stationary

states of the system having finite energy and finite heat flux are considered. The deviation of the system state and intrinsic system state is measured using a set of Lagrange coefficients. Within that a notion of a generalized absolute temperature (GAT) is introduced. GAT is a measure of the deviation of a system state from the corresponding limiting state. Besides absolute temperature, a quantity which refers to the zero energy state, two additional quantities are used in description: a GAT which refers to the maximal heat flux state, and the Lagrange coefficient γ . The similarities between different temperatures used are described, and their relation to Lagrange coefficients discussed.

The article is organized as follows. In the Section 2, after a preliminary recognition of the parameters, a system of two level atoms without fluxes is considered. Following the proposed centering of thermal properties around β , the standard statistical mechanics expression for average energy is obtained. In the Section 3 the consequences of the heat flux in the system are elaborated. Discussion of the results is given in the Section 4, while main results are summarized in the Section 5.

SYSTEM OF TWO LEVEL ATOMS EXCHANGING ENERGY WITH ELECTROMAGNETIC FIELD

In the information theory approach to statistical physics [2], one maximizes the expression for entropy S as a sum over the available states with energies ε_i , $i = 1, \dots, N$. If f_i is the distribution function, and $A^{(a)}$ relevant constraints, which are assumed expressible using one-particle quantities $A_i^{(a)}$, then for fermions one has

$$S \sim \sum_i [(1 - f_i) \ln(1 - f_i) + f_i \ln f_i], \quad (1)$$

$$A^{(a)} \sim \sum_i A_i^{(a)} f_i, \quad (2)$$

thus obtaining

$$f_i = \left[\sum_a A_i^{(a)} \alpha^{(a)} + 1 \right]^{-1}. \quad (3)$$

In (3), quantities $\alpha^{(a)}$ are Lagrange coefficients, through which the constraints (2) are taken into account. Lagrange coefficients are considered to be auxiliary quantities which are, using (2), related to macroscopic, measurable quantities.

In the case of a constant number of fermions of average energy E , (2) and (3) become

$$E = \sum_i f_i \varepsilon_i, \quad (4)$$

$$f_i = (e^{\beta \varepsilon_i} + 1)^{-1}, \quad (5)$$

respectively. For simplicity, $\hbar = 1$ and $k_B = 1$ is taken throughout the article. Alternatively to the information theory approach, energy E and other macroscopic quantities are derivable from the partition function.

In this section another way of deriving macroscopic quantities of a system is described. It is applied to a collection of mutually independent two level atoms, with energy levels ε_1 and ε_2 and level populations n_1 and n_2 , respectively. In the initial state, the system is in equilibrium with the environment, assumed to be a quasi-continuous bosonic heat bath and represented as a collection of electromagnetic (EM) modes, i.e., photons. The heat bath temperature is taken to be high enough so that the average number of photons is constant in the region of frequencies of the order of $|\varepsilon_2 - \varepsilon_1|$. In that case the equilibrium spectral density of EM field, given by the Planck formula,

$$u(\omega) = \frac{\omega^3}{\pi^2 c^3} \frac{1}{e^{\beta\omega} - 1}, \quad (6)$$

is well approximated by the classical, Rayleigh-Jeans expression

$$u(\omega) \approx \frac{\omega^2}{\pi^2 c^3} \frac{1}{\beta}. \quad (7)$$

In the initial state, therefore, the system has approximately equally populated levels, $n_1 = n_2$, and its average energy per atom, E_0 , satisfies

$$(n_1 + n_2)E_0 = n_1\varepsilon_1 + n_2\varepsilon_2 \Rightarrow E_0 = \frac{\varepsilon_1 + \varepsilon_2}{2}. \quad (8)$$

Let the heat bath subsequently cool infinitesimally. In the new state of equilibrium between the system and the EM field, the absolute temperature is slightly less than infinity, its Lagrange coefficient $d\beta$ is infinitesimal and positive. Furthermore, level populations satisfy Einstein's relation

$$n_1 u(|\varepsilon_2 - \varepsilon_1|) B = n_2 [u(|\varepsilon_2 - \varepsilon_1|) B + A], \quad (9)$$

with $A/B = \omega^3/(\pi^2 c^3)$. Combination of (7) and (9) gives

$$\frac{n_1}{n_2} = 1 + (\varepsilon_2 - \varepsilon_1) d\beta. \quad (10)$$

Because of the infinitesimalities encountered, the following substitution is applicable

$$n_i = C_i + D_i d\beta, \quad (11)$$

in which C_i and D_i are constants independent of EM field characteristics. Relations (10) and (11) are combined into

$$1 + (\varepsilon_2 - \varepsilon_1) d\beta = \frac{C_1}{C_2} + \left(\frac{D_2}{D_1} - \frac{C_1 D_2}{C_2^2} \right) d\beta, \quad (12)$$

with factors proportional to $(d\beta)^2$ neglected. It is seen that $C_1 = C_2 = 1/2$, where the equalities follow from (12) and (11), respectively. From $n_1 + n_2 = 1$ the $D_1 = -D_2$ follows, and from (12) one has

$$D_i = \frac{\varepsilon_j - \varepsilon_i}{4}, \quad i \neq j. \quad (13)$$

Expression (13) is equivalently written as $D_i = \varepsilon_j - \varepsilon_i/4 - \varepsilon_i/2 = (E_0 - \varepsilon_i)/2$. The last form is also valid in the case of three- or more-level atoms. Finally, (11) is written as

$$n_i(d\beta) = [1 - (\varepsilon_i - E_0) d\beta] n_i(0). \quad (14)$$

A special form of expression (14) will be discussed in detail in Section 4.

The infinitesimal change $d\beta$ can be considered as β/M for some finite β and a large enough number M . Then level populations after M applications of infinitesimal cooling, i.e., after cooling of environment from $\beta = 0$ to $\beta > 0$, satisfy

$$n_i = [1 - (\varepsilon_i - E_0) d\beta] \cdot \dots \cdot [1 - (\varepsilon_i - E_0) d\beta] \cdot \frac{1}{2} = \frac{1}{2} \left[1 - \frac{(\varepsilon_i - E_0) d\beta}{M} \right]^M \xrightarrow{M \rightarrow \infty} \frac{e^{-(\varepsilon_i - E_0)\beta}}{2}, \quad (15)$$

with $n_i(0) = 1/2$ used. While $\{n_i(0)\}$ is properly normalized, level population in (15) are not, which will be discussed in more detail later. Using (15), the average energy becomes

$$E = \frac{e^{-\varepsilon_1\beta} \varepsilon_1 + e^{-\varepsilon_2\beta} \varepsilon_2}{e^{-\varepsilon_1\beta} + e^{-\varepsilon_2\beta}}, \quad (16)$$

Which is the well-known statistical physics expression. In the derivation of (16), the cooling of the environment was considered, i.e., $\beta > 0$, because of what the equation (6) was applicable. Formally, the expression (16) is also obtainable for $\beta < 0$, if one does not invoke

(6) and (7), but starts from some other expression, e.g. (10). From the foregoing expressions it follows that the change in sign of β brings about inversion of the level population function.

In the present derivation of (16), the notion of partition function was not exploited. Moreover, the distribution function was not needed in order to obtain (16). Instead, the consequences of the change of environment were analyzed. Formally, the simplified, classical formula (7) is recognized as an elementary transformation of the system which, after a sequence of repetitions, brings about (16). This contributes to the recognition of the importance of coefficient β . In particular, it is interpreted here as a measure of the influence of the environment on the system. Let us elaborate that connection in more detail. The coupling to environment, linked before to energy transfer, generally is asymmetric, which induces asymmetry in the level population (the effects of particle statistics and suppressions caused by symmetry are not considered here). A system of mutually non-interacting particles, which is isolated from environment, has neither stimulated nor spontaneous channels for energy transfer. In case of a system coupled to the environment in a minimal energy state, the allowed channel for particle transfers is a spontaneous emission. In the case of a system coupled to the environment in a non-minimal energy state, i.e., the colored environment, the allowed channels additionally include stimulated processes. The stimulated processes preserve the symmetry of the level population function. Similarly, the lower the EM field intensity, the smaller the branch of stimulated processes, thus bringing about the prevalence of spontaneous emission, as well as the asymmetry in level population function thereby induced. In the case of $\beta < 0$ the asymmetry in energy transfer is realized through the diminishing of number of photons radiated from the system to environment. That is possible as suppression of spontaneous emission. The degree of asymmetry in the particle transfer is taken as the measure of environment influence. Then the influence is stronger for larger β . The influence's limit is the diverging β state, or the $T = 0$ state. The interpretation presented belongs to the equilibrium state description, in which β and T are formally equivalent quantities. However, one specific characteristic of β -centered interpretation is seen – the larger the β , the larger the environment influence.

Some of the expressions used in obtaining (15) and (16) are related to the high-temperature approximation of the EM field spectral density function (7). However, this expression was merely an auxiliary quantity, which served in formulation of the first change. For repetitive changes, the expression (15) is sufficient. The derivation before (15) was needed in order to show that the standard, equilibrium statistical mechanics expression for system quantities are obtainable following the assumed gradual intensification of the environment influence.

Until now, the only parameter representing the EM field spectral density has been β . Because of the equilibrium between the system and its environment, the same is valid for the system. Hence, the absolute temperature introduced through the relation

$$T^{-1} = \beta, \tag{17}$$

represents the value of the system's absolute temperature. But, despite the simple function relation between T and β , they differ substantially. The coefficient β is zero when there is no induced asymmetry in the level population, and its value gradually changes as the environment induces larger and larger changes in level population. Therefore, β represents a deviation of the system state from the state of uniform level population, termed here the intrinsic system state. On the contrary, absolute temperature is zero for maximally asymmetric level populations, whether approached from the side of positive or negative values. Then the influence of the environment is maximal. The value of the absolute temperature is maximal and equal to infinity for a system with a spectrum bounded from above, when the environment influence is minimal, i.e., when the level population is symmetric. Parameter β measures the deviation of an equilibrium system state from the

intrinsic system state. In the same line of thought the absolute temperature measures the deviation of the system state from the particular state of maximal level population asymmetry, i.e., from the state in which only the lowest energy level is populated. The symmetry (maximal asymmetry) of the level population is related to the maximal (minimal) entropy of the state. Hence, β measures deviation of a system state from the state of maximal entropy.

In the case analyzed, there are two limiting states – states with the lowest and largest possible energy. Regarding that, the absolute temperature measures deviation of a state from the one particular limiting state, the lower energy level. The negative absolute temperature measures deviation of a state from the other limiting state, which is here the other level, i.e., the higher energy level. In the sense, the absolute temperature and negative absolute temperature are two completely independent notions. Because of the simplicity of a canonical ensemble of two level atoms, these two temperatures are related through only a sign change. Generally, it is therefore opportune to think about two different absolute temperatures; one related to a deviation from the minimal energy state, and other related to a deviation from the maximal energy state.

It is a consequence of the physical space that the absolute temperature of the average EM field is relatively small, so that lowering the temperature, i.e., making β larger, is the asymptotic change. In addition, for a large enough class of systems, the environment EM field temperature is not high enough to bring about a level symmetry, even if it is the only energy exchange channel.

SYSTEM OF TWO LEVEL ATOMS WITH FINITE HEAT FLUX AND ENERGY CONTENT

In this section a special configuration of two level atoms is considered. Geometrically, the system resembles a well-analyzed system of harmonic oscillators [2]. In the system, N equidistant, two level atoms form a ring. The interaction between the atoms is a direct energy exchange between the nearest neighbors, with the interaction integral J . Dispersion relation of normal modes, excitons, is

$$\varepsilon_n = \varepsilon_0 - 2J \cos \frac{n\pi}{N}, \quad (18)$$

with $\varepsilon_0 = \varepsilon_2 - \varepsilon_1$, and $n = -N, \dots, -1, 0, 1, \dots, N-1$. Along with (18), the following auxiliary quantity is introduced,

$$q_n = \varepsilon_n \frac{\varepsilon_{n+1} - \varepsilon_n}{(\pi/N)} = 2J \left(\varepsilon_0 - 2J \cos \frac{n\pi}{N} \right) \sin \frac{n\pi}{N}, \quad (19)$$

with the last equation valid for $N \gg 1$. Thermodynamically, the stationary states of the system are analyzed, which are characterized by the energy content and heat flux. In the way one speaks about the “superconductor of thermal energy” [7], as the heat flux lasts indefinitely. The average energy per atom, E , and the heat flux divided by number of atoms, Q , satisfy

$$E = \sum_n \varepsilon_n f_n, \quad (20)$$

$$Q = \sum_n q_n f_n, \quad (21)$$

with the following expression for the exciton distribution function,

$$f_n = (e^{\beta\varepsilon_n + \gamma q_n} + 1)^{-1}, \quad (22)$$

in which β and γ are Lagrange coefficients, real scalars. Expressions (18-22) are discretized versions of expressions found in the literature [6]. Dependence of system energy E , determined using (18), (20) and (22), on Lagrange coefficients is shown in Figure 1 for two

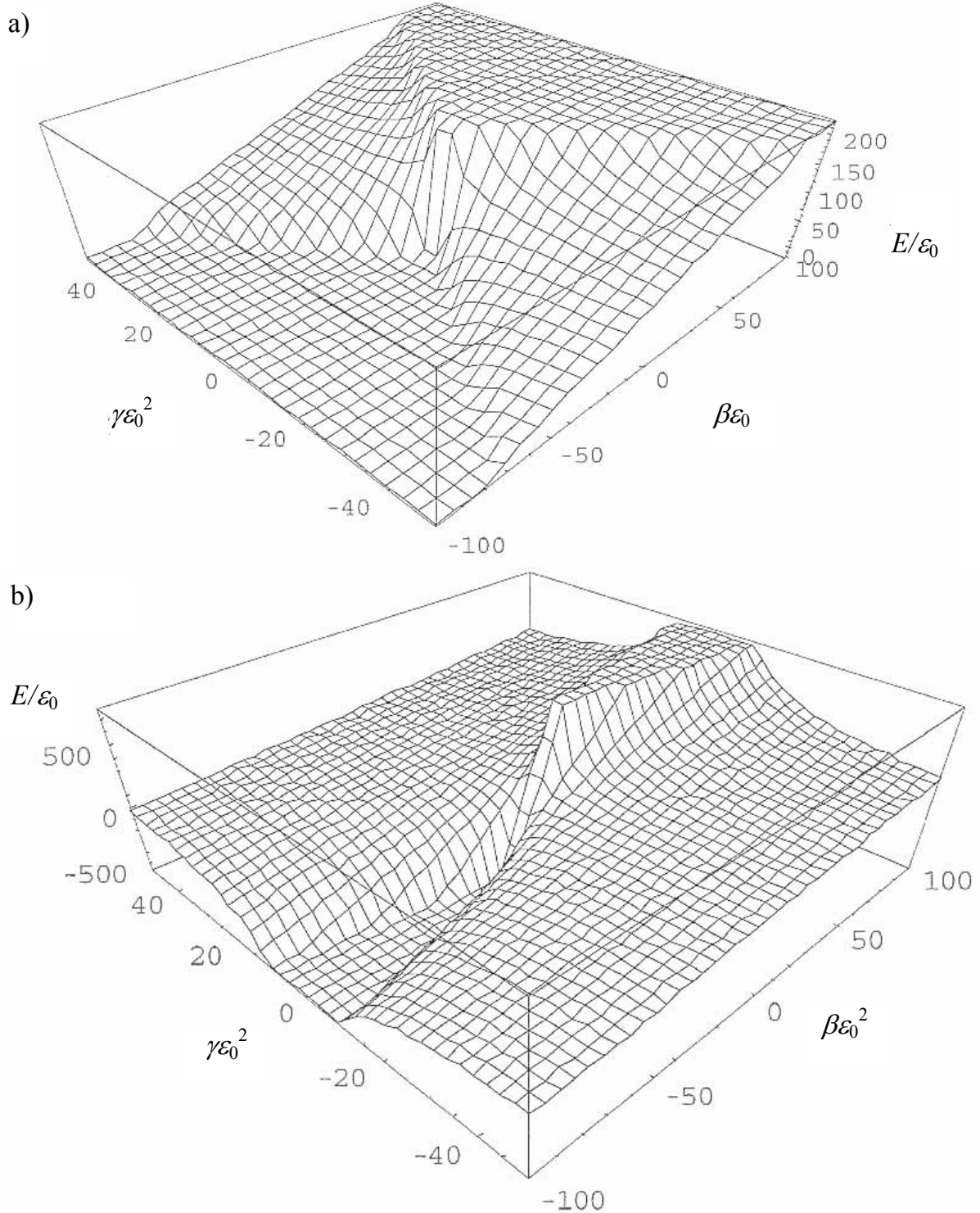


Figure 1. Energy E as a non-normalised function of β and γ for $N = 100$. Parameter $\alpha = 2J/\epsilon_0$ equals a) 1, b) 10.

cases of coupling strength $\alpha = 2J/\epsilon_0$. In the case of negligible coupling strength, energy does not depend on γ . Conversely, the larger the α , the more pronounced the dependence of energy on γ . In the following discussion the value $\alpha = 1$ is taken. In the graph relating Q and E (Fig. 2), curves of constant β and γ form two families of mutually intersecting curves. Graphs relevant for the inverse case are shown in Figure 3. In these graphs, the Lagrange coefficients are related, with explicitly shown curves of constant E and Q . While in the classical region of $\beta \rightarrow \infty$ the

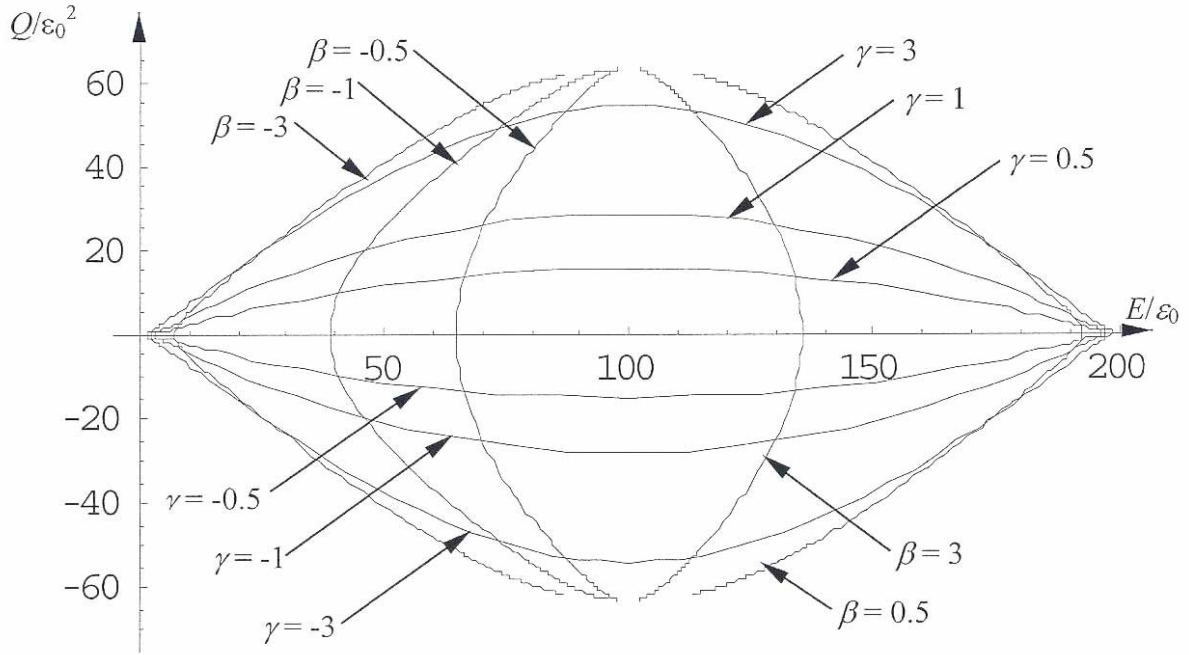


Figure 2. Curves of constant β and γ on the graph relating non-normalised heat flux Q and system energy E for $N = 100$. Units on axis are arbitrary. Curves for $\beta = 0$ and $\gamma = 0$ are parallel to vertical and horizontal axis, respectively. Convergence of curves to points of extremal Q is not shown because of numerical reasons.

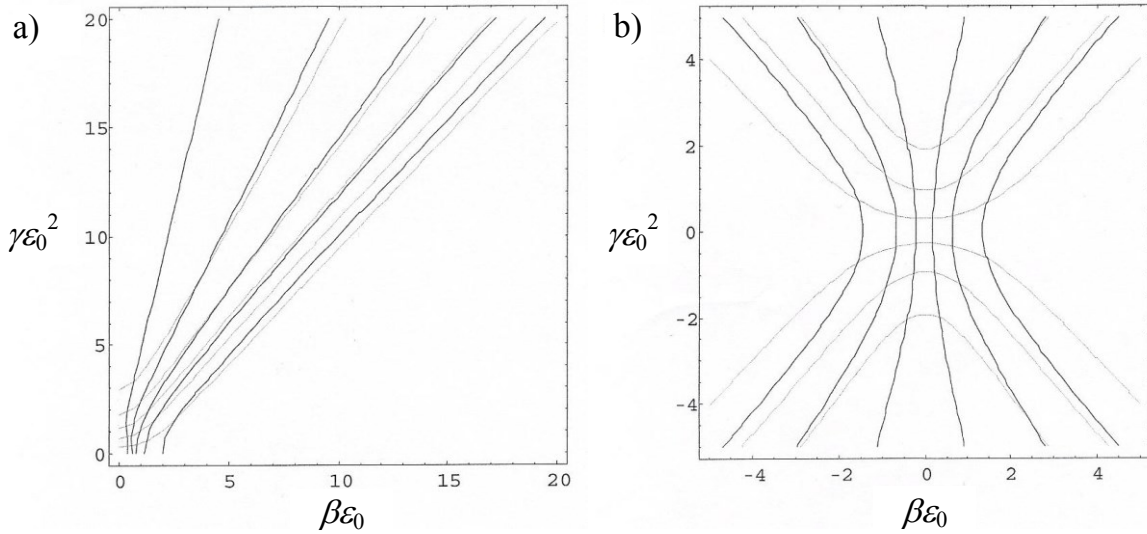


Figure 3. Curves of constant E (solid) and Q (dashed) on the graph relating Lagrange coefficients β and γ , a) global character and b) neighbourhood of the intrinsic state $\beta = \gamma = 0$.

curves of constant β and constant γ tend to be parallel, in the neighborhood of the intrinsic state they become perpendicular one to another. Therefore, in the classical region, a change of, e.g., system energy E , is accompanied by the change in the system heat flux Q . On the contrary, near the intrinsic state the change in E is considerably larger than the change in Q , thus it is possible to change E with almost negligibly changing Q .

From Eq. (22) some special cases can be inferred. First, if γ is negligible compared to β , one has periodic analogy of collection of two level atoms considered in the previous section. There are then two limiting states, with co-ordinates

$$(\varepsilon_0 \pm 2J, 0), \tag{23}$$

in the (E, Q) plane. In (23), the minus (plus) sign refers to states with minimal (maximal) energy. In the case when the system state is close enough to one of limiting states, the distribution function (22) becomes approximately

$$f_n \approx e^{-\beta \varepsilon_n}. \quad (24)$$

In the second special case, β is negligible to γ , and furthermore the system in the neighborhood of one of the limiting states is considered. Then (22) simplifies to

$$f_n \approx e^{-\gamma q_n}, \quad (25)$$

and it is clear that relevant contribution of the n -th state is q_n and not the energy ε_n . Expression (25) is interpretable as a classical distribution function of a system which has (19) as the dispersion relation. One could further introduce the equivalent absolute temperatures, $T_{\text{eq}\pm}$, measuring deviations of system states from the states with extremal heat flux values,

$$T_{\text{eq}\pm} = \pm \frac{1}{\gamma}. \quad (26)$$

From (19) it can be determined that the states with maximal contribution to the heat flux Q , having indices n_{\pm} , satisfy

$$\cos \frac{n_{\pm} \pi}{N} = \frac{1 \pm \sqrt{1 + 8\alpha^2}}{\alpha}, \quad (27)$$

with valid solution(s) satisfying $(1 - 4\alpha) \cdot \sin(n\pi/N) > 0$. Generally, this gives the two values of (19) for the limiting states

$$q_{\pm}. \quad (28)$$

Comparison of (24) and (25) on one hand, and (23) and (28) on the other hand implies that the two sets of limiting states are relatable through exchange

$$\left\{ \begin{array}{c} \beta \\ \varepsilon_0 \pm 2J \end{array} \right\} \leftrightarrow \left\{ \begin{array}{c} \gamma \\ q_{\pm} \end{array} \right\}. \quad (29)$$

Projected onto the whole system, the state without heat flux and with relatively low energy is similar to the state with maximal heat flux, because in both cases a few particles are not in states characterized by (23) or (28). For thermodynamics of states close to the limiting states, one has to take into consideration that there is a parabolic dispersion relation when γ is negligible to β , while (19) depends linearly on the index n in the case of a relatively small β and relatively large γ .

In approaching limiting states, quantities β and γ diverge. In the case of $\beta \rightarrow +\infty$ and $\gamma = 0$, the usual description invokes the limit $\beta = +\infty$, i.e., the zero energy state, as a referent state in terms of the absolute temperature, $T = 1/\beta$. In the case of $\beta \rightarrow -\infty$ and $\gamma = 0$, the limit $\beta \rightarrow -\infty$, the state of maximal energy, if expressed in terms of quantity $-T$, serves as the referent state. Cases with $\beta = 0$ and $\gamma \rightarrow \pm\infty$ have not been thoroughly examined in the literature. Such states are encountered, e.g., during intensive particle motion. Then $\gamma \rightarrow \pm\infty$ means large enough drift motion in which diffusive motion is negligible. States with diverging β and states with diverging γ , share the relatively large asymmetry of the level population function.

The plane spanned by Lagrange coefficients β and γ , contains all possible stationary states of the described system (Fig. 4). Along with the axis of β and γ , the axis for the absolute temperature and for the negative absolute temperature are shown in order to emphasize their relationship with β . States far from axis β are not easily described using the non-equilibrium absolute temperature θ as a GAT, as is seen from the corresponding distribution function (25), which is valid approximately in that case. The temperature related part is negligible then, and the reference to $\beta \rightarrow \infty$ state is not solid. From the foregoing expressions it follows that the

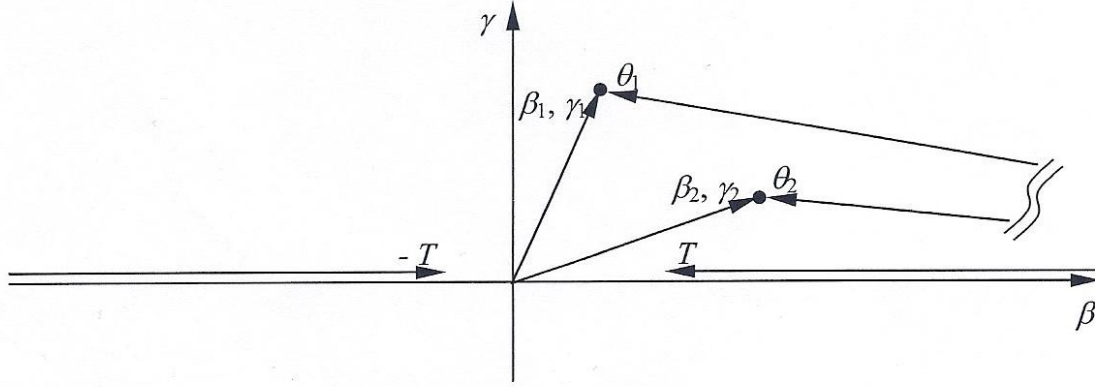


Figure 4. Comparison of different systems states as performed in the absolute temperature T , negative absolute temperature $-T$ and the Lagrange coefficient centred approach. States are denoted using non-equilibrium absolute temperature θ and a pair of Lagrange coefficients α and β .

relevant quantities are the β and γ , which are on one hand connected to T , and on the other hand to different GATs.

DISCUSSION

Expressions (14) and (15) resemble the expressions connected with generators of infinitesimal changes [9]. In particular, when there is time-homogeneity, Hamiltonian is the generator of infinitesimal translations in time. If $|\psi(t)\rangle$ is some time-dependent state vector in time t , then its value in infinitesimally later time $t + dt$ is

$$|\psi(t + dt)\rangle = (1 - iHdt)|\psi(t)\rangle \quad (30)$$

While its value in Δt later moment is

$$|\psi(t + \Delta t)\rangle = e^{iH\Delta t}|\psi(t)\rangle \quad (31)$$

The expressions (14) and (15) are obtained within the classical approach to statistical physics, in such a way that c-numbers figure in them. In the quantum mechanics, from which (30) and (31) are taken, operators are state vectors figure. A manifest difference between two groups of expressions in an imaginary unit, which is missing in previous expressions. All that is aligned with the existing recognition that β may be considered as imaginary time. In that sense, (14) is the averaged value of infinitesimal imaginary time translation,

$$\langle i|e^{-H\alpha\beta}\rho(0)|i\rangle = \langle i|(1 - Hd\beta)\rho(0)|i\rangle = \frac{1 - \varepsilon_i d\beta}{2}, \quad (32)$$

with the initial density matrix of the canonical ensemble $\rho(0) = \mathbb{E}/2$, where \mathbb{E} is 2×2 identity matrix. In (32) it was assumed that $|i\rangle \in \{|1\rangle, |2\rangle\}$ are eigenstates of the system Hamiltonian H . Overall, the repetition of imaginary time translations brings about (15). However, the similarity between (30) and (14) is not fully manifested in the derivation presented here, as (30) is a unitary transformation for hermitian H , while (14) is not. In addition, in (32) the form of time translation valid for functions is used, which is not appropriate for a density matrix. In other words, additional care should be taken in derivation of (14) if one wants to interpret it as an imaginary time translation (32). Still, one more non-manifest similarity between the real time and imaginary time translations should be mentioned: admissible values of time parameter cover the set of real numbers.

For each limiting state one can introduce a generalized absolute temperature (GAT). GAT is the quantity measuring the deviation of a system's state from some limiting state. In that way, when the scale spanned by the GAT is used, the corresponding limiting state is the referent state. The GAT is a generalization of the absolute temperature T . The absolute temperature is one realization of the GAT introduced for only one limiting state. The GAT has different realizations, each referring to different among the possible limiting states. Further examples of GATs mentioned in this article are listed in Table 1. Each GAT is introduced for a particular limiting state. In that way, as seen from Table 1, generally there are several GATs applicable for diverging $(\beta^2 + \gamma^2)^{1/2}$. In measuring GAT one encounters the similar problem as in measuring nonequilibrium temperature θ – when using a thermometer the absolute temperature is measured. Hence, there is the indirect way of measuring GATs, i.e., through determination of the exciton population function f_n , fitting it to the form (22) and using definitions in Table 1 to determine a particular GAT.

Depending on the dynamics and initial conditions, a system will evolve through regions close to different limiting states, hence the different GATs will be suitable for the description of such dynamics. While in the simpler cases this does not cause problems, in more complex cases, in which there are many limiting states as the described ones, this may bring about tedious, non-tractable calculations. In the later case it is opportune to refer to the intrinsic system state in description of system dynamics. Such a determination of a referent state of a system generally changes somewhat a written form of the relevant expressions. In Figure 4 the coordinate system defined through β and γ is shown. Two states shown have the appropriate values of Lagrange coefficients, and the values of non-equilibrium absolute temperature. It is seen that the non-equilibrium absolute temperature measures combined effects of β and γ , i.e., energy and heat flux, on the system state. The non-equilibrium absolute temperature is useful for system states close to the axis abscissa. The β and γ are useful in describing a general system state. In addition, a deviation of a system state from the intrinsic, i.e., $\beta = \gamma = 0$ state points to strength of an environment influence: states closer to the origin are less influenced by environment. In case of the usual environment with $T \approx 0$, a system in states with higher β is more aligned with the environment. A system in a state with strong fluxes, i.e., rather large value of γ , is subjected to an intense environment influence, hence is more similar to a system in low temperature states in that the variations in the level population are less pronounced. From (24) and (25) it is clear that a different approach is needed for the general description of system state instead of quantities related to a single limiting state.

Finally, from (10), (19) and (22) it is seen that the following substitution is possible

$$\frac{g_n}{\theta} = \beta \varepsilon_n + \gamma q_n, \quad (33)$$

Table 1. Temperatures encountered in the description of system's states.

Temperature	Absolute temperature	Non-equilibrium absolute temperature	Negative absolute temperature	Equivalent temperatures	
				$1/\gamma$	$-1/\gamma$
Notation	T	θ	$-T$	$T_{\text{eq+}}$	$T_{\text{eq-}}$
Nearest limiting state	$E = 0,$ $Q = 0$	$E = 0,$ $Q = 0$	$\max E,$ $Q = 0$	$\max Q$	$\min Q$
Region of suitability	$\beta \rightarrow \infty,$ $\gamma = 0$	$\beta \rightarrow \infty,$ $\gamma \approx 0$	$\beta \rightarrow -\infty,$ $\gamma = 0$	$\beta \rightarrow 0,$ $\gamma \rightarrow \infty$	$\beta \rightarrow 0,$ $\gamma \rightarrow -\infty$

for a small enough neighborhood of some limiting state, in order for the dependence of g_n on changes of β and γ to be negligible. Quantity g_n is a generalised dispersion relation which combines effects of the dispersion relation and the heat flux.

SUMMARY AND CONCLUSIONS

In this article, the Lagrange coefficient β is proposed as a referent, intensive thermal quantity, for which it may be argued that it is particularly useful in broadening the notion of temperature-like quantity out of equilibrium thermodynamics. It is argued that there is a relation between β and environment influence. The absolute temperature T is recognized as a particular realization of the GAT, which refers to the deviation of the system state from a minimal energy state. The consequences of the propulsion are discussed in the case of the ensemble of two level atoms interacting with an electromagnetic field. In cases where heat flux is considered, similar results are obtained.

The results serve as a starting point for the alternative treatment of stationary non-equilibrium states in which system states are described using β and other Lagrange coefficients instead of trying to use a temperature-related quantity. In such a treatment the emphasis of a particular limiting state is overcome, hence the asymmetry of a treatment of flux- and temperature-related variables does not exist. Furthermore, the fact that a system, in a stationary state, is not coupled to the environment in an intense enough way to establish solid relations to some environment referent point is emphasized in the formalism.

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O DEFINIRANJU REFERENTNIH TOČAKA TEMPERATURNE SKALE

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SAŽETAK

Apsolutna temperatura T raspoznatog je fizikalnog značenja u ravnotežnoj termodinamici. Skala razapeta Lagrangeovim koeficijentom β uobičajeno je pomoćna skala. U ovom radu, skala razapeta koeficijentom β je primjerena intenzivna termalna veličina za opis ravnotežnog i, primjereno poopćena, stacionarnog neravnotežnog stanja. Koeficijent β mjeri relativno odstupanje stanja sustava od stanja opisanog uniformnom distribucijskom funkcijom. Razlog odstupanja je vezanje za okolinu, koje je ostavreno izmjenom energije i koje iščezava u stanju $\beta = 0$. Kao primjer razmotren je kanonski ansambl atomā s dvije razine vezan za elektromagnetski kvazikontinuum. Predložena i uobičajena interpretacija koeficijenta β primijenjene su na stacionarna stanja tog sustava u kom slučaju se uvodi pojam poopćene apsolutne temperature. Poopćena apsolutna temperatura mjera je odstupanja stanja sustava od stanja s beskonačno intenzivnim vanjskim utjecajem.

KLJUČNE RIJEČI

neravnotežna termodinamika, ravnoteža, Lagrangeov koeficijent