Microcanonical equations for the Tsallis entropy

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Abstract

Microcanonical equations for several thermodynamic properties of a system, suitable for molecular dynamics simulations, are derived from the nonextensive Tsallis entropy functional. Two possible definitions of temperature, the usual one and a “physical” modification which satisfies the zeroth law of thermodynamics, are considered, and the results from both choices are compared. Results for the ideal gas using the first definition of temperature are provided and discussed in relation with the canonical results reported in the literature. The second choice leaves most formulae unchanged from their extensive (Shannon-Boltzmann-Gibbs) form.

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I. INTRODUCTION

In the last two decades there has been a great deal of interest in nonextensive entropies to explain physical phenomena such as anomalous diffusion, believed to be outside the scope of the conventional and highly successful Shannon-Boltzmann-Gibbs (SBG) entropy \[1\]. Among the various reported nonextensive functionals, the Tsallis entropy \[2\] has received considerable attention. It is defined as

$$S_q \{p_l\} = -k_B \sum_l p_l^q \log_q p_l,$$

where

$$\log_q x = \lim_{q' \to q} \frac{x^{1-q'} - 1}{1 - q'},$$

\(p_l\) being the probability of each microstate \(l\) accessible to the system and \(k_B\) the Boltzmann constant. This definition can be considered an uniparametric generalization of the SBG functional, which is recovered when the entropic index \(q\) equals one, as can be easily verified using L’Hôpital rule. A further generalization, not studied in this paper, replaces \(k_B\) with a generic \(k(q)\) under the weaker constraint \(k(1) = k_B\).

Most discussions about the Tsallis entropy and the theoretical and computational results from its application have been made in the context of the canonical ensemble, although a satisfactory definition of the mean energy has taken some effort to achieve \[2\]. As with ordinary extensive statistics, this ensemble is often more amenable to theoretical calculations. However, the microcanonical ensemble is clearly more directly accessible to molecular dynamics (MD) simulation, which consists simply in the integration of Newton’s Second Law, and as such gives rise automatically to the conservation of energy, but lacks the intrinsic notion of a thermostat. Thus, it is necessary to have a formalism which allows for the obtention of the thermodynamic properties of a system from microcanonical averages.

Several methods have been devised in order to obtain these formulae for the SBG functional, adjusted to different needs. For instance, Ray and Graben \[3\], guided by didactic concerns, use a method based on fluctuations which involves some arbitrary definitions and is only valid for relatively large systems. A more systematic and general method, based on Laplace transforms, was put forward by Pearson, Halocioglu and Tiller \[4\]. However, the use
of this transform is only a method of integration. The present paper applies an equivalent but more straightforward method to the Tsallis entropy, and it is structured as follows: in the next section, after reviewing some well-know features of the microcanonical ensemble, a set of formulae for thermodynamic properties such as the heat capacities and compressibility coefficient is developed using the conventional definition of temperature. These formulae are applied to the nonextensive ideal gas in order to obtain its thermal and caloric equations. After discussing an important shortcoming of this definition of temperature, the previously developed results are changed in order to reflect a physical definition of temperature. Finally, the main conclusions are summarized.

II. FORMULAE OBTAINED USING THE ORDINARY TEMPERATURE

The system to be studied consists of $N$ classical particles of mass $m$, with coordinates $(\vec{r}^N, \vec{p}^N)$ in $6N$-dimensional phase space, in a recipient of fixed volume $V$ and with a total energy $E$, resulting from a Hamiltonian which must be separable into a kinetic and a potential part which depend only on the positions and momenta, respectively:

$$E = H (\vec{r}^N, \vec{p}^N) = E_c (\vec{p}^N) + U (\vec{r}^N).$$

(2)

The probability distribution over the microstates compatible with these restrictions can be obtained using the maximum entropy (MaxEnt) method, by maximization of (1a) submitted to the normalization $\sum p_l = 1$. In this way, it is trivially obtained that all the microstates compatible with the specified thermodynamic coordinates are equiprobable. In practice, the energy of the system can only be determined (and constrained) to be in an interval $[E - \delta E, E]$, with $\delta E \ll E$ for a useful measurement. Thus, the number of microstates available to the system would be $\Gamma (E, V, N) - \Gamma (E - \delta E, V, N)$, with:

$$\Gamma (E, V, N) = \frac{1}{h^{3N}} \int \theta [E - H (\vec{r}^N, \vec{p}^N)] d\vec{r}^N d\vec{p}^N.$$  

(3)

The spatial limits of integration are $V^N$. The momenta can be integrated over the whole $\mathbb{R}^{3N}$. $\theta$ is the Heaviside step function which restricts the integration to the volume in phase space where the hamiltonian is less or equal than $E$. Finally, $h^3$ is the phase volume of an individual microstate, used to adimensionalize the number of microstates, and must be multiplied by $N!$ in the case of indistinguishable particles. Both the precise value of $h$ and
the presence of $N$ are, however, irrelevant to the following discussion. For most systems (specially for moderate and large values of $N$), $\Gamma$ is a strongly increasing function of $E$, so $\Gamma(E - \delta E, V, N) \ll \Gamma(E, V, N)$ and the number of microstates available to the system can be approximated by $\Gamma(E, V, N)$, and the probability of each of them by its inverse. Substituting this probability in (1a) a straightforward $q$-generalization of the well-known microcanonical entropy equation is obtained:

$$S_q(E, N, V) = k_B \log_q \Gamma(E, V, N).$$

In conventional thermodynamics, temperature is defined as the inverse of the partial derivative of entropy with respect to energy:

$$T = \left( \frac{\partial S_q}{\partial E} \right)^{-1}_{V,N} = \frac{\Gamma_q}{k_B \Omega},$$

where

$$\Omega = \left( \frac{\partial \Gamma}{\partial E} \right)_{V,N} = \frac{1}{h^3 N} \int \delta \left[ E - H(\vec{r}^N, \vec{p}^N) \right] d\vec{r}^N d\vec{p}^N.$$  

These equations, relating entropy and temperature with $\Gamma$ and $\Omega$, are responsible for the differences between the present development and the conventional extensive one.

The microcanonical average of a general magnitude $\chi(\vec{r}^N)$ which depends on the positions of the particles is expressed in two equivalent ways:

$$\langle \chi \rangle = \frac{1}{h^3 N \Omega} \int \chi(\vec{r}^N) \theta \left[ E - H(\vec{r}^N, \vec{p}^N) \right] d\vec{r}^N d\vec{p}^N$$

$$\langle \chi \rangle = \frac{1}{h^3 N \Omega} \int \chi(\vec{r}^N) \delta \left[ E - H(\vec{r}^N, \vec{p}^N) \right] d\vec{r}^N d\vec{p}^N.$$  

The equivalence is based on the hypothesis that $\Gamma$ is a strongly increasing function of $E$, so only the contribution to it from the higher energies, $\Omega \delta E$, must be taken into account, to a good approximation. In the remaining of this paper, only the second of these formulae will be used.

In order to obtain a microcanonical formula for any thermodynamic variable, it is necessary to express it as a function of $\Gamma$ or its partial derivatives, like it has already been done for temperature. The pressure, isocoric heat capacity and Grünessein parameter are likewise straightforwardly written as.
\[ p = T \left( \frac{\partial S}{\partial V} \right)_{E,N} = \frac{1}{\Omega} \left( \frac{\partial \Gamma}{\partial V} \right)_{E,N} \] (9)

\[ C_V = \left( \frac{\partial T}{\partial E} \right)_{V,N}^{-1} = \left[ T \left( \frac{q\Omega}{T} - \frac{1}{\Omega} \left( \frac{\partial \Omega}{\partial E} \right)_{V,N} \right) \right]^{-1} \] (10)

\[ \gamma = V \left( \frac{\partial p}{\partial E} \right)_{V,N} = \frac{V}{\Omega} \left[ \left( \frac{\partial \Omega}{\partial V} \right)_{E,N} - p \left( \frac{\partial \Omega}{\partial E} \right)_{V,N} \right] \] (11)

Other variables often used in tables and experiments, but not so immediately translated into microcanonical language are the isobaric heat capacity, coefficient of thermal expansion and isothermal compressibility:

\[ C_p = \left( \frac{\partial E}{\partial T} \right)_{p,N}, \alpha = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_{p,N}, \kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_{T,N} \] (12)

This is because of the fact that the constraints more easily applied to a system in the laboratory (constant temperature or pressure) are not those of the microcanonical ensemble (constant energy or volume). However, the previous variables can be related to

\[ \alpha_E = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_{E,N} = \left[ VT \left( \frac{q}{T} \left( \frac{\partial \Gamma}{\partial V} \right)_{E,N} - \frac{1}{\Omega} \left( \frac{\partial \Omega}{\partial V} \right)_{E,N} \right) \right]^{-1} \] (13)

\[ B_E = -V \left( \frac{\partial p}{\partial V} \right)_{E,N} = \frac{V}{\Omega} \left[ p \left( \frac{\partial \Omega}{\partial V} \right)_{E,N} - \left( \frac{\partial^2 \Gamma}{\partial V^2} \right)_{E,N} \right] \] (14)

using the following identities, obtained from standard relations among derivatives:

\[ \kappa_T = \frac{1}{B_E + \frac{C_V}{\alpha_E V}} \] (15)

\[ \alpha = \kappa_T \left( \frac{\gamma C_V}{V} - \alpha_E B_E \right) \] (16)

\[ C_p = C_V \left( 1 - \frac{\alpha}{\alpha_E} \right). \] (17)

It is necessary to find a way to express the derivatives of \( \Gamma \) and \( \Omega \) in such a way that they can be calculated directly during a MD simulation. For this purpose, one can observe that the integration in (3) can be performed the following way due to the form of the hamiltonian in eq. (2):
\[ \int_{H(\vec{r}^N, \vec{p}^N)} d\vec{r}^N d\vec{p}^N = \int_{U(\vec{r}^N) \leq E} \left[ \sum_{j=1}^{N} \sum_{i=1}^{3} \frac{p_i^2}{2m} \leq E - U(\vec{r}^N) \right] d\vec{p}^N d\vec{r}^N. \]

The inner integral in the right-hand side of this equation is clearly the volume of a 3N-dimensional sphere of radius \( R = \sqrt{2m(E - U(\vec{r}^N))} \), which equals \( \frac{4N}{(3N)^2} R^{3N} \). Substituting this into the previous equation, eq. \( \text{(3)} \) becomes

\[ \Gamma (E, V, N) = \frac{(2m\pi)^{3N}}{h^{3N}} \int_{V^N} \theta [E - U(\vec{r}^N)] \left[ E - U(\vec{r}^N) \right]^{\frac{3N}{2} - 1} d\vec{r}^N. \] (18)

Using an almost identical course of reasoning and the formula for the surface (instead of the volume) of the \( n \)-dimensional sphere, eqs. \( \text{(6)} \) and \( \text{(8)} \) can be reexpressed as:

\[ \Omega (E, V, N) = \frac{(2m\pi)^{3N}}{h^{3N}} \int_{V^N} \theta [E - U(\vec{r}^N)] \left[ E - U(\vec{r}^N) \right]^{\frac{3N}{2} - 1} d\vec{r}^N. \] (19)

\[ \langle \chi \rangle = \frac{(2m\pi)^{3N}}{\Omega h^{3N}} \left( \frac{3N}{2} - 1 \right) \int_{V^N} \chi(\vec{r}) \theta [E - U(\vec{r}^N)] \left[ E - U(\vec{r}^N) \right]^{\frac{3N}{2} - 1} d\vec{r}^N. \] (20)

These expressions are also valid for the extensive case (since they do not depend on the choice of entropy functional as long as the latter preserves the microcanonical distribution) and were already provided by Pearson et al. \([4]\) using the Laplace transform method.

A first practical result can be extracted from these transformations by setting \( \chi(\vec{r}) = E - U(\vec{r}) \) (the kinetic energy expressed as a function of the positions):

\[ \langle E_c \rangle = \frac{(2m\pi)^{3N}}{\Omega h^{3N}} \left( \frac{3N}{2} - 1 \right) \int_{V^N} \theta [E - U(\vec{r}^N)] \left[ E - U(\vec{r}^N) \right]^{\frac{3N}{2} - 1} d\vec{r}^N, \]

and comparing this to eq. \( \text{(15)} \), concluding that \( \langle E_c \rangle = \frac{3N}{2} \frac{\Gamma}{\Omega} \). Combining this with the definition of temperature given in \( \text{(5)} \) an expression for the average kinetic energy as a function of the temperature can be formulated:

\[ \langle E_c \rangle = \frac{3N}{2} k_B T T^{q-1}, \] (21)
which can be considered a $q$-generalization of the theorem of equipartition of energy. The extensive equation is straightforwardly recovered in the $q \to 1$ limit. Equation (21) can be used to calculate the microcanonical temperature during a simulation, but it suffers from the drawback of having an explicit dependence on $\Gamma$, an integral not usually employed directly in the field of MD. $\Gamma$ can be calculated, for a given set of parameters, from a numerical approximation of integral (18). Unfortunately, the complexity of this calculation grows exponentially with $N$ and the integrand is highly discontinuous, which may preclude microcanonical calculations for large systems in the Tsallis formalism. Furthermore, a magnitude which depends on the absolute entropy seems unphysical.

The equation for the pressure can be obtained by substituting (18) in (9) (taking into account for the derivation that both the limits and the integrand depend on $V$) and comparing with (6), which gives:

$$p = \frac{NT}{\Omega V} - \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle = \frac{2}{3} \frac{\langle E_c \rangle}{V} - \frac{1}{3V} \sum_i \left\langle \nabla_i U \cdot \tilde{r}_i \right\rangle. \quad (22)$$

By differentiating (6) with respect to $E$ and comparing it with the result of substituting $\chi = E_c^{-1} = \left[ E - U (\tilde{r}^N) \right]^{-1}$ into (20), one arrives at

$$\left( \frac{\partial \Omega}{\partial E} \right)_{V,N} = \Omega \left( \frac{3N}{2} - 1 \right) \langle E_c^{-1} \rangle,$$

and eq. (10) can be rewritten as

$$C_V = \left[ T \left( \frac{3Nq}{2 \langle E_c \rangle} - \left( \frac{3N}{2} - 1 \right) \langle E_c^{-1} \rangle \right) \right]^{-1}. \quad (23)$$

To calculate the next variable of interest, $\gamma$, there is only an ingredient lacking according to eq. (11), the partial derivative of $\Omega$ with respect to the volume. Using the same method as for the pressure, this parameter is found to be equal to

$$\left( \frac{\partial \Omega}{\partial V} \right)_{V,N} = \frac{N}{V} \left( \frac{3N}{2} - 1 \right) \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} E_c^{-1} \right\rangle,$$

so

$$\gamma = N - V \left( \frac{3N}{2} - 1 \right) \left[ p \langle E_c^{-1} \rangle + \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} E_c^{-1} \right\rangle \right]. \quad (24)$$

No new derivatives are needed to rewrite expression (13) for $\alpha_E$:

$$\alpha_E = \left[ VT \left( \frac{3Nq}{2 \langle E_c \rangle} + \left( \frac{3N}{2} - 1 \right) \left( \frac{\partial U}{\partial V} \right)_{E,N} E_c^{-1} \right) \right]^{-1}. \quad (25)$$

Finally, differentiating (18) two times with respect to volume
\[
\frac{1}{\Omega} \left( \frac{\partial^2 \Gamma}{\partial V^2} \right)_{E,N} = \frac{N p}{V} - \frac{2 \langle E_c \rangle}{3 V^2} + \frac{N}{V} \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle + \left\langle \left( \frac{\partial^2 U}{\partial V^2} \right)_{E,N} \right\rangle - \left( \frac{3N}{2} - 1 \right) \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N}^2 \right\rangle - E^{-1}
\]

which, after substitution in (14), gives the formula for \( B_E \):

\[
B_E = V \left[ \left( \frac{3N}{2} - 1 \right) \left( \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle - p \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle \right) - \frac{2 \langle E_c \rangle}{3 V^2} - \frac{N}{V} \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle - \left\langle \left( \frac{\partial^2 U}{\partial V^2} \right)_{E,N} \right\rangle \right] .
\]

(26)

Partial derivatives with respect to volume can easily be transcribed using gradients as it was done in eq. (22).

These particular expressions have been chosen so all of them except (21) are formally independent of \( \Gamma \); hence the only additional difficulty for a nonextensive simulation is the calculation of the temperature, which has already been discussed. All the formulae either are independent of \( q \), and thus valid also for the extensive case, or recover the SBG expression in the \( q \to 1 \) limit.

The ideal gas and other simple systems are often used as examples in textbooks because their phase-space volumes can be calculated analytically. In particular, for the perfect gas, it is possible to take \( U = 0 \), so \( E \geq 0 \) and the integrals over real space in the previous section become trivial:

\[
\Gamma = \frac{(2m\pi E)^{3N}}{h^{3N} \left( \frac{3N}{2} \right)!} V^N
\]

\[
\Omega = \frac{(2m\pi)^{3N} E^{2N} V^N}{h^{3N} \left( \frac{3N}{2} - 1 \right)!} ,
\]

results which can be substituted in eq. (11) to obtain the caloric equation of state:

\[
E = \left\{ \left( \frac{3N}{2} \right)^q k_B T \left[ \frac{(3N/2 - 1)!}{(2m\pi)^{3N/2} V^N} \right]^{q-1} \right\}^{\frac{1}{2(q-1)+1}} .
\]

(28)

Using (22) and (21), the thermal equation of state can likewise be obtained:

\[
p = \frac{N k_B T}{V} \left[ \frac{(2m\pi)^{3N}}{h^{3N} \left( \frac{3N}{2} \right)!} V^N \right]^{q-1} \left\{ \left( \frac{3N}{2} \right)^q k_B T \left[ \frac{(3N/2 - 1)!}{(2m\pi)^{3N/2} V^N} \right]^{q-1} \right\}^{\frac{q-1}{q+1}} .
\]

(29)
It is easy to see that as $q \to 1$ these equations tend to the well-known extensive ones. Important simplifications arise also when $N$ is large. These two limits, however, do not commute. More about this can be found in the canonical treatment by Abe in [5]. A different microcanonical treatment has been proposed by Parvan [6], who includes an extensive thermodynamical variable $\zeta = \frac{1}{q} - 1$ to the description of a system in order to recover the extensivity in the thermodynamic limit.

III. FORMULAE OBTAINED USING THE PHYSICAL TEMPERATURE

The consideration of the difficulty of obtaining $\Gamma$ by performing the integration in eq. (18) may suggest the idea of setting the system at a given temperature by putting it in contact with a thermostat before starting the microcanonical simulation, so both $T$ and $\langle E_c \rangle$ are known and $\Gamma$ can be calculated using eq. (21). However, this approach fails because the condition of thermal equilibrium between two systems does not imply that they are at the same temperature defined by eq. (5), as discussed by Abe et al. in Ref. [7]. Thus this definition can be rejected as unphysical. The correct physical temperature can easily be shown to be

$$T_{phys} = \left( 1 + \frac{1-q}{k_B S_q} \right) T = \Gamma^{1-q} T,$$  \hspace{1cm} (30)

which has as an immediate consequence, taking equations (5) and (21) into account, that this physical temperature, as a function of phase space integrals, is independent of $q$, as noted by Toral [8]. Thus, this temperature can be seen as the usual derivative of the Boltzmann entropy. This has led Gross [9] to conclude that the Boltzmann entropy is enough to describe every hamiltonian system at equilibrium, extensive or not. This conclusion has been disputed by Wang [10], and is not applicable to the aforementioned Parvan formalism [6]. However, a detailed discussion is clearly outside the objectives of this paper.

With this definition, the equipartition theorem recovers its familiar form:

$$T_{phys} = \frac{\Gamma}{k_B \Omega} \hspace{1cm} (31)$$

$$\langle E_c \rangle = \frac{3N}{2} k_B T_{phys}. \hspace{1cm} (32)$$
In particular, eq. (31) is identical to the one obtained using the SBG entropy. Thus, the expressions given by Pearson for the pressure, isocoric heat capacity and Grüneisen parameter, as well as the auxiliary variables $\alpha_E$ and $B_E$, or equivalently the $q \to 1$ ($T \to T_{phys}$) limits of the ones given in the previous section, are still valid:

\[
\begin{align*}
    p &= -\left( \frac{\partial E}{\partial V} \right)_{E,N} = \frac{Nk_B T_{phys}}{V} - \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle, \\
    C_{V,phys} &= \left( \frac{\partial E}{\partial T_{phys}} \right)_{V,N} = k_B \left[ \left( \frac{2}{3N} - 1 \right) \left\langle E_c \right\rangle \left\langle E_{c}^{-1} \right\rangle + 1 \right]^{-1}, \\
    \gamma &= V \left( \frac{\partial p}{\partial E} \right)_{V,N} = N - V \left( \frac{3N}{2} - 1 \right) \left[ p \left\langle E_{c}^{-1} \right\rangle + \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} E_{c}^{-1} \right\rangle \right], \\
    \alpha_{E,phys} &= \frac{1}{V} \left( \frac{\partial V}{\partial T_{phys}} \right)_{E,N} = \left[ VT_{phys} \left( \frac{3Np}{2\left\langle E_c \right\rangle} + \left( \frac{3N}{2} - 1 \right) \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} E_{c}^{-1} \right\rangle - \frac{N}{V} \right) \right]^{-1}, \\
    B_E &= -V \left( \frac{\partial p}{\partial V} \right)_{E,N} = V \left[ \left( \frac{3N}{2} - 1 \right) \left\langle \left( \frac{\partial^2 U}{\partial V^2} \right)_{E,N} E_{c}^{-1} \right\rangle - p \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} E_{c}^{-1} \right\rangle \right] \\
    &+ \frac{2}{3} \frac{\left\langle E_{c} \right\rangle}{V} \left\langle \left( \frac{\partial U}{\partial V} \right)_{E,N} \right\rangle - \left\langle \left( \frac{\partial^2 U}{\partial V^2} \right)_{E,N} \right\rangle.
\end{align*}
\]

The only obstacle to simply adopt all the extensive formulae is the definition of pressure as a derivative of entropy. To keep its physical meaning, the new definition of temperature requires that pressure is expressed as

\[
p = T \left( \frac{\partial S_q}{\partial V} \right)_{E,N} = \frac{T_{phys}}{1 + \frac{1}{k_B} S_q} \left( \frac{\partial S_q}{\partial V} \right)_{E,N},
\]

which means that derivatives involving both $T_{phys}$ and $p$ must be changed in order to reflect this fact. This affects thermodynamic equations (15), (16) and (17). Since $T_{phys}$ is a function of $S_q$ and $T$, it is easy to use the chain rule to relate the physical variables to the unphysical ones for which equations have already been developed in the previous section:
The thermodynamic behaviour of a system described by the Tsallis entropy has been studied in the microcanonical ensembles. Two possible definitions of temperature have been considered, resulting in two different sets of formulae. These microcanonical formulae can be used to obtain thermodynamic information (heat capacities, pressure, dilatation coefficients, etc.) from mechanical averages available during a MD simulation. However, if the first definition of temperature is used, which amounts to a direct generalization of the conventional one, these thermodynamic magnitudes depend on phase-space integrals which are not easily calculated. The second definition of temperature is designed to satisfy the zeroth law of thermodynamics and addresses this problem but only partially, returning some formulae to their extensive ($q = 1$) form. This is explained by the fact that the physical temperature is, for any value of $q$, a derivative of the SBG entropy, a relation clearly seen in the microcanonical formalism.

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