

# A Proposal of an Isothermal $q$ -EoS for Solids at High Pressures

*Uma Proposta de uma  $q$ -EoS Isotérmica para Sólidos em Altas Pressões*

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We present a new approach to the isothermal equation of state for solids when subjected to high pressures. The central point lies in the fact that the solid subjected to high pressures presents non-linear elastic behavior. We show how the connection between the  $q$ -deformed finite deformation theory and the mathematical formalism of Non-Extensive Statistical Mechanics, as postulated by Tsallis [1], allows us to achieve a  $q$ -deformed equation of state. We also establish the associated  $q$ -deformed interatomic potential and discuss its relation to the Grüneisen parameter.

**Keywords:** Isothermal EoS; Finite Strain; High Pressure; Solids.

Apresentamos uma nova abordagem para a equação de estado isotérmica para sólidos quando estão submetidos a altas pressões. A questão central reside no fato que um sólido submetido a altas pressões exibe um comportamento elástico não-linear. Mostramos como a conexão entre a teoria de deformação finita  $q$ -deformada e o formalismo matemático da Mecânica Estatística Não-Extensiva, proposta por Tsallis [1], nos permite alcançar uma equação de estado  $q$ -deformada. Também estabelecemos o potencial interatômico  $q$ -deformado associado e discutimos sua relação com o parâmetro de Grüneisen.

**Palavras-chaves:** EoS Isotérmica; Deformação Finita; Alta Pressão; Sólidos.

## I. A Brief Review of the Isothermal $EoS$ for Solids under High Pressure

The study of the behavior of solids when they are subjected to high or even extreme pressures has been of great interest in many research fields from Condensed Matter Physics to the Physics of the Earth's Interior. The works of several researchers [2]-[46] on these areas have shed light on crucial questions on this behavior for solids as well as other materials. One of the fundamental goals has been to achieve an isothermal equation of state ( $EoS$ ) capable of to describe the behavior of a wide class of known materials.

A theme from the elasticity theory, the solids under high pressure have been investigated since the precursor works of Lord Kelvin and A. Love [47; 48]. A disruption on the classical theory of elasticity began with the works of F. Murnaghan [49]-[51] who established a linear relation for the bulk modulus,

$B(P)$ . The classical theory of elasticity has two fundamental principles: (i) the deformations (strains) are uniquely determined by the stresses and are reversible, and (ii) the strains are limited to linear elasticity. The latter is removed when adopting the Finite Strain Theory (FST) [49]. Here the Murnaghan theory is established admitting that the initial stress is a large hydrostatic pressure. The first practical expressions for finite strains go back to the works of A.F. Birch [52]-[54]. In 1981 F. Stacey [4] made clear what is the fundamental assumption in FST: it is the formal relationship between the compression and the coordinate displacement [9].

A.F. Birch improved the Murnaghan theory of finite strain to study the compressibility of materials in Earth's interior, on its phases, lower mantle and outer core and he brought his equations of state of 2nd, 3rd, and 4th order [52]-[54]. It was A. Keane [55], after A.F. Birch, that shed light on the important role performed by the parameter  $B'_\infty$  in the description of the of solids subjected to very high pressures, as highlighted by F. Stacey [11].

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The bulk modulus,  $B$  (whose inverse is the compressibility,  $K$ ), can be deduced from an isothermal equation of state and this is a central result together its first,  $B'(P)$ , and second,  $B''(P)$ , derivatives for the elastic characterization of solids in very high pressures [56]. Over time, experiments made it possible to achieve ever higher pressures (present works in the literature report pressures so high as 1 TPa [57; 58]) and all three quantities ( $B_0$ ,  $B'_0$ ,  $B''_0$ ) have been obtained by the Seismological data from shock wave measurements using different techniques of measurements: static [5], ultrasonic [6; 59] and the model-independent infrared [18].

Recently, some authors [27; 32] have argued that a better approach to an isothermal equation of state could come from a relationship containing these three parameters ( $B_0$ ,  $B'_0$ , and  $B''_0$ ). Thus, the prospect is that proposals for *EoS* with three parameters could better describe the appropriate limit at high pressures. But, in this scheme, each advance in order needs a new parameter.

At the moment, the literature has been show a large number of proposals for isothermal equations of state, at least 36 equations are known [31; 42], and as highlighted by F. Stacey these are all empirical equations of state. Stacey himself makes a proposal [22] known as the reciprocal equation  $B'$  which has the expected asymptotic behavior, that is, the expected value for  $B'_\infty$ , although at low pressures this equation does not provide a good description of the pressure versus volume relationship.

F. Stacey enumerates three criteria [42] that any *EoS* must satisfy to be considered as a good proposal. We bring all of the three in the following. The first criterion is an algebraic identity,

$$\lim_{P \rightarrow \infty} P [B'(P)/B(P)] = 1, \quad (1)$$

which is based on the argument that in deep regions of the Earth, as the core and the lower mantle,  $B'(P)$  must be nearer of the value of  $B'_\infty$  than of  $B'_0$ . The second criterion is given by the thermodynamic limit (see the reference [22])

$$\lim_{P \rightarrow \infty} B'(P) \equiv B'_\infty > 5/3, \quad (2)$$

and the third criterion involves the asymptotic pressure limit for Grüneisen parameter [44],

$$\lim_{P \rightarrow \infty} \gamma(P) \equiv \gamma_\infty = (B'_\infty/2) - 1/6, \quad (3)$$

which is the Slater limit. We will demonstrate that our *q-EoS* satisfy all of the three relations above. We also will show that our purpose for the *q-EoS*

with two parameters is in completely agreement with the known data in the literature [10; 60].

When we consider solids under high pressure, we need to take into account the long-range interactions and this is one of the main features of the Non-Extensive Statistical Mechanics. The atoms becomes each time more closed one to another with the increasing of pressure, so the interaction among the first neighbors must be replaced by an interaction that also consider the atoms that were initially distant. Therefore, we have a nonlinear behavior of the physical system.

In Section II we revisit the Murnaghan *EoS* and rewrite his formulation by using the deformed *q*-Logarithm [1; 61; 62]. To do this, a crucial step is establish the relationship between the strain and the parameter *q*, and how the *q*-Logarithm function comes in to support this development. Therefore, this relationship carries the nonlinear condition of the theory considered here. The pressure, as expected, is a monotonically function of the relative volume *v*. Some of the relevant results of the formulation developed here appears on the relationships involving the parameter *q* with the first derivative of the bulk modulus at  $P = 0$ ,  $B'_0$ , as well as with its asymptotic value,  $B'_\infty$ . So, the *q* parameter depends on the value of  $B'_0$  and connects both regions of low and high pressure.

The knowledge of  $B_0$  and  $B'_0$  determines the *q* parameter that governs the *EoS*. So, the parameter *q* works as a *signature* for the specific behavior of a given solid when subjected to high pressures. This behavior also contains the tail power law and it is achieved in a direct way using the *EoS* written in the *q*-Exponential form.

Once established the general relationship between the strain and the parameter *q*, we seek the *q-EoS* with two parameters from the expansion of the Helmholtz free energy given as a function of power series of deformation in the Section III. The *q-EoS* so obtained now including a correction term that seeks to better describe the real behavior of solids under high pressures. Therefore, a second key concept in this work is the system energy as a function of the deformation.

The calculation of the bulk modulus and its derivatives (first and second) is carry out in the Subsection III.3. We present the results for the bulk modulus in the both limits: at the origin and at the asymptotic. Both limits are related with the parameter *q*. In turn, the asymptotic limit is obtained from a quadratic equation and its roots are related with the exponents in the interatomic potential. This is the goal of the Section IV. But, before

that, in the Subsection III.4, we bring the formulation for the new *EoS* expressed as a q-Deformed Exponential, i.e., we get an expression for  $v$  as a function of  $P$ . As previously commented, it is this form that the asymptotic behavior for the *EoS* exhibits the power tail law in the extreme pressure regime.

We follow with the approach of the interatomic potential in the Section IV. We show that the q-*EoS* can be obtained from an appropriate choosing of the interatomic potential. This potential has a form that resembles that one of the Mie potential, but now including the q-deformation parameter. From this relation the Lennard-Jones potential is encompassed, and also the Birch second order equation of state as well as the Ulmann and Pan'kov *EoS*.

A connection with the Grüneisen parameter is discussed in Section V. We consider the approach established by V.N. Zharkov and V.A. Kalinin [63] to get the formulations of Slater and that of Vashchenko-Zubarev in such a way to encompass the q-*EoS*. We show how this can be done through the associated q-deformed interatomic potential as well as how to get the parameters  $\gamma_0$  and  $\gamma_\infty$ .

The Section VI presents a comparison test for the new q-*EoS* with some *EoSs* known at literature to exhibits the performance of the q-*EoS*. We raise some considerations and perspectives of future works in Section VII.

**II. The Murnaghan's *EoS* in the Tsallis's q-Deformed Formulation**

We begin revisiting the isothermal *EoS* for high pressures as proposed by F. Murnaghan [49; 51]. Our goal is rewrite this equation by using the deformed q-Logarithm function as establish in references [1], [64]-[66]. To perform this, we recover the particular solution of the Bernoulli Differential Equation [67]-[69],

$$v^{(1-n)}(P) = (1 - n) [\kappa - A P] , \tag{4}$$

with  $n$  being a real number,  $v = V/V_0$  is the relative volume and the constant  $A$  attend to the inequality  $A > 0$ . As can be seen, we are left with three unknown parameters:  $n$ ,  $\kappa$  (dimensionless), and  $A$ . We must recover the initial volume,  $V_0$ , or the relative volume equal to unit, when  $P = 0$ , so

$$P \rightarrow 0 , v \rightarrow 1 \Rightarrow \kappa = (1 - n)^{-1} , \tag{5}$$

consequently, the equation (4) gives

$$-A P = \frac{v^{1-n} - 1}{1 - n} . \tag{6}$$

The expression on the right side of (6) can be identified with the definition of the q-Logarithm function [1; 62; 69]

$$\ln_q x \equiv \frac{x^{1-q} - 1}{1 - q} , \tag{7}$$

where  $q > 1$  and  $0 < x < 1$  characterizes the case of interest here. If we change  $n$  by  $q$  we get

$$P(v) = -(1/A) \ln_q v . \tag{8}$$

We highlight that the negative of q-Logarithm of the relative volume,  $v$ , is a monotonically increasing function, since  $0 < v \leq 1$  and  $q > 1$ . In this work we are assuming that the solid does not suffer a phase transition while the pressure is increasing.

The constant  $A$  in (8) can be determined from the definition of *Isothermal Bulk Modulus*

$$B_T \doteq -v \left( \frac{\partial P}{\partial v} \right) \Big|_{T=0} . \tag{9}$$

Thus, if we calculate the derivative above by using the definition of q-Logarithm in (7) then arises

$$B_T = \frac{1}{A} v^{1-q} = \frac{1}{A} [1 + (1 - q) \ln_q v] , \tag{10}$$

an expression whose value in the limit  $v \rightarrow 1$  (corresponding to  $P \rightarrow 0$ ) provides

$$B(0) \doteq B_0 = 1/A . \tag{11}$$

Therefore, we achieve the final expression for the Murnaghan *EoS* in the q-deformed form,

$$P(v) = B_0 (-\ln_q v) . \tag{12}$$

On the other hand, the bulk modulus gives

$$B_T(v) = B_0 v^{1-q} = B_0 [1 + (1 - q) \ln_q v] , \tag{13}$$

and from its first derivative immediately follows

$$\frac{\partial B_T}{\partial v} = (1 - q) B_0 v^{-q} = (1 - q) \frac{B_T(v)}{v} . \tag{14}$$

we notice that we can use the *EoS* itself to rewrite the bulk modulus in (13) and its first derivative in (14) now as functions of pressure

$$B_M(P) = B_0 + (q - 1) P , \tag{15}$$

$$B'_M(P) \doteq \frac{\partial B_M}{\partial P} = (q - 1) , \tag{16}$$

where the subscript  $M$  means the Murnaghan case. The equation (15) shows that the bulk modulus is a monotonically increasing function of pressure, and

being a smooth function we can calculate all their derivatives, but the first derivative already provides a constant value in the Murnaghan case.

The value of the asymptotic limit (the behavior when  $P$  goes to infinity) of  $B'_M$  is equal to  $B'_0$ ,

$$B'_0 = (q - 1) = B'_\infty, \tag{17}$$

so,  $B'_\infty$  is the value for the derivative of the bulk modulus in the asymptotic limit. By the other side, the second derivative of the bulk modulus just leaves the value zero,

$$B''_M(P) = 0. \tag{18}$$

It is a immediate result from relation (17) that the parameter  $q$  is given by

$$q = B'_0 + 1 = B'_\infty + 1. \tag{19}$$

Therefore, we can put (15) in following form

$$B_M(P) = B_0 + B'_0 P. \tag{20}$$

As expected, the bulk modulus a linear function of pressure as stated by F. Murnaghan [50]. The relation (19) shows the value of the parameter  $q$  expressed as a function of the elastic properties of the system under study,  $(B_0, B'_0)$ .

At this point, we want to bring another form for  $EoS$  in (12) establishing its inverse relation, that is, how  $v$  is a function of  $P$ . This inverse relation is precisely the  $q$ -Exponential function defined as

$$\exp_q x \equiv [1 + (1 - q)x]^{1/(1-q)}. \tag{21}$$

Consequently, applying (21) to the equation (12) we arrive at the desired function  $v(P)$ ,

$$v(P) = \exp_q(-P/B_0). \tag{22}$$

The above equation shows the behavior for relative volume as a monotonically decreasing function of pressure, with no cutoff, for  $q > 1$ , and equally important to mention is that the equation (22) brings, intrinsically, the power tail law. This asymptotic behavior [69] is explicitly given below by

$$\lim_{P \rightarrow \infty} v(P) \sim \left[ \frac{B_0}{(q-1)P} \right]^{1/B'_\infty}. \tag{23}$$

Then, we conclude that even for Murnaghan  $EoS$ , in the extreme pressure regime the relative volume function,  $v(P)$ , becomes a power law.

In the next section, we build an extension of Murnaghan equation in such a way that it encom-

passes the results from Birch-Murnaghan theory, that is, the second order Birch-Murnaghan equation and goes beyond.

### III. A Propose of a $q$ - $EoS$ with Two Parameters

An intense research has taken place in the last decades focusing on the searching for an isothermal  $EoS$  with three-parameter [4]-[70]. Apparently, one might think that there is a disadvantage of our proposal with respect to the other  $EoS$ s in literature, as the  $q$ - $EoS$  has only two parameter and we already know  $EoS$  with three parameters. But, in the Section VI we show that the  $q$ - $EoS$  exhibits a performance comparable to the Birch-Murnaghan third order  $EoS$ .

We generalize the results of the finite strain theory and build a relationship between the strain and the relative volume through the real parameter  $q$  ( $> 1$ ). Then, starting with the Helmholtz free energy, we will show that it is enough to admit terms up to second order in the power expansion of the deformation to get a simple but powerful equation of state that describes the behavior of a solid subjected to high, even extreme pressures.

#### III.1. The Theory of Finite Strain in the Tsallis's $q$ -Deformed Functions

Our starting point is the relation demonstrated by F. Murnaghan [51] and the practical expressions proposed by A. Birch [54] in 1952, between the ratio of volumes in the strained state,  $V$ , and the volume in the unstrained state,  $V_0$ , with the coordinate displacement [4; 9]

$$v \equiv \frac{V}{V_0} = (1 + 2\epsilon)^{3/2}, \tag{24}$$

where  $\epsilon$  is the strain. Since we are considering materials in compression the strains are positive, thus we redefine the strain  $f_L = -\epsilon$ , so

$$v = (1 - 2f_L)^{3/2}. \tag{25}$$

The relation in (25), as pointed by L. Knopoff [71; 72], is not the unique as many different relations can be proposed depending on the reference state which is chosen. As stated by the equation (25) we have the Lagrange strain, while if we choose

$$v = (1 + 2f_E)^{-3/2}, \tag{26}$$

then, we have the Euler strain. Now, we propose that the relations in (25) and (26) can be cast in a

single expression that encloses both the Euler and Lagrange strains, but not only these two values as well as all values in between so

$${}_s f = \left( v^{-s/3} - 1 \right), \tag{27}$$

therefore, now  $s$  is a real number. For  $s = -2$  we recover the Lagrange strain while for  $s = 2$  the Euler strain. We rewrite the relation (27) in connection with the Tsallis q-Logarithm as

$$-3 f(v) = \frac{v^{1-(1+s/3)} - 1}{1 - (1 + s/3)}. \tag{28}$$

So, let's defining

$$q = 1 + s/3, \tag{29}$$

then we reach the desired relation for  $f(v)$ ,

$$f(v) = - (1/3) \ln_q v. \tag{30}$$

The q-Logarithm is a monotonically increasing function of  $v > 0$ , without cutoff  $\forall q$ . When  $q = 0$ , the q-Logarithm reduces to linear functions, while in the limit for  $q = 1$  it becomes the ordinary logarithm function. If  $q > 1$ , then the function  $(\ln_q v)$  approaches asymptotically to  $1/(q - 1)$  (see reference [69] for more details). For  $s \in [-2, 0)$ , what it takes place, for example, for the Lagrange strain, then  $0 < q < 1$  and the q-Logarithm is a monotonically increasing function without cutoff. A summary of values for  $q$  to some known strains is presented in the Table I.

[ q ]	[ s ]	Asymptote	Strain
1/3	-2	no	Lagrange
2/3	-1	no	-
1	0	no	Hencky
4/3	1	yes	-
5/3	2	yes	Euler

TABLE I – This table shows the values for the parameter  $q$  corresponding to some strains  $s$ .

Throughout this work we assume that  $q > 1$ . The equation (30) is the main result in the next developments where the Helmholtz free energy is taking as the approach to establish the new q-EoS.

### III.2. The Isothermal EoS from Helmholtz Free Energy

An approach widely used to get an isothermal EoS for  $P(v)$  follows from the relation of pressure

with the Helmholtz free energy,  $\mathcal{F}$ ,

$$P(V) = - \left( \frac{\partial \mathcal{F}}{\partial V} \right)_T. \tag{31}$$

The Helmholtz free energy is builded as a power expansion of the deformation,  $f$ , and its convergence, as physically expected, is justified since the contributions from the terms of high powers in the expansion provide decreasing contributions [9]. In this way, the Helmholtz free energy expression is

$$\mathcal{F}(V) = \mathcal{F}_0 + a_1 f + \frac{1}{2} a_2 f^2 + \mathcal{O}(f^3), \tag{32}$$

where the constant term  $\mathcal{F}_0$  can be put equal zero because the absolute value of  $\mathcal{F}$  is arbitrary. On the other side, the coefficients  $a_1$  e  $a_2$  are given by

$$a_1 = \left( \frac{\partial \mathcal{F}}{\partial f} \right) \Big|_{V=V_0}, \quad a_2 = \frac{1}{2!} \left( \frac{\partial^2 \mathcal{F}}{\partial f^2} \right) \Big|_{V=V_0}. \tag{33}$$

If we consider the uncompressed state at  $V = V_0$  and  $P = 0$ , then the coefficient  $a_1$  is zero, so we are left with the quadratic term and upper power terms. In this work, we consider terms up to the second degree in (32), and as we will see, this is enough to generate an EoS that gives a good account the experimental data available in literature, while this does not constitute a limit to the degree, so

$$\mathcal{F}(V) \simeq (1/2) a_2 f^2(V). \tag{34}$$

The Isothermal EoS can be immediately obtained using the relation (31),

$$P(V) = a_2 f(\partial f / \partial V). \tag{35}$$

We rewrite the relation (35) as a function of the relative volume,  $v \doteq (V/V_0)$ , instead of the volume  $V$  itself. Then, the equation (35) turns into

$$P(v) = \frac{a_2}{V_0} f(v) \left( \frac{\partial f(v)}{\partial v} \right). \tag{36}$$

Now, we recover the relation (30) that connects the deformation with the q-Logarithm function to calculate the expression in (36), then

$$P(v) = - \left( \frac{a_2}{9V_0} \right) v^{-q} \ln_q v. \tag{37}$$

The constant  $a_2$  can be determined using the definition of isothermal bulk modulus,  $B_T$ , in (9), so

$$B_0 = - v \left( \frac{\partial P(v)}{\partial v} \right) \Big|_{T, v=1} \Rightarrow a_2 = 9B_0 V_0. \tag{38}$$

Substituting (38) in (37) we have reached the final form for the Isothermal q-*EoS* for high pressures

$$P(v) = B_0 v^{-q} (-\ln_q v). \quad (39)$$

Comparing (39) with the Murnaghan *EoS* in (12) we can see that the term  $v^{-q}$  in the first one brings a correction to the pressure that grows as the compression increases. So, it is expected that the q-*EoS* and Murnaghan *EoS* give different results for compressions above to 50% of the initial volume (see Figure 1). The q-*EoS* in (39) shows a performance very close to the Birch-Murnaghan third order *EoS* (see Section VI).

### III.3. The Expressions for the Bulk Modulus and Its Derivatives

Now, we calculate the expression for the isothermal bulk modulus,  $B_T$ , from the definition in (9) and taking the *EoS* given in (39), so we get

$$\left(\frac{\partial P}{\partial v}\right)_T = -(q/v)P(v) - B_0 v^{-2q}, \quad (40)$$

and then, we immediately have

$$B_T(v) = B_0 v^{-q} + (2q - 1)P(v). \quad (41)$$

There is an alternative expression for  $B_T$ . Since

$$v^{-q} = 1 - q \ln_{(q+1)} v, \quad (42)$$

we can rewrite the equation (41) as follow

$$B_T(v) = B_0 + (2q - 1)P(v) - qB_0 \ln_{(q+1)} v. \quad (43)$$

Both equations (42) and (43) show that  $B_T$  is a monotonically increasing function of pressure, besides when  $v \rightarrow 1$  (or equivalently,  $P \rightarrow 0$ )

$$B_T(v \rightarrow 1) = B_0. \quad (44)$$

Next, we calculate the derivative of (41),

$$\left(\frac{\partial B_T}{\partial v}\right) = (3q - 1) \left(\frac{\partial P}{\partial v}\right)_T + q(2q - 1) \frac{P}{v}, \quad (45)$$

and taking into account the result below,

$$(\partial B_T \partial v) = B'_T(P) (\partial P \partial v)_T, \quad (46)$$

we arrive at an expression for the derivative of the bulk modulus that depends only on quantities that are functions of pressure,  $P$ ,

$$B'_T(P) = (3q - 1) - q(2q - 1) \left(\frac{P}{B_T(P)}\right). \quad (47)$$

Two fundamental limits can be highlighted from (47), the first one is obtained when  $P \rightarrow 0$

$$B'_0 = (3q - 1). \quad (48)$$

The second one is the asymptotic limit ( $P \rightarrow \infty$ ) which leads to a quadratic equation for  $B'_\infty$ ,

$$[B'_\infty]^2 - (3q - 1)[B'_\infty] + q(2q - 1) = 0, \quad (49)$$

and whose roots are:

$$B'_\infty (+) = (2q - 1), \text{ and } B'_\infty (-) = q. \quad (50)$$

These two roots for  $B'_\infty$ , when we subtract the unity, give directly the exponents for the interatomic potential associated to the *EoS* under analysis (see Section IV)

$$(2q - 1) - 1, \text{ and } q - 1. \quad (51)$$

As we will see in the Section IV, the first root is related with the exponent of the repulsive part on the interatomic potential. So, in the regime of very high pressures it is this root that rules the asymptotic behavior for  $B'_\infty$ .

The relations (48) and (50) show that the proposed *EoS* actually is a two parameter equation of state as if we have  $B_0$  and  $B'_0$  or  $B_0$  and  $q$  all the other parameters are determined. On the other hand, with the identification in (48) and assuming  $B'_\infty = (2q - 1)$ , the equation (47) becomes

$$B'_T(P) = B'_0 - q B'_\infty \frac{P}{B_T(P)}. \quad (52)$$

Now, we search for the Stacey first criterion in (1). To get this, we rewrite (47) as follows

$$P \frac{B'_T(P)}{B_T(P)} = \frac{1}{qB'_\infty} (B'_0 - B'_T(P)) B'_T(P), \quad (53)$$

and taking the limit  $P \rightarrow \infty$  and considering the L'Hopital rule we recover the desired result in (1).

The Stacey second criterion imposes a lower boundary value to  $q$  parameter according to (50):

$$B'_\infty = 2q - 1 > 5/3 \Rightarrow q > 4/3. \quad (54)$$

The above result must be verified from the application of the q-*EoS* in (39) to real physical systems.

The second derivative of the bulk modulus,  $B''_T(P)$ , follows immediately

$$B''_T(P) = -q \frac{B'_\infty}{B_T(P)} \left[1 - P \frac{B'_T(P)}{B_T(P)}\right]. \quad (55)$$

From (55) we can obtain the relation:

$$[B'_T(P)]^2 + B_T(P) B''_T(P) = B'_0 B'_T(P) - q B'_\infty. \tag{56}$$

The previous relationship can be compared with its analog from Keane's equation [4; 55]. If we calculate the second derivative from Keane's *EoS* and take into account the equation (51), we get an expression that differs one to another only in the second term in the right side of (56). In the case of the Keane equation appears the full function given by  $-q B'_T(P)$ . A comparative of our *q-EoS* with some known equations of state in the literature will be discussed in the section IV.

Now, we back to the equation (56) and we analyse its limits. The first one is the limit at the origin

$$B''_0 = -q (B'_\infty/B_0), \tag{57}$$

which shows that the signal of  $B''_0$  is always negative unless  $B'_\infty$  changes its signal. In the other side, the asymptotic limit of (56) becomes

$$B''_\infty \simeq q (2q - 1)^2 \frac{P}{(B_\infty)^2} \rightarrow 0. \tag{58}$$

Therefore, the second derivative of the bulk modulus goes to zero at the infinity. The power law tail will be investigated in the next subsection.

### III.4. The Proposed *EoS* in Its q-Exponential Version

We begin the approach of the q-Exponential version from the differentiation of (39),

$$-(dP/B_0) = [-qv^{q-1} \ln_q v + v^{-2q}] dv, \tag{59}$$

and after some manipulation we obtain

$$\left[ -\frac{1}{B_0} + (2q - 1) \frac{P}{B_0 B_T(P)} \right] dP = v^{-q-1} dv. \tag{60}$$

The expression in (60) obeys Bernoulli's Non-linear differential equation as follows

$$(dv/dP) = Q(P) v^n, \tag{61}$$

where  $n = q + 1$  and the function  $Q(P)$  is

$$Q(P) = -\frac{1}{B_0} + (2q - 1) \frac{P}{B_0 B_T(P)}. \tag{62}$$

For a particular solution for equation (61) we have

$$v(P) = [1 - q g(P)]^{-1/q} \equiv \exp_{(q+1)}[-g(P)], \tag{63}$$

where the function  $g(P)$  has the form

$$g(P) = \int_0^P d\xi Q(\xi) = \frac{P}{B_0} - \frac{B'_\infty}{B_0} I(P), \tag{64}$$

and  $I(P)$  being the integral

$$I(P) = \int_0^P d\xi \frac{\xi}{B_T(\xi)}, \tag{65}$$

which can be calculated by using the relation in (47). Then, we get

$$I(P) = (1/qB'_\infty) [B_M(P) - B_T(P)], \tag{66}$$

where  $B_M(P)$  is the relation in (20). We see that the expression (66) has the correct limit, i.e., it leads to the Murnaghan result when  $B_T(P) = B_M(P)$ . Besides,  $I(P)$  turns completely known if we have  $B_T(P)$ . Therefore, the relation  $v(P)$  is

$$v(P) = \exp_{(q+1)} \left[ -\frac{P}{B_0} + \frac{1}{qB_0} (B_M(P) - B_T(P)) \right]. \tag{67}$$

A final point here is about the asymptotic form of equation (63), that is, how the power law tail arises in the high pressure regime. Following the same procedure as done in (23) we get

$$\lim_{P \rightarrow \infty} v(P) \sim \left[ \frac{(B_0/q)}{P + B_T(P) - B_M(P)} \right]^{1/q}. \tag{68}$$

Thus, to advance get an explicit expression for asymptotic limit of the function  $v(P)$  it is necessary a proposal for the bulk modulus  $B_T(P)$ .

Next, we establish another important connection of the proposed *EoS*. We present the appropriate interatomic potential that recover the equation of state given by equation (39).

### IV. The Interatomic Potential Associated with the Proposed *EoS*

So far, the connection we have established for the proposed *EoS* comes from Finite Strain Theory (TFS) together with the Helmholtz energy expansion. Next, we take the approach of interatomic potential and show how the *q-EoS* stems from as a specific form of the Mie interatomic potential (a two-body potential). First

$$\Phi(v) = -C_1(q) v^{-(q-1)} + C_2(q) v^{-2(q-1)}, \tag{69}$$

and remembering that (for cubic lattices, see [9]),

$$(a/r) = v^{-1/3}, \tag{70}$$

the interatomic potential can be rewritten

$$\Phi(r) = -C_1(q) \left(\frac{a}{r}\right)^{3(q-1)} + C_2(q) \left(\frac{a}{r}\right)^{6(q-1)}. \quad (71)$$

We proceed with the calculation of the *EoS* from the definition below

$$P(v) = -\frac{1}{V_0} \left(\frac{d\Phi}{dv}\right) = \frac{(1-q)}{V_0} [C_1(q)v^{-q} - 2C_2(q)v^{1-2q}]. \quad (72)$$

When, we are considering the limit  $P \rightarrow 0$ , or  $v \rightarrow 1$ , it comes up the relationship for the constants

$$C_1(q) = 2C_2(q). \quad (73)$$

The equation of state *EoS* takes the form

$$P(v) = (q-1)(C_1(q)/V_0)[v^{1-2q} - v^{-q}]. \quad (74)$$

On the other hand, the  $q$ -dependent constant,  $C_1$ , follows from the bulk modulus definition in (9)

$$C_1(q) = \frac{V_0 B_0}{(q-1)^2}. \quad (75)$$

Substituting (75) in (72) we achieve the  $q$ -*EoS*,

$$P(v) = B_0 v^{-q} (-\ln_q v). \quad (76)$$

Therefore, we precisely recover the expression for  $q$ -*EoS* in (39), as it was expected.

The interatomic potential in (71) exhibits a constrain between the exponents through the parameter  $q$ , precisely the exponent in the repulsive part is the double of the attractive part. In this way, the potential in (71) becomes the  $q$ -deformed Mie potential (we remember that  $q > 1$ ). If we take the following relations:

$$n_q/3 = 2(q-1), \quad \text{and} \quad m_q/3 = (q-1), \quad (77)$$

then, we can obtain the form for  $q$ -*EoS* derived from the  $q$ -deformed Mie potential,

$$P(v) = \frac{3B_0}{(n_q - m_q)} \left( v^{-(1+n_q/3)} - v^{-(1+m_q/3)} \right). \quad (78)$$

Some important fundamental potentials and *EoSs* known in the literature can be cast in this special form given by (78). We can cite, for example, the Lennard-Jones potential (which takes into account the *Van der Waals* interaction), the second-order Birch *EoS* and the Ulmann-Pan'Kov *EoS* [73].

The Table II shows the map of  $(q-1)$  values for some known interatomic potentials and *EoSs*,

according the relations in equation (77).

$(q-1)$	$m_q$	$n_q$	Potential or <i>EoS</i>
1/3	1	2	<i>Special Born-Mie</i>
2/3	2	4	<i>Second-order Birch</i>
2	6	12	<i>Lennard-Jones</i>
$> 1$	$m$	$2m$	<i>Ulmann and Pan'kov</i>

TABLE II – The map of values of  $q$  with the interatomic potentials and *EoSs*.

We rewrite the final form of the potential in (69) observing the result in (73)

$$\Phi(v) = \frac{V_0 B_0}{(q-1)^2} \left[ \frac{1}{2} v^{-2(q-1)} - v^{-(q-1)} \right]. \quad (79)$$

A brief discussion on the relation of the proposed  $q$ -*EoS* with the thermodynamical Grüneisen parameter,  $\gamma$ , it is the goal in the next section.

## V. The Grüneisen Parameter and Its Relation with the Proposed *EoS*

The last connection we establish here is related with the Grüneisen parameter, as it becomes known after the work of E. Grüneisen [74]. The Grüneisen parameter has been important since meaningful changes in density of solids take place in the regime of high pressures and temperatures [42], [75]-[89].

In particular, the *quasiharmonic* approximation in the high- and low-temperature limits yields the Mie-Grüneisen equation of state [63]. This equation of state has two terms:

$$P = P_{pot}(V) + \frac{\gamma}{V} E_{lv}, \quad (80)$$

where  $P_{pot}$  is the contribution to the pressure due to potential, called potential pressure, and depends only of the volume, while the second term is the energy of the lattice vibrations and the  $\gamma$  parameter compounds this part. To obtain the  $\gamma$  parameter from (80) it demands the knowledge of the contribution of energy due to lattice vibrations, what has been a hard task. Instead, we will resort the approximate formulations.

Three classical formulations that constitutes approximate methods and which have had an important impact on understanding of the Grüneisen parameter are the models due to J.C. Slater [75], J.S. Dugdale and D.K.C. MacDonald [76] (this approach was corrected by Rice, McQueen and Walsh [77]), and V.Y. Vashchenko and V.N. Zubarev [78], the latter known as the *Free Volume Approximation*.

Those classical approaches give the Grüneisen parameter as a function of the volume of system and the isothermal pressure,  $P_{pot}$ . A vibrational analysis based on the nature of the interatomic “spring” and the characteristic spatial measure of the lattice to compares the three above formulations and highlights their differences was done by Segletes [79], who showed that the empirical formulations builded on the shock Hugoniot data suffers from thermodynamics inconsistencies due to the decoupling of the mechanics of lattice compression.

Here we consider the Slater and Vashchenko-Zubarev formulas according to the Zharkov-Kalinin approach [63] and apply the new q-EoS to find out whether it is consistent with the result of these formulations, or whether new results emerge. The thermal Grüneisen parameter,  $\gamma_0$ , is defined by

$$\gamma_0 = V (\partial P / \partial \mathcal{U})_V, \tag{81}$$

where  $\mathcal{U}$  is the internal energy. From (81) we have

$$\gamma_T = V \left( \frac{\partial P}{\partial S} \right)_V \left( \frac{\partial S}{\partial \mathcal{U}} \right)_V. \tag{82}$$

Taking into account the Maxwell relation

$$(\partial P / \partial S)_V = - (\partial T / \partial V)_S, \tag{83}$$

we can rewrite (82) as

$$\gamma_T = - \frac{V}{T} \left( \frac{\partial T}{\partial V} \right)_S = - \left( \frac{\partial \ln T}{\partial \ln V} \right)_S. \tag{84}$$

This equation is fundamental in the study of adiabatic temperature gradient for the Geophysics of the interior of planets, specially the Earth [9]. Another interesting relation that can be obtained from (81), taking into account the definition

$$(\partial P / \partial T)_V = \alpha B_T, \tag{85}$$

where  $B_T$  is the isothermal bulk modulus and  $\alpha$  is the volume coefficient of thermal expansion, is

$$\gamma_T = \alpha V (B_T / C_V). \tag{86}$$

In (86),  $C_V$  is the specific heat at constant volume. The experimental data for the thermal expansion coefficient and the specific heat at high pressures are not yet accessible (as far as we know). For this reason, we can only use the equation (86) to determine the thermodynamic Grüneisen parameter at normal atmospheric pressure,  $\gamma_0$ .

Our goal is to use the q-EoS in (76) to find out whether the formulas for Slater approximation

and for Vashchenko-Zubarev Approximation hold the known results. For the Slater formula [9]

$$\gamma^{sl} = - \frac{V}{2} \frac{(\partial^2 P_{pot} / \partial V^2)}{(\partial P_{pot} / \partial V)} - \frac{2}{3}, \tag{87}$$

or using the new variable  $v$  we get

$$\gamma^{sl} = - \frac{v}{2} \frac{(\partial^2 P_{pot} / \partial v^2)}{(\partial P_{pot} / \partial v)} - \frac{2}{3}. \tag{88}$$

Taking the derivative of (88) and observing (76)

$$\left( \frac{\partial P_{pot}}{\partial v} \right) = - \left( \frac{B_T}{v} \right), \tag{89}$$

so, the second derivative follows

$$(\partial^2 P_{pot} / \partial v^2) = (B_T / v^2) (1 + B'_T (P)). \tag{90}$$

Substituting (89) and (90) in (88), we obtain

$$\gamma^{sl} (q, P) = (1/2) B'_T (P) - (1/6). \tag{91}$$

The above expression immediately allows to evaluate the two limits:  $P \rightarrow 0$  and  $P \rightarrow \infty$ . The first limit provides the value for  $\gamma_0^{sl}$

$$\gamma_0^{sl} = (3/2) q - 2/3 = (1/2) B'_0 - 1/6, \tag{92}$$

where we taking into account the relation in (48). The second limit is the asymptotic limit

$$\gamma_\infty^{sl} = q - 2/3 = (1/2) B'_\infty - 1/6. \tag{93}$$

Now, we consider the Vashchenko-Zubarev formula, also called the Free-Volume Approximation, which is given as a function of  $v$

$$\gamma^{vz} = - \frac{v}{2} \frac{(\partial^2 (P_{pot} v^{4/3}) / \partial v^2)}{(\partial (P_{pot} v^{4/3}) / \partial v)}. \tag{94}$$

Substituting  $P_{pot}$  in equation (76) we have

$$\gamma^{vz} (q, v) = - (1/6) + (1/2) \chi_1 (q, v), \tag{95}$$

where the function  $\chi_1 (q, v)$  is

$$\chi_1 (q, v) = \left( \frac{q-1}{3q-4} \right) \left[ \left( 1 - v^{(q-1)} \right) - 3 \right]^{-1}. \tag{96}$$

The result, observing (76), becomes

$$\left( \partial (P_{pot} v^{4/3}) / \partial v \right) = v^{1/3} [(4/3) P - B_T (P)], \tag{97}$$

while, for its second derivative with respect to  $v$

$$\left(\frac{\partial^2 (P_{pot} v^{4/3})}{\partial v^2}\right) = \frac{1}{3v} \left(\frac{\partial (P_{pot} v^{4/3})}{\partial v}\right) - v^{-2/3} B_T \left(\frac{4}{3} - B'_T\right). \quad (98)$$

The expression for  $\gamma^{vz}$  follows from (98) and (97)

$$\gamma^{vz}(q, P) = \frac{(\frac{1}{2}) B'_T - \frac{5}{6} + \frac{2}{9} (P/B_T)}{1 - \frac{4}{3} (P/B_T)}. \quad (99)$$

Thus, the corresponding limits to (92) and (93) are:

$$\gamma_0^{vz} = (1/2) B'_0 - (5/6) \quad , \quad (100)$$

$$\gamma_\infty^{vz} \doteq \gamma_\infty = (1/2) B'_\infty - (1/6) \quad . \quad (101)$$

Both limits have the expected results and for the asymptotic limit one has the Slater limit [75]. Therefore, the formulation of the  $q$ - $EoS$  encompasses the Stacey third criterion, that is, the Slater limit.

Physical Quantity	Relation with $q$
$q$ - $EoS$	$P(v) = B_0 v^{-q} (-\ln_q v)$
$B'_0$	$(3q - 1)$
$B'_\infty$	$(2q - 1)$
$B''_0$	$-q (B'_\infty/B_0)$
$\gamma^{vz}(q, P)$	Equation (99)
$\lambda(q, P)$	Equation (102)
$x(q, P)$	Equation (103)

TABLE III – All physical quantities related with the  $q$  parameter and calculated in this work.

In this point we recover the expression in (96) to determine the functions  $\lambda$  and  $x$  (this corresponds to the function  $q$  used by Stacey in his papers [29; 44]). The first one takes the form

$$\lambda = v \left(\frac{\partial \ln x}{\partial v}\right) = -\frac{1}{2} (B'_\infty - 1) \left[\frac{\eta + 1}{\mu} - 1 + \left(\frac{\eta}{\mu}\right) \frac{1 - (\eta/\mu)}{(2/3) \left(\frac{B'_0}{B'_\infty - 1}\right) + (\eta/\mu)}\right]. \quad (102)$$

For the function  $x$ , we get

$$x = v \left(\frac{\partial \ln \gamma}{\partial v}\right) = -\left(\frac{\eta}{\mu}\right) \left[\frac{1 - (\eta/\mu)}{(1/3) + (\eta/\mu)}\right], \quad (103)$$

where  $(\eta/\mu)$  is

$$(\eta/\mu) = \left[1 - \left(\frac{B'_0 - 3}{3B'_\infty + 2}\right) v^q - 1\right]^{-1}. \quad (104)$$

Now, we bring together all the physical quantities calculated until now and related with the parameter  $q$  and summarize them in the Table III.

### VI. Comparison of the $q$ - $EoS$ with Others $EoS$ s Known in the Literature

As mentioned in the Introduction, there exist, at least, thirty six proposals of equations of state for solids under high pressure. One of this compilation can be found in the reference [31]. Here, we chose three particular  $EoS$ s: Murnaghan (M), third-order Birch-Murnaghan, and Vinet (V) to compare their with our propose of the  $q$ - $EoS$ . This comparison is presented in the Figure 1.

The comparative graph was build for the functional metallic oxide  $MgO$  with the data being generated by each of the equations of state from the knowledge of the parameters  $B_0$  and  $B'_0$ . The proposed  $q$ - $EoS$  in (39), which is an equation of state with two parameters, exhibits a performance equivalent to the third-order Birch-Murnaghan  $EoS$ .

In the Table IV presents a first comparative characterization to some chosen solids from the values for the following parameters:  $q$ ,  $B'_\infty$ ,  $B''_0$ ,  $\gamma_0^{vz}$ ,  $\gamma_\infty$ ,  $x_0$  and  $\lambda_0$ .

### VII. Some Considerations and Discussions

We have shown how to obtain the  $q$ - $EoS$ , i.e., the  $q$ -deformed isothermal equation of state in (39) from a  $q$ -deformed finite strain theory and the free energy approach. This is the central result of this work, an  $EoS$  that seeks to describe the behavior of a solid subjected to high pressures and even ultra-high pressures. Yet, we also can relate this  $q$ - $EoS$  to an appropriated  $q$ -deformed interatomic potential, the  $q$ -deformed Mie interatomic potential, where the parameter  $q$  is a real number ( $q > 1$ ) and therefore this interatomic potential changes for different  $q$ 's. As we have seen, the  $q$ -deformed interatomic potential includes the special case of Lennard-Jones potential, but we have some other possible variances of that. We are still working on the consequences of this identification [90; 91].

Besides, the second order Birch-Murnaghan  $EoS$  as well as the Ullman-Pan'kov potential are equally obtained from the proposal of the  $q$ -interatomic potential in (79). The third-order Birch-Murnaghan  $EoS$  is not encompass in this scheme, but possibly the next order of  $q$ - $EoS$  could accomplish this.

As we demonstrate in this work, all of three Stacey criteria (1)-(3) are satisfied by the  $q$ - $EoS$  as well as by its associated interatomic potential.

In particular, the second criterion is entirely satisfied when we apply the q-EoS for elements and compounds as exemplified by the Table IV.

The goal of the next work is precisely to investigate the third order q-EoS and this work is in progress [92]. We search for an EoS that can perform equivalently, or even better, than third-order

Birch-Murnaghan EoS and without its limitations, such as the impossibility of assuming the value 4 for the first derivative of the bulk module. Maybe it be possible to build an q-EoS whose order,  $n$ , of the EoS itself functions as a parameter. There is also the generalization of the Mie potential itself. All these questions will be approached in future works.

Material	$B_0$	$B'_0$	q	$B'_\infty$	$B''_0$	$\gamma_0^{uz}$	$\gamma_\infty$	$x_0$	$\lambda_0$
$MgO^{(a)}$	160.64	4.35	1.78	2.57	-0.028	1.342	1.117	0.131	1.552
$NaCl^{(a)}$	23.70	5.14	2.05	3.09	-0.267	1.737	1.380	0.215	2.258
$Au^{(a)}$	160.44	6.56	2.52	4.04	-0.063	2.447	1.853	0.369	3.525
$CaO^{(b)}$	110.70	4.40	1.80	2.60	-0.042	1.367	1.133	0.137	1.597
$Al_2O_3^{(c)}$	254.40	4.28	1.76	2.52	-0.017	1.304	1.092	0.124	1.485

TABLE IV – The map of values for the parameters calculated from the knowledge of  $B_0$  (GPa) and  $B'_0$ . The parameter  $B''_0$  has units of  $(GPa)^{-1}$ . (a) T. Katsura, Y. Tange. Minerals **9**, (2019) [41]. (b) S. Speziale, S.R. Shieh, T.S. Duffy. J. Geophys. Research **111**, B02203 (2006). [35]. (c) T.J. Ahrens (Editor). Washington: American Geophysical Union (1995) [10].

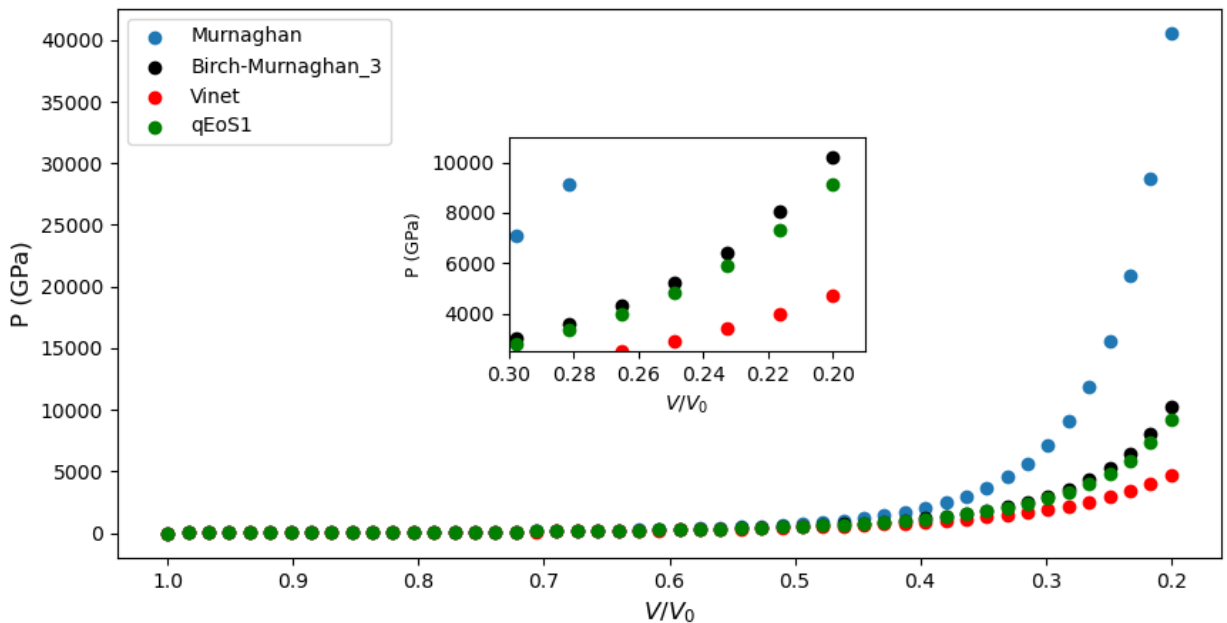


FIGURE 1 – A comparison of four equations of state for the metallic oxide  $MgO$ : Murnaghan (M), third-order Birch-Murnaghan (B-M(\_3)), Vinet (V), and the proposed q-EoS. The data are generated from the knowledge of  $B_0$  and  $B'_0$  for the  $MgO$  (see the reference [36]).

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