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Article

Thermodynamics of Fluid Elements in the Context of Turbulent Isothermal Self-Gravitating Molecular Clouds

Sava Donkov [1,*], Ivan Zh. Stefanov [2] and Valentin Kopchev [3]

1 Institute of Astronomy and NAO, Bulgarian Academy of Sciences, 72 Tzarigradsko Chausee Blvd., 1784 Sofia, Bulgaria
2 Department of Applied Physics, Faculty of Applied Mathematics, Technical University-Sofia, 8 Kliment Ohridski Blvd., Sofia 1000, Bulgaria; izhivkov@tu-sofia.bg
3 Department of Applied Physics, Faculty of Applied Mathematics, Technical University-Sofia, 8 Kliment Ohridski Blvd., Sofia 1000, Bulgaria; kopchev@tu-sofia.bg
* Correspondence: sddonkov@astro.bas.bg

Abstract: In the present work we suggest a new approach for studying the equilibrium states of an hydrodynamic isothermal turbulent self-gravitating system, as statistical model for a molecular cloud. The main hypothesis is that the local turbulent motion of fluid elements is purely chaotic and can be regarded as a perfect gas. Then the turbulent kinetic energy, per one fluid element, can be substituted for the temperature of chaotic motion of the fluid elements. Using this we write down effective formulae for internal and total energy and the first principal of thermodynamics. Then we obtain expressions for entropy, free energy, and Gibbs potential. Searching for equilibrium states we explore two possible systems: the canonical ensemble and the grand canonical ensemble. Studying the former we conclude that there is no extremum for the free energy. In the latter system we obtain a minimum for the Gibbs potential when macro-temperature and pressure of the cloud are equal to those of the surrounding medium. This minimum corresponds to a possible stable local equilibrium state of our system.

Keywords: molecular clouds; fluids; turbulence; self-gravity; thermodynamics

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1. Introduction

This paper is dedicated on the idea to consider the local turbulent motion of fluid elements, in the case of purely saturated isothermal turbulence which demonstrates an inertial range of scales, as a perfect gas and make use of the thermodynamic laws to obtain conclusions for the dynamical state of a turbulent self-gravitating fluid. Molecular clouds (MCs) are entities in the cold neutral interstellar medium that perfectly match this aim. They are (supersonically) turbulent, self-gravitating and isothermal [1] fluids consisting mostly by molecular hydrogen [2–4]. Their turbulence is driven at scales several times larger than the cloud size and, also, cloud's scales and subscales, for several orders of magnitude, belong to an inertial range [2–4], which is well defined in both cases – for subsonic isothermal turbulence [5,6], as well for supersonic isothermal turbulence [7–9]. Magnetic fields and new-born stars also play a significant role in their physics, but we neglect them in our considerations in order to simplify the first step to a fiducial model.

It is easy for one to see the advantage of use of the thermodynamic laws for studying the dynamical states of a MC, regarded as an ideal gas of fluid elements. The idea to apply thermodynamic models for studying dynamical stability of physical systems consisting of macro-particles (for example: stars, galaxies and etc.) comes from the works of [10–14] and more recently from the works by [15–20]. Although this approach is fairly developed, there are many uncertainties regarding one to one correspondence between thermodynamic equilibrium and dynamical stability, also, the thermodynamic ensembles of self-gravitating systems are not equivalent (for discussion on these topics see [14,15] and [21], and references therein). In spite of the latter we find that the simplicity of the thermodynamic

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is a very attractive alternative for studying the hydrodynamical turbulent systems, of course, with a caution. In this work we focus on searching of possible equilibrium states (stable and/or unstable) of the system. For example, the problem with stability of a molecular cloud against collapse or dispersing is a key issue concerning star-formation [2–4,22]. This issue can be explored observationally, through numerical experiments, or analytically. Here we study it analytically by using thermodynamic potentials like energy, entropy, free energy, and Gibbs potential as tools to make conclusions about stability of a cloud.

In the base of our model we adopt the idea that the turbulent kinetic energy can be substituted for the temperature (hereafter macro-temperature or temperature of the macro-gas). This idea was firstly suggested by [23] in order to investigate the instability and fragmentation of star-forming clouds by use of turbulent-entropic instability as a thermodynamic tool. In the present work starting from the above assumption we write down the internal and total energy, per one fluid element, of a turbulent self-gravitating and isothermal MC. We also presume that there exists an inertial range for the turbulence and its averaged velocity dispersion obeys a scaling law in this range. The latter determines, also, a scaling relation for the macro-temperature. The natural variables for the thermodynamic system in regard are macro-temperature and number density. That's why starting from the first principle of thermodynamics we succeeded to obtain the explicit equation for entropy at an arbitrary scale in the inertial range (see Section 4.1).

In these variables (macro-temperature and number density) the natural thermodynamic potential is free energy and hence we deal with a canonical ensemble. We obtain the free energy in an explicit form in equation (11). Then we seek for extrema of the latter potential and conclude that it may have a minimum when macro-temperature of the cloud is equal to the macro-temperature of the surrounding medium, playing a role of a large "thermal" reservoir. Obtaining the derivative in regard to number density we see that the free energy is a monotonically increasing function and hence it does not get extrema. All possible states of the canonical ensemble are unstable, because if one perturb the number density then the cloud will disperse or collapse, depending on its Jeans' mass.

Then extending our considerations we study the case of grand canonical ensemble, which corresponds to Gibbs potential (see equation 13) in variables: macro-temperature and pressure. Seeking for extrema we conclude that Gibbs potential has a local minimum when the macro-temperature and pressure of the macro-gas in our cloud are equal to the corresponding quantities for the surrounding medium. In this case the cloud may resides in a stable dynamical equilibrium.

The paper structure is as follows: in the next Section 2 we make a short retrospection (in regard to our point of view) of the main works in the field, and try to find the place of our study; in Section 3 we present the model and give the equations for internal and total energy, and also make the assumptions for our mean field consideration; in Section 4 we write down the first principle for the model and obtain the explicit form of the entropy (Section 4.1), then we get the formulae for the free energy (Section 4.2) and the Gibbs potential (Section 4.3); after that, in Section 4.4, we consider the cloud stability in two cases: canonical ensemble (Section 4.4.1), and grand canonical ensemble (Section 4.4.2); in Section 5 we comment on the basis of the model and main results (Section 5.1), on the statistical interpretation of entropy, free energy, and Gibbs potential (Section 5.2), and on the possible caveats (5.3); finally, in Section 6, we give our conclusions.

2. The General Frame

The thermodynamics of self-gravitating systems started with Antonov's [10] discovery that, when a self-gravitating system, with a mass M, is confined within a box of radius R, no maximum entropy state can exist below a certain critical energy $E = -0.335GM^2/R$. Hence the system, regarded as a microcanonical ensemble, does not have an equilibrium state. This very interesting result was further developed by Lynden-Bell and Wood [12], who guessed that for $E < -0.335GM^2/R$ the system would collapse and overheat. This is called "gravo-thermal catastrophe" or "Antonov's instability". In [12] they have related this phenomenon to the property of self-gravitating systems to have negative specific

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heats. The gravo-thermal catastrophe picture is expected to play a crucial role in the evolution of globular clusters. It is found that the collapse proceeds self-similarly and that the central density becomes infinite in a finite time. This instability has been known as "core collapse" and many globular clusters have probably endured core collapse [24]. In the case of dense clusters of compact stars (neutron stars or stellar mass black holes), the gravo-thermal catastrophe should probably lead to the formation of supermassive black holes of the size to explain quasars and AGN.

Later Katz [11] has investigated, on a theoretical point of view, the stability of isothermal spheres with a very powerful method extending Poincare's theory of linear series of equilibrium. He found that instability sets at the point of minimum energy. Padmanabhan [13] has reconsidered this stability analysis. He has studied the sign of the second variations of entropy and reduced the problem of stability to an eigenvalue equation. His considerations leads to the same stability limit as Katz, but in addition Padmanabhan's method gives the form of perturbation that induces instability in the critical point. This perturbation presents a "core-halo" structure. Padmanabhan has performed his analysis in microcanonical ensemble in which the energy and mass are fixed. The microcanonical ensemble is perhaps the most relevant for studying stellar systems like elliptical galaxies or globular clusters [24]. In addition, from the statistical mechanics point of view, only the microcanonical ensemble is rigorously justified for non extensive systems, as discussed in the review of Padmanabhan [14]. However, it is possible to consider formally a canonical or grand canonical ensemble, where the temperature is fixed instead of energy. Here we should mention the works of de Vega, Sanchez and Combes [18,19], where these authors have developed a theory of the cold neutral interstellar medium, and especially of the MCs, using the formalism of the renormalization field theory group. They have considered the medium (MC) as a gas, composed by micro-particles (atoms or molecules), which are in thermal equilibrium. These particles interacting with each other through Newtonian gravity. The turbulence is not accounted. They have shown that this non-relativistic self-gravitating gas in thermal equilibrium with variable number of particles (they have regarded the system as a grand canonical ensemble) is exactly equivalent to a field theory of a single scalar field with exponential self-interaction. They have analysed this field theory perturbatively and non-perturbatively through the renormalization group approach. As a main result they have succeeded to get the scaling relations for mass of the cloud: $M(R) \sim R^d$, and for velocity dispersion: $\Delta v(R) \sim R^q$, where R is the characteristic size of the system. Moreover, assuming virialization of the gas, they obtained the relation for the scaling exponents: $q = (d-1)/2$. Mean field theory in their approach yields for the scaling exponents $d = 2$ and $q = 1/2$, accordingly. So they theoretically derived the fractal structure of MCs and fiducial values for scaling exponents, assuming the self-gravitating medium to be in thermal equilibrium and steady state, without turbulence. Also, in the paper by de Vega and Sanchez [20], the authors have built the statistical mechanics of non-relativistic self-gravitating gas in thermal equilibrium (again without accounting for the turbulence), using Monte Carlo simulations, analytic mean field methods and low density expansions. The system is shown to possess an infinite volume limit, both in the canonical and in the microcanonical ensemble when $N, V \to \infty$, keeping $N/V^{1/3}$ fixed. They have computed the equation of state, the entropy, the free energy, the chemical potential, the specific heats, the compressibility, the speed of sound and have analysed their properties, signs and singularities. They have shown, as well, that the system suggests a fractal structure with fractal dimension $1 \lesssim d \leqslant 3$, with d slowly decreasing with increasing density.

The canonical ensemble has been addressed theoretically by Chavanis [15] who found an analytical solution for the marginally stable perturbations using the method developed by Padmanabhan [13]. The constant $T, P-$ case, that is the grand canonical ensemble, has been addressed previously with synthetic arguments by Bonnor [25] and Ebert [26], and also by Yabushita [27] who studied the stability of the system numerically, by Lombardi and Bertin [28] who extended the analysis by Bonnor [25] to the non-spherically symmetric case, and by Chavanis [16] who gave an analytical solution for the case of marginally stable perturbations using the same method as he had used for the canonical ensemble.

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It is well known, for self-gravitating systems, that the thermodynamic ensembles do not coincide in the whole range of parameters [14]. Using toy-models Padmanabhan [14] has demonstrated that the region of negative specific heats possible in the microcanonical ensemble is replaced by a phase transition in the canonical ensemble. This phase transition separates a dilute "gaseous" phase from a dense "collapsed" phase. Since these toy models are not very realistic, the self-gravitating gas was also studied in a mean field approximation. In this consideration, an isothermal sphere is stable if and only if it is a local maximum/minimum of an appropriate thermodynamic potential (the entropy in the microcanonical ensemble and the free energy in the canonical ensemble). As expected from physical grounds, phase transition occurs when the gaseous sphere stops to be a local maximum/minimum of this potential and becomes a saddle point.

Other problems arise, when one uses the equation of Boltzmann entropy to calculate the critical points and eventually equilibrium states and saddle points of a self-gravitating thermodynamic system. For example this is the approach in works of Antonov [10], Lynden-Bell and Wood [12], and Chavanis [15]. As it is commented, in detail, in Sormani and Bertin [21], The Boltzmann entropy is equivalent to classical thermodynamic entropy ($\mathrm{d}S = \delta Q/T$) and hence is valid, if and only if the system has locally an equation of state of ideal gas, and also the system is in hydrostatic equilibrium. Although due to attractive gravitational force the pressure should decrease compared to that of ideal gas. Hence, strictly speaking, the equation of state can not be defined in terms of local quantities. A different way to justify the use of Boltzmann entropy was suggested by Padmanabhan [14], by means of so-called mean field approximation. However, the range of applicability of this approximation is still not clear.

In the frame, sketched above, our model can be characterized as a thermodynamic picture of a hydrodynamical turbulent isothermal self-gravitating system (molecular cloud in the cold neutral media) which presumes an ideal gas equation of state, that is valid locally. Also the system is in steady state, assuming hydrostatic equilibrium, and gravity is presented by mean field approximation. The novel contribution is that the ideal gas is composed by fluid elements, which chaotic motion is due to turbulence. The latter is suggested firstly by Keto et al. [23], but their approach and study are different. Accounting for the inertial range of turbulence and fractal structure of the cloud we obtain scaling laws for the temperature and self-gravity potential, accordingly. Then we explicitly write down the total energy and derive formulae for the entropy, free energy and Gibbs potential. Analysing canonical and grand canonical ensembles we conclude that for the former there does not exist an equilibrium state for the system, but for the latter there is a critical point, which is a local minimum from a thermodynamic point of view, and may be a possible hydrodynamical stable equilibrium. These considerations we regard as to be of use in suggested by us thermodynamic picture of turbulent self-gravitating MCs.

3. Set Up of the Model

We consider a cloud of molecular gas. This gas is isothermal with Kelvin temperature T. We model the gas as a turbulent self-gravitating fluid. The turbulence is fully developed and saturated. We suppose there exists an inertial range for turbulence in the interval: $l_{\mathrm{up}} \geq l \geq l_{\mathrm{d}}$, where l is the scale of consideration. l_{up} is the upper scale of the inertial range and l_{d} is the scale at which the turbulence starts to dissipate. We presume that this inner part with characteristic size l_{d} has very small volume and mass in regard to the whole cloud with size l, hence: $l \gg l_{\mathrm{d}}$. We suppose, as well, the cloud to be a homogeneous entity with an averaged number density $n = n(l)$. The latter, of course, is a very rough approximation (in regard to the very fragmented structure of molecular clouds), but our model is based on the theory of simple thermodynamic systems and this simplification is needed, at this first step.

We assume also that for the turbulence, in the inertial range, holds a scaling law:

$$\sigma(l) = u_0 l^{\beta} \,, \tag{1}$$

where $\sigma(l)$ is the 3D turbulence velocity dispersion, $u_o \sim 1$ is a normalizing coefficient and $0 < \beta \leq 1$ is a scaling exponent [8,29–31].

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We presume that the cloud is submerged in a very large, but not infinite[1], medium which plays a role of reservoir of thermal and turbulence energy for it. This medium has some averaged number density n_0, Kelvin temperature T_0, and 3D turbulence velocity dispersion σ_0. Also, in the volume of molecular cloud, this medium creates gravitational potential $\varphi_{\rm m} = {\rm const}$.

Our main hypothesis is that the macroscopic motion of the fluid elements caused by the turbulence in the inertial range is locally purely chaotic and can be regarded as a motion in an ideal gas containing of fluid elements treated as particles without internal degrees of freedom. In this sense we can introduce the notion of macro-temperature θ (the temperature of the chaotic motion of fluid elements) which is related to the velocity dispersion σ through the following expression:

$$\frac{1}{2}m\sigma(l)^2 \equiv \frac{3}{2}\kappa\theta(l)\,, \tag{2}$$

where m is the mass of the fluid elements, and κ is the Boltzmann constant. The equation (2) means that the turbulent kinetic energy, per one fluid element, at scale l is equivalent to the kinetic energy of the chaotic motion of the gas of fluid elements, which we term as a "macro-gas". This equation must be considered as an averaged relation (at regarded scale l), because according to our assumption the motion of the fluid elements is only locally purely chaotic.

Make use from equations (1) and (2) one obtains for the macro-temperature θ the following scaling law:

$$\theta(l) = \frac{m}{3\kappa}\sigma(l)^2 = \frac{mu_0^2}{3\kappa}l^{2\beta}\,. \tag{3}$$

Therefore if one accounts for the turbulent kinetic energy, thermal energy (energy of the molecule motion)[2], and gravitational energy, one can write down the following expressions for the internal and total energy of the macro-gas, per one fluid element, accordingly:

$$u = \varepsilon_{\rm turb} + \varepsilon_{\rm th} = \frac{3}{2}\kappa\theta + \frac{3}{2}\frac{m}{m_0}\kappa T\,, \tag{4}$$

and

$$\varepsilon = \varepsilon_{\rm turb} + \varepsilon_{\rm th} + \varepsilon_{\rm grav} = u + \varepsilon_{\rm grav} = \frac{3}{2}\kappa\theta + \frac{3}{2}\frac{m}{m_0}\kappa T + m\varphi\,, \tag{5}$$

where m_0 is the mean molecular mass of the gas, and $\varphi = \varphi_{\rm m} + \varphi_{\rm s}$ is the total gravitational potential in the cloud's volume caused by both: the surrounding medium ($\varphi_{\rm m}$) and the self-gravity of the cloud ($\varphi_{\rm s}$).

In principle, in the expression for the internal energy of one thermodynamic system take part the kinetic energy of the particles, their internal energy (already neglected in our considerations as it was mentioned above), if they are not simple material points, and the potential energy of their interaction. In our model the interaction between the fluid elements is only due to gravitational attraction. This interaction, in a small volume, is negligible in comparison to their kinetic energy. But one can not neglect the gravitational energy of these elements caused by the self-gravity of the whole cloud. So we account for it including in the equation (5) (for the total energy, per a fluid element) the total potential φ. The latter means that we consider every fluid element as it is submerged in an averaged external gravitational field caused by the surrounding medium and the self-gravity of the cloud. For self-gravity we assume that $\varphi_{\rm s} \propto n(l)l^2$, which is natural from dimensional considerations. Accounting for a fractal nature of molecular clouds we use the scaling law for the mass of our cloud: $M(l) \propto l^\gamma$, to obtain that $n(l) \propto l^{\gamma-3}$ and hence one can write for the self-gravity the following simple expression:

[1] To avoid the so called "Jeans swindle": the assumption for infinite homogeneous medium is actually not really consistent, because the Poisson equation cannot be solved unless the medium density is zero.

[2] Hereafter we will omit this term, because we suppose $T = {\rm const.}$ and regard fluid elements as a simple particles.

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$$\varphi_{\rm s} = Bn^{\delta} \ , \ \delta = \frac{\gamma - 1}{\gamma - 3} \ , \tag{6}$$

where $B < 0$ is a negative constant, and the mass scaling exponent varies in the range: $1 \le \gamma < 3$. The latter is in agreement with the literature (see the review by Hennebelle and Falgarone [3]).

One more point has to be clarified in the context of the above. The self-gravity of large systems is one of the major issues, which arise, if they are regarded as thermodynamic systems. This is due to two reasons. The first one is that the gravitation causes a long acting force, which can violate the thermodynamic limit hypothesis[3]. We avoid this problem assuming that the cloud and the surrounding medium (which is very large in regard to the cloud) are nearly homogeneous, and if the cloud's size changes with a small amount $\mathrm{d}l$ (hence the density will changes also small, according to: $\mathrm{d}n \propto l^{\gamma-4}\mathrm{d}l$), then the thermodynamic limit will holds. The second one is that the formula for the self-gravitational energy depends on N^2 (where N is the number of particles in the system) and therefore the total energy (and hence the other thermodynamic potentials) of the whole system are not additive. That is why we adopt in our treatment to consider the thermodynamic potentials not for the whole system, but rather per fluid element (see for example the book of Shapiro and Teukolsky [32]). The latter allows us to consider the gravitational energy as caused by some external averaged field, where a fluid element is submerged, and hence this energy is already additive.

4. Results

4.1. The First Principle and the Entropy of Macro-Gas

In the context of previous Section the first principle of thermodynamics of fluid elements, written per one fluid element, reads as follows:

$$\mathrm{d}\varepsilon = \theta \mathrm{d}s - P\mathrm{d}(1/n) \ , \tag{7}$$

where s is the entropy per one fluid element, $P = n\kappa\theta$ is the pressure of macro-gas expressed through the equation of state, and n is the number density ($1/n$ has a meaning of volume per one fluid element).

If one accounts that from equation (5) it stems $\mathrm{d}\varepsilon = (3/2)\kappa\mathrm{d}\theta + mB\delta n^{\delta-1}\mathrm{d}n$, then using (7) it is easy to obtain that:

$$\mathrm{d}s = \frac{3}{2}\frac{\kappa}{\theta}\mathrm{d}\theta + \left[\frac{mB}{\theta}\delta n^{\delta-1} - \frac{\kappa}{n}\right]\mathrm{d}n \ . \tag{8}$$

Integrating the latter equation from scale of dissipation $l_{\rm d}$ to the considered scale l one obtains an equation for entropy, as follows:

$$s(\theta, n) = \frac{3}{2}\kappa\ln(\theta/\theta_{\rm d}) - \kappa\ln(n/n_{\rm d}) + \frac{mB}{\theta}\left(n^{\delta} - n_{\rm d}^{\delta}\right) \ , \tag{9}$$

where $\theta_{\rm d}$ and $n_{\rm d}$ are, accordingly, the macro-temperature and number density at dissipation scale. Also we assume that $s_{\rm d} = s(\theta_{\rm d}, n_{\rm d}) = 0$ which plays the role of third principle of the thermodynamics of fluid elements.

4.2. Free Energy

Free energy, per one fluid element, can be defined through the following expression [4] :

$$f \equiv \varepsilon - \theta s \ \Rightarrow \ \mathrm{d}f = -s\mathrm{d}\theta - P\mathrm{d}(1/n) \ . \tag{10}$$

3 The thermodynamic limit hypothesis presumes that if the volume of the system V and the number of particles N in it tend to infinity simultaneously, then the number density $n = N/V$ keeps a constant value.

4 For the obtaining the differential forms of free energy and Gibbs potential see the calculations in App.A

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To obtain the explicit form of free energy we make use of equations (5) and (9). The formula for $f(\theta, n)$ is as follows:

$$f(\theta, n) = \frac{3}{2}\kappa\theta[1 - \ln(\theta/\theta_{\mathrm{d}})] + \kappa\theta \ln(n/n_{\mathrm{d}}) + m\left[Bn_{\mathrm{d}}^{\delta} + \varphi_{\mathrm{m}}\right] . \tag{11}$$

4.3. Gibbs potential

Gibbs potential, per one fluid element, reads as follows:

$$g \equiv \varepsilon - \theta s + P/n \quad \Rightarrow \quad \mathrm{d}g = -s\mathrm{d}\theta + (1/n)\mathrm{d}P . \tag{12}$$

To obtain the explicit form of Gibbs potential we make use of equations (5), (9), and the equation of state: $P = n\kappa\theta$. The formula for $g(\theta, n)$ is as follows:

$$g(\theta, n) = \frac{3}{2}\kappa\theta[1 - \ln(\theta/\theta_{\mathrm{d}})] + \kappa\theta[1 + \ln(n/n_{\mathrm{d}})] + m\left[Bn_{\mathrm{d}}^{\delta} + \varphi_{\mathrm{m}}\right] . \tag{13}$$

It is interesting to note that both potentials: free energy (equation 11) and Gibbs potential (equation 13) depend only on the constant part, in regard to n, of gravitational potential.

4.4. Stability Analysis

Using the model presented in Section 3 and the equations of thermodynamics of fluid elements obtained above in this Section 4 one can make a stability analysis of the considered molecular cloud in the context of the thermodynamics of macro-gas. In this Section we do the analysis in two different cases. In the first case we regard the cloud as a macro-gas contacting with a huge reservoir (the surrounding medium) at fixed temperature θ_0 and fixed number density n_0 - this realises a case of canonical ensemble. Hence the relevant potential is the free energy. The second case is a grand canonical ensemble: the cloud contacts with a huge reservoir at fixed temperature θ_0 and fixed pressure P_0; the relevant potential is the Gibbs potential, accordingly.

About the following considerations we refer the reader to the book by Reif [33], Chapter 8.

4.4.1. Canonical Ensemble

In this case the cloud is regarded as a macro-gas contacting with a large surrounding medium at fixed macro-temperature θ_0 and fixed number density n_0. The free energy, written in the off-equilibrium form[5] reads:

$$f_0(\theta, n) = \varepsilon(\theta, n) - \theta_0 s(\theta, n) ,$$

and it will be varied as a function of θ, which plays a role of parameter determining the state of the system (our cloud). Therefore we take the first derivative of $f_0(\theta, n)$ in regard to θ (see equations 7 and 8) and seeking for extrema. This is as follows:

$$\left(\frac{\partial f_0}{\partial \theta}\right)_n = \left(\frac{\partial \varepsilon}{\partial \theta}\right)_n - \theta_0 \left(\frac{\partial s}{\partial \theta}\right)_n = \frac{3}{2}\kappa - \frac{3}{2}\kappa\frac{\theta_0}{\theta} = 0 .$$

[5] The detailed derivation of the off-equilibrium form for the Gibbs potential is performed in App.B. The derivation for the free energy is not made, because the calculations in the case of canonical ensemble are (a subcase and) simpler than that for the grand canonical ensemble.

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Hence the free energy might have an extremum for macro-temperature $\theta = \theta_0$. One needs of the second derivative of $f_0(\theta, n)$ in regard to θ to say what kind of extremum this may be. It is obvious that the second derivative at temperature $\theta = \theta_0$ is positive:

$$\left(\frac{\partial^2 f_0}{\partial \theta^2}\right)_n = \frac{3}{2}\frac{\kappa}{\theta_0} > 0\,.$$

This corresponds to a possible minimum of the free energy. The conclusion is that if the system (our cloud) resides at macro-temperature $\theta = \theta_0$, then it can be in a stable dynamical equilibrium. To complete this study one has to calculate the derivatives of $f_0(\theta, n)$ in regard to n, at temperature $\theta = \theta_0$. They are as follows:

$$\left(\frac{\partial f_0}{\partial n}\right)_\theta = \left(\frac{\partial \varepsilon}{\partial n}\right)_\theta - \theta_0\left(\frac{\partial s}{\partial n}\right)_\theta = \frac{\kappa\theta_0}{n}\,,$$

and

$$\left(\frac{\partial^2 f_0}{\partial n^2}\right)_\theta = -\frac{\kappa\theta_0}{n^2}\,.$$

From the above formulae it stems that there are no extrema for the free energy in regard to n. $f_0(\theta, n)$ is an increasing function of variable n and the first derivative decreases and tends to zero.

Hence the free energy does not have extrema in two variable space (θ, n), the critical point for the temperature $\theta = \theta_0$ there exists, but regarding to the number density n the free energy is a monotonically increasing function. Therefore there is no a local equilibrium state for the system (our cloud) regarded as a canonical ensemble.

4.4.2. Grand canonical ensemble

In the second case the cloud is considered as a macro-gas contacting with a large surrounding medium at fixed macro-temperature θ_0 and fixed pressure P_0. The Gibbs potential, written in the off-equilibrium form[6] reads:

$$g_0(\theta, n) = \varepsilon(\theta, n) - \theta_0 s(\theta, n) + P_0(1/n)\,,$$

and it will be varied, separately, as a function of θ and n, which are the variables determining the state of the cloud.

So we take the first derivative of $g_0(\theta, n)$ in regard to θ (see equations 7 and 8) and seeking for extrema. This is as follows:

$$\left(\frac{\partial g_0}{\partial \theta}\right)_n = \left(\frac{\partial \varepsilon}{\partial \theta}\right)_n - \theta_0\left(\frac{\partial s}{\partial \theta}\right)_n = \frac{3}{2}\kappa - \frac{3}{2}\kappa\frac{\theta_0}{\theta} = 0\,.$$

Hence the Gibbs potential might have an extremum for macro-temperature $\theta = \theta_0$. We need of the second derivative of $g_0(\theta, n)$ in regard to θ to say what kind of extremum this is. For one it is easy to see that the second derivative at temperature $\theta = \theta_0$ is positive:

$$\left(\frac{\partial^2 g_0}{\partial \theta^2}\right)_n = \frac{3}{2}\frac{\kappa}{\theta_0} > 0\,.$$

This means that if the cloud resides at macro-temperature $\theta = \theta_0$, then it might be in a stable dynamical equilibrium, because the Gibbs potential may have a minimum.

Suppose that the macro-temperature of cloud is considered fixed at $\theta = \theta_0$. Then the variation of Gibbs potential is only due to n. The first derivative in regard to n, accordingly reads:

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[6] See the App.B

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$$\left(\frac{\partial g_0}{\partial n}\right)_\theta = \left(\frac{\partial \varepsilon}{\partial n}\right)_\theta - \theta_0\left(\frac{\partial s}{\partial n}\right)_\theta - \frac{P_0}{n^2} = 0 + \frac{\kappa\theta_0}{n} - \frac{P_0}{n^2} = 0\,.$$

But the pressure of macro-gas in the cloud, at considered conditions, is $P = n\kappa\theta_0$. Therefore the condition for an extremum, in regard to variable n, is: $P = P_0$. The second partial derivative of $g_0(\theta, n)$ about n, under the conditions: $\theta = \theta_0$ and $P = P_0$, reads:

$$\left(\frac{\partial^2 g_0}{\partial n^2}\right)_\theta = -\frac{\kappa\theta_0}{n^2} + 2\frac{P_0}{n^3} = \frac{P_0}{n^3} > 0\,.$$

The mixed second derivatives of Gibbs potential are obviously zero and therefore the functional determinant built up from the second partial derivatives of $g_0(\theta, n)$, calculated at $\theta = \theta_0$ and $P = P_0$, will be:

$$D = \left(\frac{\partial^2 g_0}{\partial \theta^2}\right)_n \left(\frac{\partial^2 g_0}{\partial n^2}\right)_\theta - \left(\frac{\partial^2 g_0}{\partial \theta \partial n}\right)\left(\frac{\partial^2 g_0}{\partial n \partial \theta}\right) = \frac{3}{2}\frac{\kappa}{\theta_0}\frac{P_0}{n^3} > 0\,.$$

Hence, if the parameters of our system are set at: $\theta = \theta_0$ and $P = P_0$, then it resides in a local stable dynamical equilibrium.

The considered cases, namely of canonical and grand canonical ensembles, are appropriate to real molecular clouds, because at their boundaries occurs phase transition between atomic warm neutral media and molecular cold neutral media of the ISM [2–4]. This transition is a non-linear process attended with a jump in number density of the gas [7] at constant pressure [2–4].

5. Discussion

5.1. Basic Assumptions and Main Results

In this paper we have made an attempt at applying the powerful tools of thermodynamic equilibrium analysis to study the dynamical state of turbulent isothermal self-gravitating hydrodynamical systems presented by MCs. In the base of our model we put the assumption that the turbulent kinetic energy can be locally substituted for the macro-temperature of purely chaotic turbulent motion of fluid elements, an idea first arisen by [23]. Setting up the model we also presume there is an inertial range of spatial scales for this turbulence, which is substantiated for subsonic [5,6] as well as for supersonic [7–9] case. The latter presumption seems to be not needed for our considerations but it provides a continuity for θ and n in regard to the scales of consideration. This is very important for a cloud's stability in the inertial range (see Section 4.4.2). Also we regard our cloud to be submerged in a very large, but not infinite, medium which serves as a reservoir of turbulent (and also thermal) energy and supplies confining pressure for the system. We give, also, an account for the gravity of surrounding medium and for the self-gravity of cloud, as well, assuming they cause potentials in the cloud's volume. The latter is the so called "averaged field approach".

Starting from the model, shortly reminded above, we have succeeded to write down the internal and total energy and the first principle, per fluid element. Make use of them we have obtained the explicit equations for entropy, and for free energy, and Gibbs potential, as well. The latter two potentials are tools for studying cloud's stability in the cases of canonical and grand canonical ensembles, accordingly.

Considering canonical ensemble we have set to the conclusion that the system does not have a stable equilibrium state, although the free energy has a minimum when the macro-temperature is equal to the temperature of reservoir, because, with respect to the number density, $f(\theta, n)$ is a strictly increasing function. Hence, though one can set the system at macro-temperature $\theta = \theta_0$, if there happens a small perturbation in n, then the cloud will tend to get less or more dense (depending on its Jeans' mass, in regard to its density and Kelvin temperature), and finally it will disperse or collapse.

7 Note that the number density of molecular gas is proportional to the number density of macro-gas through a constant m/m_0.

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Contrary to the above case, if one considers a grand canonical ensemble, the system can be set at a stable dynamical equilibrium state. Gibbs potential has a local minimum for $\theta = \theta_0$ and $P = P_0$. This means that, although there may be happened small perturbations in macro-temperature and/or density, the cloud will come always back to the equilibrium state.

How can one understand these ensembles and corresponding conditions for θ, n and P, in the context of the cloud's hydrodynamics? Since we deal with equilibrium thermodynamics one natural way to interpret our model is to compare it with the terms of the virial theorem. This theorem has two forms: Eulerian and Lagrangian, depending on the chosen coordinate system. We decided to use the Eulerian form, because it is more appropriate for stationary systems. It reads:

$$\frac{1}{2}\ddot{I} = 2(\tau - \tau_S) + w - \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_S \rho r^2 \vec{u}\cdot \mathrm{d}\vec{S}\,, \tag{14}$$

where $\vec{r}$ is a radius-vector (with absolute value $r = |\vec{r}|$) from the origin of the Eulerian coordinate system, $\vec{u}(\vec{r},t)$ is the velocity field (with absolute value $u = |\vec{u}|$) in the fluid and $\rho(\vec{r},t)$ is the density field. The terms in equation (14) have the explicit form and physical meaning as follows:

$$I = \int_V \rho r^2 \mathrm{d}V\,, \tag{15}$$

is the moment of inertia of the fluid in the volume V, calculated about the origin, and $\ddot{I}$ is its second time derivative;

$$\tau = \int_V \left(\frac{1}{2}\rho u^2 + \frac{3}{2}P_{\mathrm{th}}\right)\mathrm{d}V\,, \tag{16}$$

is the total kinetic plus thermal energy of the fluid (P_{th} is the thermal pressure);

$$\tau_S = \int_S \vec{r}\cdot\Pi\cdot \mathrm{d}\vec{S}\,, \tag{17}$$

is the confining pressure on the volume surface, including both the thermal pressure and the ram pressure of any gas flowing across the surface; where $\Pi_{ij} = \rho u_i u_j + P_{\mathrm{th}}\delta_{ij}$ is the general form of the fluid pressure tensor;

$$w = -\int_V \rho\vec{r}\cdot\vec{\nabla}\varphi\,\mathrm{d}V\,, \tag{18}$$

is the gravitational energy of the cloud, where the potential φ accounts for both self-gravity of the cloud and gravity of the external matter. The last term on the r.h.s. in equation (14) represents the rate of change of the momentum flux across the cloud surface.

We have to point out that the terms concerning thermal energy and pressure (in equations 16 and 17), due to the microscopic motion of the fluid molecules, are not in question. They have their standard interpretation. It needs to be clarified the terms concerning kinematics and dynamics of the fluid elements. Let us begin with gravitational term (equation 18). This is a volume energy term which is accounted in our model trough the mean field potential φ in the equation (5) for total energy. Then it appears in the equations (11) and (13) for free energy and Gibbs potential, accordingly. The terms containing macro-temperature in equations (5), (11), and (13) correspond to the volume kinetic term in equation (16). The ram pressure term in equation (17) can be linked to the boundary condition for the pressure P_0, of the reservoir, in the case of grand canonical ensemble. Accordingly, the boundary conditions for the macro-temperature θ_0 (in both cases: canonical and grand canonical ensembles) and for the number density n_0 (canonical ensemble), of the reservoir, can be associated with the momentum flux across the cloud surface (the last term in the equation 14), because this flux transfers also kinetic energy, and can be caused by macro-temperature and/or number density gradients.

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Finally one might conclude, although there is not a complete correspondence between our model and dynamical balance presented by the virial theorem, the suggested thermodynamic anzac has a potential to describe equilibrium states of hydrodynamical self-gravitating systems. For the full picture, of course, one must regard the thermodynamics of micro-particles (atoms and/or molecules), as well.

5.2. Number of Microstates

In this section we shed light on our results for the entropy in terms of statistical mechanics. The explicit form of equation (9) gives one an opportunity to obtain, also, formula for the number of microstates which correspond to a given macrostate, in the case of isolated system. From Boltzmann theory we know that this number is:

$$W = \exp(Ns/\kappa)\,,$$

where N is the number of fluid elements in the cloud with characteristic size l.

Then it is not difficult for one, making use of equation (9), to obtain:

$$\begin{aligned} W(l) = \\ = \left(\frac{l}{l_{\mathrm{d}}}\right)^{3N\beta} \left(\frac{l}{l_{\mathrm{d}}}\right)^{(3-\gamma)N} \exp\left(N\frac{m(\varphi_{\mathrm{s}}(l)-\varphi_{\mathrm{s}}(l_{\mathrm{d}}))}{\kappa\theta}\right) \\ = \left(\frac{l\sigma(l)}{l_{\mathrm{d}}\sigma_{\mathrm{d}}}\right)^{3N} \left(\frac{l}{l_{\mathrm{d}}}\right)^{-\gamma N} \exp\left(N\frac{m(\varphi_{\mathrm{s}}(l)-\varphi_{\mathrm{s}}(l_{\mathrm{d}}))}{\kappa\theta}\right). \end{aligned} \tag{19}$$

It is interesting to note that at the last row of the above equation the physical meaning of the multipliers is as follows: the first one is a number of microstates due to the chaotic turbulent motion of the fluid elements in 6D phase-space of the turbulent system, the second one comes from the fractal structure of the cloud, and the last one is due to self-gravity.

The equation (19) shows that the first two multipliers (at the second row) in the function $W(l)$ strictly increases when l increases, while the last multiplier (accounting for the self-gravity) has the opposite behaviour. It can be mentioned also that $W(l_{\mathrm{d}}) = 1$.

It is worth to note, also, that if we deal with canonical or grand canonical ensemble the corresponding probability of an equilibrium macrostate of the system will be proportional to $\sim \exp(-Nf(\theta,n)/\kappa\theta)$ or to $\sim \exp(-Ng(\theta,n)/\kappa\theta)$, accordingly. And the state with maximal probability realises for the minimum of corresponding potential.

5.3. Caveats

In this Section we intend to consider possible caveats in regard to presented model.

The first one cause the very basis of the model. This is the assumption that we can substitute the turbulent kinetic energy for the macro-temperature of chaotic motion of fluid elements. The latter substitution is justifiable only locally, due to the turbulent cascade has subscales at a given scale and according to equation (3) the macro-temperature will be different at different subscales. Also if the turbulence is supersonic, there exist shock fronts, and the flow can be intermittent. That is why to spread the obtained macro-temperature for the whole cloud is a bit speculative. To justify this presumption we have specified that it is made in an averaged sense, i.e. we calculate the temperature at every local place, in regard to the turbulent motion of fluid elements related to the cloud's scale l, averaged the obtained values and attribute it as a temperature for the entire cloud, which is summarized in the equation (2). In other words we consider our system as a physically homogeneous entity, neglecting shocks and other contrasts in density field, and intermittency as well.

The second caveat, stemming from the first one, is supposition for homogeneous medium in and outside the cloud. This is a needed condition for one thermodynamic systems to be simple. But we

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know that clouds and their surroundings are strongly self-gravitating objects. Hence the assumption for homogeneity will be broken. That is why we adopt it as a rough, but needed, at this first step approximation.

The above two caveats can be partially avoided if one considers not the whole cloud, but rather a smaller volume in the cloud, in which the inhomogeneities can easily be neglected (this approach is developed in [34]). This alternative model is simpler but does not allow one to make clear conclusions for the whole system.

The third caveat is the hypothesis that equilibrium thermodynamics is relevant to dynamical states of MCs. Some authors ([22,35,36] and references there in) claim that MCs are dynamical self-gravitating objects that are in a state of hierarchical gravitational collapse at all scales and never be at steady state. In our model the turbulence plays a leading role in the cloud's dynamics together with the self-gravity. Hence one can relates the evolutionary stage of the cloud to its late period. So if one considers probability density functions of surface mass density or mass density, from observations [37–39] and/or simulations [39–42], then notices that these probability distributions demonstrate stable shapes and slopes, for several dynamical timescales, especially at late stages of cloud's evolution. So the equilibrium thermodynamic is appropriate to describe just these, probably stable, late stages of MCs' life-cycle.

At the end of this Section we conclude that the presented in this work novel approach to study possible equilibrium states of hydrodynamical turbulent isothermal self-gravitating systems has its reason, although there are valid caveats that one can arise.

6. Conclusion

In the present paper we suggest a model for studying equilibrium dynamical states of an hydrodynamical isothermal turbulent self-gravitating system, presented by a molecular cloud, making use of the principles and tools of equilibrium thermodynamics. In the basis we put the simple idea that the local turbulent motion of fluid elements is purely chaotic and can be regarded as an ideal macro-gas. Starting from this point we write down explicitly the formulae for internal and total energy and for the first principle, per one fluid element. Using them we obtain expressions for entropy, free energy, and Gibbs potential, per one fluid element. Then we study two possible thermodynamic ensembles, describing our cloud: canonical, and grand canonical. Exploring them for equilibrium states we find that the model of canonical ensemble does not have an extremum for the free energy. At its turn the model of grand canonical ensemble exhibits a local minimum of the Gibbs energy and is appropriate to describe a stable state of our cloud. Although there exist several valid caveats against the model we consider it as an original approach for studying the equilibrium states of regarding systems.

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Abbreviations

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The following abbreviations are used in this manuscript:

MC(s)	Molecular Cloud(s)
ISM	Interstellar Medium
6D phase-space	six-dimensional phase-space
AGN	Active Galactic Nuclei

Appendix A. Legendre Transformations for the Free Energy and Gibbs Potential

Here we shortly remind the reader how one can obtain the differential forms of free energy and Gibbs potential (equations 10 and 12, accordingly), if one has the differential form for the total energy: $\mathrm{d}\varepsilon = \theta \mathrm{d}s - P\mathrm{d}(1/n)$, which is in fact the first law of thermodynamics (equation 7).

Let us start with the free energy. Its formula reads: $f \equiv \varepsilon - \theta s$. Hence, for the total differential one obtains: $\mathrm{d}f = \mathrm{d}\varepsilon - s\mathrm{d}\theta - \theta\mathrm{d}s = \theta\mathrm{d}s - P\mathrm{d}(1/n) - s\mathrm{d}\theta - \theta\mathrm{d}s = -s\mathrm{d}\theta - P\mathrm{d}(1/n)$, where the last equality coincides with equation (10).

In turn the Gibbs potential defines as: $g \equiv \varepsilon - \theta s + P(1/n)$. Therefore one easy calculates the total differential: $\mathrm{d}g = \mathrm{d}\varepsilon - s\mathrm{d}\theta - \theta\mathrm{d}s + P\mathrm{d}(1/n) + (1/n)\mathrm{d}P = \theta\mathrm{d}s - P\mathrm{d}(1/n) - s\mathrm{d}\theta - \theta\mathrm{d}s + P\mathrm{d}(1/n) + (1/n)\mathrm{d}P = -s\mathrm{d}\theta + (1/n)\mathrm{d}P$. And, this time, in the last equality we obtain equation (12).

Appendix B. The Off-Equilibrium Form of the Gibbs Potential

In the following considerations we use the book [33], Chapter 8.3.

Let us denote our system (cloud) as system A. We suppose that A is maintained under conditions of both constant macro-temperature and constant pressure (of the macro-gas). The situation implies that the system A is in contact with a very large reservoir A' (this is the surrounding medium of the cloud) which is at a constant temperature θ_0 and at a constant pressure P_0. The system A can exchange "heat" (that is turbulent energy) with A' but the latter is so large, that its temperature θ_0 remains unchanged. Also, the volume V of A can change at the expense of the reservoir A' and hence the system A doing work on the reservoir, but again A' is so large that its pressure P_0 remains constant.

Let us denote with $A^0 = A + A'$ the "sum" of two systems: A and its surrounding medium A'. Apparently, A^0 can be regarded as an isolated system. Then, for the change of its entropy ΔS^0 during any spontaneous process, one has:

$$\Delta S^0 = \Delta S + \Delta S' \geq 0\,, \tag{A1}$$

where ΔS and $\Delta S'$ are the changes of entropy of the systems A and A', during the same process, accordingly. So, if A absorbs "heat" Q in this process, then A' absorbs "heat" $-Q$ and undergoes corresponding entropy change: $\Delta S' = (-Q)/\theta_0$. At the same time the first law of the thermodynamics written for A reads:

$$Q = \Delta E + P_0 \Delta V\,, \tag{A2}$$

where ΔE is the change of total energy of A, and $P_0\Delta V$ is the work done by A against the constant pressure P_0 of the reservoir A', in the process in regard. Hence one can obtain:

$$\begin{aligned}\Delta S^0 = \Delta S - \frac{Q}{\theta_0} &= \frac{1}{\theta_0}[\theta_0 \Delta S - Q] = \frac{[\theta_0 \Delta S - (\Delta E + P_0 \Delta V)]}{\theta_0} \\ &= -\frac{\Delta[E - \theta_0 S + P_0 V]}{\theta_0} = -\frac{\Delta G_0}{\theta_0}\,,\end{aligned}$$

where we have used the fact that θ_0 and P_0 are both constant and introduced the definition:

$$G_0 = E - \theta_0 S + P_0 V\,, \tag{A3}$$

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for the off-equilibrium Gibbs potential. This reduces the ordinary Gibbs energy $G = E - \theta S + PV$ for the system A when the temperature and pressure of the latter are equal to those of the reservoir A'. With Gibbs energy written in this off-equilibrium form one can study the conditions for equilibrium of the grand canonical ensemble. From equation (A1) it is obvious that during the spontaneous process one must have: $\Delta G_0 \leq 0$, and hence G_0 must be minimal for a stable equilibrium.

One more point has to be clarified. If one has divided the equation (A3) by the total number N of the fluid elements in the system A (our cloud), and taking into account that $V/N = 1/n$, then one obtains the equation $g_0 = \varepsilon - \theta_0 s + P_0(1/n)$, for off-equilibrium Gibbs energy per one fluid element, from Section 4.4.2.

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