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A Three Parameter q-EoS for Solids under High Pressures

Uma q-EoS a Três Parâmetros para Sólidos sob Altas Pressões

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Here we generalize the main result obtained in the previous work [1], the q-EoS, to an arbitrary order n for a solid subjected to high pressures. It is the connection between the finite strain and the parameter q, this last in the context of the mathematical formulation of the Non-Extensive Statistical Mechanics as postulates by C. Tsallis [2], that allows to develop this approach. In the lines of the previous work, we determine the relationship with the q-deformed interatomic potential at order n. Also, we discuss the connection with the Grüneisen parameter.

Keywords: Isothermal EoS; Three Parameters; High Pressure; Solids.

Generalizamos aqui o principal resultado do trabalho anterior [1], a q-EoS, para uma ordem arbitrária n de um sólido submetido a altas pressões. É a conexão entre a deformação finita e o parâmetro q, este último no contexto da formulação matemática da Mecânica Estatística Não-Extensiva, como postulada por C. Tsallis [2], que permite desenvolver esta abordagem. Seguindo as linhas do trabalho anterior, determinamos a relação com o potencial interatômico q-deformado em ordem n. Também discutimos a conexão com o parâmetro de Grüneisen.

Palavras-chaves: EoS Isotérmica; Três Parâmetros; Alta Pressão; Sólidos.

I. Introduction

In a previous work [1], we show how the mathematical formulation of the Nonextensive Statistical Mechanics by Tsallis [2], [3]-[8] did lead us to establish a physical description for solids under high pressure. The Theory of Finite Strain [9]-[14] brought the fundamental connection with the q-deformation parameter and the expansion from the Helmholtz free energy did allow to achieve an isothermal q-Equation of State (from now on simply q-EoS). We retrieved the main result in the reference [1]:

$$\mathrm{P}\,(\upsilon) = \mathrm{B}_0\;\upsilon^{-\mathrm{q}}\;\left(-\ln_{\mathrm{q}}\upsilon\right)\;, \tag{1}$$

where B_0 is the bulk modulus at $\mathrm{P}=0$, q is the deformation parameter and $\upsilon = V/V_0$ is the relative volume. This q-EoS is an isothermal equation of state for the high pressure regime, with two parameters $(\mathrm{B}_0, \mathrm{B}_0')$ or equivalently $(\mathrm{B}_0, \mathrm{q})$. Other parameters, like the second derivative of bulk modulus, B_0'', are determined from the value taken by the parameter $\mathrm{q}\,(>1)$ as we shown in reference [1].

In this work, we follow the previous procedure to establish an equation of state for the next order (the contribution of the cubic term) of $\ln_{\mathrm{q}}\upsilon$ in the Helmholtz free energy expansion, and doing so, we obtain a q-EoS with three parameters: $(\mathrm{B}_0, \mathrm{B}_0', \mathrm{B}_0'')$, or equivalently $(\mathrm{B}_0, \mathrm{B}_0', \mathrm{q})$. The functional expression for this q-EoS maintains an analogy with the form of the third-order Birch-Murnaghan equation of state, as shown in the Section II.

The literature presents an increasing number of proposals of isothermal equations of state for solids at high pressure as has been compiled by F. Stacey [15; 16]. At least, a number of 36 EoSs are known in the literature and these EoS attempt to fit the experimental data and bring a description for the behaviour of solids under high pressure. F. Stacey also sets a proposal for an EoS known as the reciprocal B' equation (RKP) and it has the expected asymptotic behaviour, although at low pressures the equation does not present a good description for the relationship of pressure versus volume [17].

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We recover the connection between the strain and the q-deformed parameter in Section II. Continuing, in subsection II.2, we develop the proposal of an isothermal equation of state with three parameters using the Helmholtz free energy given as an expansion of the q-strain. This approach lead us to a *EoS* that resembles the third-order Birch-Murnaghan, but now in the context of the q-deformation. We continue with the calculation of the bulk modulus and their first and second derivatives in the Subsection II.2. However, as we will see, this approach exposes a loss of connection between the parameter q and the first derivative of the bulk modulus at zero pressure, B_0'. It is the expression for $B'(\upsilon)$ that reveals a way to restore the relationship between q and B_0' and this observation simplifies all calculations from then on.

After to calculate the function $B_T'(P)$ we present the results for the two limits of derivative of the bulk modulus: at origin and its asymptotic limit. The interesting point here is that the values for the asymptotic limit of function $B_T'(P)$ are still obtained from a quadratic equation for B_∞', precisely as it took place for the q-*EoS* with two parameters [1]. Besides, the roots from this quadratic equation maintain a relationship with the exponents in the q-deformed interatomic potential.

In the Section III we achieve the q-*EoS* at order n, an *EoS* with three parameters: B_0, q, and the order n. Besides, the result for B_∞' previously obtained brings up a question: does the proposal of q-*EoS* in order n (the Helmholtz free energy now includes terms until n) also leads to a quadratic equation for B_∞'? We carried out this investigation to recognizes the consequences of this quadratic equation and we find that the relationship between the parameter q and B_0' is kept valid even at order n.

The interatomic potential is builded as a two-body potential with an attractive part and a repulsive one. This is established in the Section IV. Also in this section, we show how the q-*EoS* can obtained from an appropriate chose of the interatomic potential and this last one maintains a correspondence with the general form of the Mie potential. Some known potentials in the literature are encompasses into the scheme of the q-interatomic potential and as an example we cite the Lennard-Jones potential and also certain equations of state like the Birch *EoS* and also the Bardeen *EoS*.

A connection with the Grüneisen parameter is worked out in the Section V. We start from the formulation of Vashchenko-Zubarev for Grüneisen parameter and demonstrate that the q-*EoS* has consistent with the *Free-Volume Approximation* and its limit at origin $\gamma_0\,(P \to 0)$ as well as with the asymptotic limit $\gamma_\infty\,(P \to \infty)$. We present an expression for γ^{vz} as a function of the relative volume, υ, that maintains a close analogy with the expression brought by Alt'shuler and Collaborators [18], and we can verify that the higher order of the q-*EoS* the better it is the description of the γ function.

We highlight that all the three Stacey criteria are still valid here in the context of the n-q-*EoS* in the limits discussed in the reference [1].

The Section VI presents some tests for the new n-q-*EoS*. In special, we show a table with the theoretical values obtained from the parameters B_0 and B_0'', as q, γ_0, γ_∞ among others, for some chosen materials and we bring a graphical comparative of the q-*EoS* with some *EoS*s known at literature. We make a few considerations in the Section VII and also some comments on the future of this research.

II. A Propose of a q-*EoS* with Three Parameters

An intense research has take place in the few last decades, focusing on the searching for an isothermal *EoS* with three-parameter that better describes the behaviour of solids under high pressures [19]-[67]. Among them, the works of P.B. Roy and S.B. Roy [49; 53] have justifying the necessity of an *EoS* with three parameters (B_0, B_0', B_0'') for a apropriate description of the solids in high pressures. In comparing their *EoS* with others known in the literature, they reported a difficulty with the accuracy of the available experimental data which had present very distinct values by different measure techniques (static measurement [27], ultrasonic [28] and the model-independent infrared [41]).

Starting from the expansion of the Helmholtz free energy as established in work [1], we take the next order in the expansion, that is, the third order of the strain, and build an equation of state that has three parameters and maintains a similarity with the third-order Birch-Murnaghan *EoS*.

We recall below the main relation established in reference [1] that connects the deformation with the q-Tsallis logarithm

$$-3\,f(\upsilon) = \frac{\upsilon^{1-(1+s/3)} - 1}{1-(1+s/3)}\ . \tag{2}$$

So, defining the Tsallis's q parameter as $q = 1+s/3$, and assuming that $q > 1$, we achieve to the desired result

$$f(\upsilon) = (1/3)\,(-\ln_q \upsilon)\ . \tag{3}$$

The q-Logarithm is a monotonically increasing function of υ, $\forall$ q. For q = 0, the q-Logarithm reduces to linear functions, while for the limit q $\to$ 1 it turns on the ordinary logarithm function.

When $\{s \in [-2, 0)\}$, what takes place, for example, in the Lagrangian strain, the q-Logarithm is a monotonically increasing function and for q > 1 it has an asymptote at $1/(q-1)$ (see reference [6] for more details).

The equation (3) is the central relation in the development where we take the Helmholtz free energy as the approach to get the new *EoS*. In the Table I we present the values for q to the parameter s for some known strains and its possible asymptotes.

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*.

In this work we assume that the parameter q > 1.

II.1. The Three Parameter *EoS* from Helmholtz Free Energy

We recover the approach established on paper [1] to get a three parameter q-*EoS* for $P(V)$ using the Helmholtz free energy, $\mathcal{F}$, from

$$P(V) = -\left(\frac{\partial \mathcal{F}}{\partial V}\right)_T . \quad (4)$$

The Helmholtz free energy is builded as a power expansion of the deformation, f, that is, a series of terms with alternating signs, then the third order term competes with the second order term, so there is not just an addition of contributions. The Helmholtz free energy expression is

$$\mathcal{F}(V) = \mathcal{F}_0 + a_1 f + \frac{1}{2!} a_2 f^2 + \frac{1}{3!} a_3 f^3 + \mathcal{O}\left(f^4\right), \quad (5)$$

where the constant term $\mathcal{F}_0$ can be put equal zero as the absolute value of $\mathcal{F}$ is arbitrary. Besides, the coefficient a_1 is zero in the equilibrium condition. So a_2 and a_3 are given by

$$a_2 = \frac{1}{2!}\left(\frac{\partial^2 \mathcal{F}}{\partial f^2}\right)\bigg|_{V_0}, \text{ and } a_3 = \frac{1}{3!}\left(\frac{\partial^3 \mathcal{F}}{\partial f^3}\right)\bigg|_{V_0}. \quad (6)$$

We taking terms up to order three in the expansion (5), and with this procedure we generate an *EoS* that gives account in a better way the experimental data available in literature. Therefore, it has

$$\mathcal{F}(V) \simeq (1/2)\, a_2 f^2(V) + (1/6)\, a_3 f^3(V). \quad (7)$$

The Isothermal q-*EoS* can be immediately written using the relation (4)

$$P(V) = a_2\, f\,(\partial f/\partial V) + (1/2)\, a_3\, f\,(\partial f/\partial V). \quad (8)$$

We rewrite the relation in (8) as a function of the relative volume, $\upsilon \doteq (V/V_0)$, instead of the volume V itself. So, the equation (8) turns into

$$P(\upsilon) = -\frac{2a_2}{V_0}\, f(\upsilon)\left(\frac{\partial f(\upsilon)}{\partial \upsilon}\right)\left[1 + \frac{3a_3}{2a_2} f(\upsilon)\right]. \quad (9)$$

Now, we recover the relationship (3) that connects the deformation with the q-Logarithm function to calculate the expression in (9)

$$P(\upsilon) = \frac{2a_2}{9V_0}\, \upsilon^{-q}\, (-\ln_q \upsilon)\left[1 + \frac{a_3}{2a_2}(-\ln_q \upsilon)\right]. \quad (10)$$

The constant a_2 can be determined using the definition of the *Isothermal Bulk Modulus*

$$B_T(\upsilon) = -\,\upsilon\left(\frac{\partial P(\upsilon)}{\partial \upsilon}\right)\bigg|_{T,\upsilon=1}, \quad (11)$$

and taking the initial condition: $\upsilon = 1$ (corresponding to $P = 0$), we get the constant a_2

$$a_2 = (9/2)\, V_0 B_0 . \quad (12)$$

The Isothermal q-*EoS* in (10) becomes

$$P(\upsilon) = B_0\, \upsilon^{-q}\, (-\ln_q \upsilon)\left[1 + \frac{a_3}{9V_0B_0}(-\ln_q \upsilon)\right], \quad (13)$$

while the expression for $B(\upsilon)$ is

$$B(\upsilon) = B_0 \upsilon^{-q}\left[-\left(\frac{a_3}{27V_0B_0}\right) q\, \upsilon^{1-2q}(-\ln_q \upsilon) + [1 + (2q-1)(-\ln_q \upsilon)]\left(1 + \frac{a_3}{2a_2}(-\ln_q \upsilon)\right)\right].$$

The constant a_3 follows from the derivative of the bulk modulus, $B'(\upsilon)$, observing the relation below

$$B'_T(P) = -1 - \upsilon\, \frac{\left(\partial^2 P/\partial \upsilon^2\right)_T}{(\partial P/\partial \upsilon)_T}. \quad (14)$$

Calculating the second derivative and taking the limit $P \to 0$, one gets

$$a_3 = (9/2)\, V_0 B_0\, [B'_0 - (3q-1)]. \quad (15)$$

Then, we achieve the form for the third order q-*EoS*,

$$\mathrm{P}\,(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}}\ \left(-\ln_{\mathrm{q}}\upsilon\right)\left(1-\delta\left(-\ln_q\upsilon\right)\right), \quad (16)$$

where the parameter δ is

$$\delta = -\left(1/2\right)\left[\mathrm{B}_0' - \left(3\mathrm{q}-1\right)\right]. \quad (17)$$

As we can see, the presence of δ undoubtedly excludes a possible relationship between B_0' and q, and thus we lose the analagous relationship established in reference [1]. In fact, this result reveals a behavior for the q-*EoS* that resembles that one for the third-order Birch-Murnaghan *EoS*.

We list the expressions for the first and second derivatives of $\mathrm{P}\,(\upsilon)$ in order to facilitate obtaining the first derivative of the bulk modulus, B_{T}',

$$\left(\frac{\partial \mathrm{P}}{\partial \upsilon}\right)_{\mathrm{T}} = -\mathrm{B}_0\upsilon^{-2\mathrm{q}}\Lambda_1\left(\upsilon\right), \quad (18)$$

$$\left(\frac{\partial^2 \mathrm{P}}{\partial \upsilon^2}\right)_{\mathrm{T}} = \mathrm{B}_0\upsilon^{-2\mathrm{q}}\left[\left(\frac{2\mathrm{q}}{\upsilon}\right)\Lambda_1 - \left(\frac{\partial\Lambda_1}{\partial\upsilon}\right)\right]. \quad (19)$$

where for the function Λ_1

$$\Lambda_1\left(\upsilon\right) = 1 - 2\delta\left(-ln_{\mathrm{q}}\upsilon\right) + \left(\mathrm{q}/\mathrm{B}_0\right)\upsilon^{2\mathrm{q}-1}\mathrm{P}\left(\upsilon\right). \quad (20)$$

Therefore, we can rewriting (14) as

$$\mathrm{B}_{\mathrm{T}}'\left(\upsilon\right) = \left(2\mathrm{q}-1\right) - \frac{\partial \ln\Lambda_1\left(\upsilon\right)}{\partial\ln\upsilon}. \quad (21)$$

We show the calculation of the bulk modulus and their derivatives with some detail in the next.

II.2. The Bulk Modulus and Its Derivatives

An immediate expression for the bulk modulus, B, comes up when we substitute (18) in its definition in (11)

$$\mathrm{B}_{\mathrm{T}}\left(\upsilon\right) = \mathrm{B}_0\upsilon^{1-2\mathrm{q}}\Lambda_1\left(\upsilon\right), \quad (22)$$

with $\Lambda_1\left(\upsilon\right)$ is given by (20). Carrying on some manipulations we can achieve a very interesting alternative form for the bulk modulus

$$\mathrm{B}_{\mathrm{T}}\left(\upsilon\right) = \left(3\mathrm{q}-2\right)\mathrm{P}\left(\upsilon\right) + \Lambda_2\left(\upsilon\right)\mathrm{B}_0\upsilon^{-\mathrm{q}}, \quad (23)$$

where the function $\Lambda_2\left(\upsilon\right)$ is

$$\Lambda_2\left(\upsilon\right) = 1 + \left[\mathrm{B}_0' - 2\left(2\mathrm{q}-1\right)\right]\left(-\ln_{\mathrm{q}}\upsilon\right). \quad (24)$$

The function $\Lambda_2\left(\upsilon\right)$ reveals a surprising possibility: we can to recover the relationship between q and B_0' if we chose

$$\mathrm{B}_0' = 2\left(2\mathrm{q}-1\right). \quad (25)$$

This arbitrariness does not take place with the relation in (17), because such a choice would did turn null the contribution of the term a_3 itself. The consequences of the choice in (25) is worked out in detail in the next section when we calculate a general expression for the isothermal *EoS* at order n.

The equations (22) and (23) show that the isothermal bulk modulus, B_{T}, is a monotonically increasing function of the relative volume. Besides when $\upsilon \to 1$ (corresponding to $\mathrm{P} \to 0$)

$$\mathrm{B}\left(\upsilon \to 1\right) = \mathrm{B}_0. \quad (26)$$

Next, we calculate the first derivative of Eq.(23) taking into account the relation in (25)

$$\left(\frac{\partial \mathrm{B}_{\mathrm{T}}}{\partial \upsilon}\right) = -\mathrm{B}_0'\ \frac{\mathrm{B}_{\mathrm{T}}}{\upsilon} + \mathrm{q}\left(3\mathrm{q}-2\right)\frac{\mathrm{P}\left(\upsilon\right)}{\upsilon}, \quad (27)$$

and making use of the variable transformation $\upsilon \to \mathrm{P}$ in the first derivative, we get

$$\left(\frac{\partial \mathrm{B}_{\mathrm{T}}}{\partial \mathrm{P}}\right) \doteq \mathrm{B}_{\mathrm{T}}'\left(\mathrm{P}\right) = \mathrm{B}_0' - \mathrm{q}\left(3\mathrm{q}-2\right)\frac{\mathrm{P}}{\mathrm{B}_{\mathrm{T}}\left(\mathrm{P}\right)}. \quad (28)$$

The expression for $\mathrm{B}_{\mathrm{T}}'\left(\mathrm{P}\right)$ is ready for an analysis of its asymptotic limit ($\mathrm{P} \to \infty$) (or equivalently, $\upsilon \to 0$). This leads to a quadratic equation for B_∞'

$$\left[\mathrm{B}_\infty'\right]^2 - 2\left(2\mathrm{q}-1\right)\left[\mathrm{B}_\infty'\right] + \mathrm{q}\left(3\mathrm{q}-2\right) = 0, \quad (29)$$

whose two roots are:

$$\mathrm{B}_{\infty\,(+)}' = \left(3\mathrm{q}-2\right), \text{ and } \mathrm{B}_{\infty\,(-)}' = \mathrm{q}. \quad (30)$$

These two roots for B_∞' are related to the exponents in the interatomic potential associated with *EoS* (see section IV). In the regime of high pressures is the largest root (in the repulsive part of the interatomic potential), that governs the asymptotic behavior for $\mathrm{B}_{\mathrm{T}}'\left(\mathrm{P}\right)$. The second derivative of the bulk modulus, $\mathrm{B}_{\mathrm{T}}''\left(\mathrm{P}\right)$, follows from equation (28)

$$\mathrm{B}_{\mathrm{T}}\left(\mathrm{P}\right)\mathrm{B}_{\mathrm{T}}''\left(\mathrm{P}\right) = -\mathrm{q}\mathrm{B}_\infty'\left(1 - \frac{\mathrm{B}_{\mathrm{T}}'\left(\mathrm{P}\right)}{\mathrm{B}_{\mathrm{T}}\left(\mathrm{P}\right)}\,\mathrm{P}\right), \quad (31)$$

or even, making use of equation (28)

$$\left[\mathrm{B}_{\mathrm{T}}'\left(\mathrm{P}\right)\right]^2 + \mathrm{B}_{\mathrm{T}}\left(\mathrm{P}\right)\mathrm{B}_{\mathrm{T}}''\left(\mathrm{P}\right) = \mathrm{B}_0'\mathrm{B}_{\mathrm{T}}'\left(\mathrm{P}\right) - \mathrm{q}\mathrm{B}_\infty'. \quad (32)$$

In the limit $\mathrm{P} \to 0$, we find the parameter B_0'' as

$$\mathrm{B}_0'' = -\mathrm{q}\left(\mathrm{B}_\infty'/\mathrm{B}_0\right). \quad (33)$$

Initially, the q-*EoS* established in (16) is a three parameter *EoS* since to know it completely is necessary to provide the values of B_0, B_0' and B_0'', or

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equivalently, B_0, B_0', and q. But, the relation in (25) reduces it to an *EoS* with two parameters.

The formulation presented here raises a central question: is the quadratic equation for the parameter B_∞' a general result even in high orders of the q-*EoS*? If the answer is yes, the order of the q-*EoS* will works as the third parameter $(\mathrm{B}_0, \mathrm{q}, n)$, and the associated interatomic potential could be build from the two roots of the quadratic equation for B_∞' as powers of υ. These facts lead us to investigate in detail a general expression for q-*EoS*.

III. The Isothermal q-*EoS* in Order n

The results obtained in the paper [1] and those in equations (29) and (30) have suggested that the quadratic equation for B_∞' is a general result even in order n. If we assume that the expansion for the Helmholtz free energy now includes terms on $\mathrm{f}(\upsilon)$ up to the order n (we are in the nonlinear behaviour when high pressures take place on the solid), then the q-*EoS* in (16) takes on the general form

$$\mathrm{P}(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}} \sum_{j=1}^{n} \delta_j^{(n)} \left(-\ln_q \upsilon\right)^j , \tag{34}$$

with the condition $\delta_1^{(n)} = 1$. The expression in (34) comes from the expansion in (5) when it is generalized to order n. The value of n defines the order of the q-*EoS*. So, for $n = 1$ we get the first order

$$\mathrm{P}(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}} \left(-\ln_q \upsilon\right), \tag{35}$$

which gives the q-*EoS* with two parameters $(\mathrm{B}_0, \mathrm{B}_0')$, or equivalently, $(\mathrm{q}, \mathrm{B}_0)$. This equation of state was the subject of study in the paper [1].

In turn, now assuming $n = 2$ in equation (34), we recover the q-*EoS* in (16) with three parameters, which is the second order q-*EoS*

$$\mathrm{P}(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}} \left[\delta_1^{(2)} \left(-\ln_q \upsilon\right) + \delta_2^{(2)} \left(-\ln_q \upsilon\right)^2\right], \tag{36}$$

where $\delta_2^{(2)} = \delta$ in (17). Substituting the definition for $\ln_\mathrm{q} \upsilon$ in (36) we have

$$\begin{aligned} \mathrm{P}(\upsilon) \ =\ & \frac{\mathrm{B}_0\ \upsilon^{-\mathrm{q}}}{(\mathrm{q}-1)^2} \left[\delta_2^{(2)} \upsilon^{2-2\mathrm{q}} + \left(\delta_2^{(2)} - (\mathrm{q}-1)\right)\right. \\ & + \left.\left((\mathrm{q}-1) - 2\delta_2^{(2)}\right) \upsilon^{1-\mathrm{q}}\right]. \end{aligned} \tag{37}$$

Since we have a freedom of choice, the coefficient of the last term in (37) can be equated to zero, so

$$\delta_2^{(2)} = (1/2)\,(\mathrm{q}-1)\,. \tag{38}$$

The condition in (38) restates the relationship between B_0' and q. From equation (17) we obtain

$$\mathrm{B}_0' = 2\,(2\mathrm{q}-1)\,. \tag{39}$$

Therefore, the second order q-*EoS* in (37) reduces to an *EoS* with two parameters and only the first two terms remain (precisely, the roots of the quadratic equation for B_∞'). Then, the expression for the second order q-*EoS* is

$$\mathrm{P}(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}} \ \left(-\ln_{(2\mathrm{q}-1)} \upsilon\right)\ . \tag{40}$$

We now develop the expression of $\mathrm{P}(\upsilon)$ for $n = 3$ and in this case we get two equations for the δ's

$$(i) \quad (\mathrm{q}-1)\,\delta_2^{(3)} - 3\delta_3^{(3)} = 0, \tag{41}$$

$$(ii) \quad 3\delta_3^{(3)} - 2\,(\mathrm{q}-1)\,\delta_2^{(3)} + (\mathrm{q}-1)^2 = 0, \tag{42}$$

whose solution leads to the q-*EoS* as

$$\mathrm{P}(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}} \ \left(-\ln_{(3\mathrm{q}-2)} \upsilon\right)\ . \tag{43}$$

In turn, for $n = 4$ the calculation brings a q-*EoS* with three relations involving the δ's

$$(i) \qquad (\mathrm{q}-1)\,\delta_3^{(4)} - 4\delta_4^{(4)} = 0, \tag{44}$$

$$(ii) \qquad 6\delta_4^{(4)} - 3\,(\mathrm{q}-1)\,\delta_3^{(4)} + (\mathrm{q}-1)^2\,\delta_2^{(4)} = 0, \tag{45}$$

$$\begin{aligned} (iii) \qquad & -4\delta_4^{(4)} + 3\,(\mathrm{q}-1)\,\delta_3^{(4)} - 2\,(\mathrm{q}-1)^2\,\delta_2^{(4)} \\ & + (\mathrm{q}-1)^3 = 0. \end{aligned} \tag{46}$$

Thus, when we take a given order n and using the previous argument, we can achieve a general expression for the coefficients in equation (34)

$$\delta_j^{(n)} = \frac{(n-1)!}{j!\,(n-j)!}\,(\mathrm{q}-1)^{j-1}\ , \tag{47}$$

with $j = 1, 2, 3, \ldots, n$. If we substitute (47) in the equation (34) we obtain the q-*EoS* of order n

$$\mathrm{P}(\upsilon) = \mathrm{B}_0\ \upsilon^{-\mathrm{q}} \left(-\ln_{\mathrm{q}^\star} \upsilon\right)\ , \tag{48}$$

where $\mathrm{q}^\star = n\mathrm{q} - (n-1)$. In its general form, the q-*EoS* in (34) has three parameters: B_0, q, and the order n. But, if we choose a given order, then the equation of state reduces to one with two parameters $(\mathrm{B}_0, \mathrm{B}_0')$.

From equation (48) we highlight the following points: (a) the equations in (35), (40) and (43), they induce a search for an expression of q-*EoS* in order n, (b) the functional form for the q-*EoS* maintains a close similarity with that one for the first order, $n = 1$, and (c) in this new functional form for $\mathrm{P}(\upsilon)$ we recover the relationship between B_0' and q.

An immediate question that arises from this section is: what does the order n in q-*EoS* mean? As we have seen, when $n = 2$ we obtain an *EoS* that has a performance equivalent to the third-order Birch-Murnaghan *EoS* (see Figure 1 on the left) and the former has no problem assuming the value 4 as a possible value for its first derivative of the bulk modulus, $B(P)$, something that does not happen with the third-order Birch-Murnaghan *EoS*.

The treatment of the interatomic potential in the section IV will shed light on the physical meaning of the order n. As we will see, the order n increases the magnitude of the repulsive part in the new q-deformed Mie potential.

Before that, we establish in the next the formulas for the bulk modulus and its first and second derivatives assuming the n-q-*EoS*.

III.1. The Bulk Modulus and Its Derivatives from the *EoS* at Order n

Now, we calculate the expressions for the first and second derivatives of the Bulk Modulus from the q-*EoS* at order n in (48), we get

$$\mathrm{B}_{\mathrm{T}}^{(n)}(v) = [(n+1)\,\mathrm{q} - n]\,\mathrm{P}(v) + \mathrm{B}_0 v^{-\mathrm{q}} \;, \quad (49)$$

and developing the first derivative we obtain

$$\left(\frac{\partial \mathrm{B}_{\mathrm{T}}^{(n)}}{\partial v}\right) = [(n+2)\,\mathrm{q} - n]\left(\frac{\partial \mathrm{P}}{\partial v}\right)_{\mathrm{T}} + \mathrm{q}\,[(n+1)\,\mathrm{q} - n]\,(\mathrm{P}(v)/v) \;. \quad (50)$$

The next step is to make a change of variable, $v \to \mathrm{P}$, in the function $\left(\partial \mathrm{B}_{\mathrm{T}}^{(n)}/\partial v\right)$, so

$$\mathrm{B}_{\mathrm{T}}'^{(n)}(\mathrm{P}) = [(n+2)\,\mathrm{q} - n] - \mathrm{q}\,[(n+1)\,\mathrm{q} - n]\left(\mathrm{P}/\mathrm{B}_{\mathrm{T}}^{(n)}(\mathrm{P})\right) \quad (51)$$

Then, for $\mathrm{P} = 0$ we find $\mathrm{B}_0'^{(n)}$ to any order n

$$\mathrm{B}_0'^{(n)} = (n+2)\,\mathrm{q} - n, \quad (52)$$

while for the asymptotic limit $\mathrm{P} \to \infty$ we achieve a quadratic equation for $\mathrm{B}_\infty'^{(n)}$ from (51)

$$\left[\mathrm{B}_\infty'^{(n)}\right]^2 + b\left[\mathrm{B}_\infty'^{(n)}\right] + c = 0, \quad (53)$$

where $b = -(n+2)\,\mathrm{q} + n$ and $c = \mathrm{q}\,[(n+1)\,\mathrm{q} - n]$. The two distinct roots of the quadratic equation above are the possible values for $\mathrm{B}_\infty'^{(n)}$

$$\mathrm{B}_{\infty\,[+]}'^{(n)} = n\,(\mathrm{q}-1) + \mathrm{q} \;, \quad \text{and} \quad \mathrm{B}_{\infty\,[-]}'^{(n)} = \mathrm{q}. \quad (54)$$

As we had highlighted in the paper [1], the root $\mathrm{B}_{\infty\,[+]}'^{(n)}$ governs the behaviour of a solid in high pressures. It is the repulsive part of potential that maintains the stability of solid. Thus, we designate now the root $\mathrm{B}_{\infty\,[+]}'^{(n)}$ simply by $\mathrm{B}_\infty'^{(n)}$. We proceed with the calculation of the second derivative of $\mathrm{B}_{\mathrm{T}}^{(n)}(\mathrm{P})$

$$\mathrm{B}_{\mathrm{T}}^{(n)}(\mathrm{P})\,\mathrm{B}_{\mathrm{T}}''^{(n)}(\mathrm{P}) = -\mathrm{q}\,[(n+1)\,\mathrm{q} - n] \times \left(1 - \frac{\mathrm{B}_{\mathrm{T}}'^{(n)}(\mathrm{P})}{\mathrm{B}_{\mathrm{T}}^{(n)}(\mathrm{P})}\,\mathrm{P}\right). \quad (55)$$

Assuming $\mathrm{P} = 0$ we get the expression for $\mathrm{B}_0''^{(n)}$

$$\mathrm{B}_0''^{(n)} = -\mathrm{q}\left(\mathrm{B}_\infty'^{(n)}/\mathrm{B}_0\right) \;. \quad (56)$$

Since q and B_0 are positive quantities, the sign of $\mathrm{B}_0''^{(n)}$ is completely defined by the sign of $\mathrm{B}_\infty'^{(n)}$.

The equation (55) can be written in an alternative form if we substitute the equation for $\mathrm{B}_{\mathrm{T}}'(\mathrm{P})$ as given by (51) into (55), therefore

$$\left[\mathrm{B}_{\mathrm{T}}'^{(n)}\right]^2 + \mathrm{B}_{\mathrm{T}}^{(n)}\mathrm{B}_{\mathrm{T}}''^{(n)} = \mathrm{B}_0'^{(n)}\mathrm{B}_{\mathrm{T}}'^{(n)} - \mathrm{q}\mathrm{B}_\infty'^{(n)} \;. \quad (57)$$

As was done in paper [1], the equation (57) can be compared with the Keane equation [19]. Even at order n, the difference between (57) and Keane equation relies on the last term. For the Keane equation appears the complete function $\mathrm{B}_{\mathrm{T}}'^{(n)}$ itself.

We show the relationship between the q-interatomic potential and the roots of $\mathrm{B}_\infty'^{(n)}$ in (54) in the next section.

IV. The Interatomic Potential Associated with the Proposed n-q-*EoS*

Here, we intent to establish the interatomic potential, $\Phi(v)$, associated with the n-q-*EoS* in (48). The starting point is the expression below

$$\Phi(v) = \Phi_0 + V_0\mathrm{B}_0\sum_{j=1}^{n}\frac{\delta_j^{(n)}}{(j+1)}\,(-\ln_{\mathrm{q}} v)^{j+1} \;, \quad (58)$$

and substituting (47) for $\delta_j^{(n)}$ in (58) and choosing

$$\Phi_0 = -\frac{V_0\mathrm{B}_0}{(n+1)\,(\mathrm{q}-1)^2}, \quad (59)$$

we get the expression for $\Phi(v)$

$$\Phi(v) = \frac{V_0\mathrm{B}_0}{n\,(\mathrm{q}-1)^2}\left[\frac{1}{(n+1)}v^{(n+1)(1-\mathrm{q})} - v^{(1-\mathrm{q})}\right]. \quad (60)$$

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Since $(a/\mathrm{r}) = \upsilon^{-1/3}$ is valid for cubic lattices [32], the q-deformed interatomic potential turns in

$$\Phi(\mathrm{r}) = \frac{V_0 \mathrm{B}_0}{n(\mathrm{q}-1)^2} \left[\frac{1}{(n+1)} \left(\frac{a}{\mathrm{r}}\right)^{3(n+1)(\mathrm{q}-1)} - \left(\frac{a}{\mathrm{r}}\right)^{3(\mathrm{q}-1)} \right] . \quad (61)$$

Assuming the following identities

$$n_{\mathrm{q}}/3 = (n+1)(\mathrm{q}-1)\,, \text{ and } m_{\mathrm{q}}/3 = (\mathrm{q}-1)\,, \quad (62)$$

the potential $\Phi(\mathrm{r})$, in the Mie form, becomes

$$\Phi(\mathrm{r}) = \frac{9a^3 \mathrm{B}_0}{m_{\mathrm{q}}(n_{\mathrm{q}} - m_{\mathrm{q}})} \left[\left(\frac{m_{\mathrm{q}}}{n_{\mathrm{q}}}\right) \left(\frac{a}{\mathrm{r}}\right)^{n_{\mathrm{q}}} - \left(\frac{a}{\mathrm{r}}\right)^{m_{\mathrm{q}}} \right] . \quad (63)$$

Also, substituting the two relations in (62) into the equation (60) and performing the derivative with respect to υ, we get the n-q-*EoS* expressed as a function of the parameters m_{q} and n_{q}

$$\mathrm{P}(\upsilon) = \frac{3\mathrm{B}_0}{(n_{\mathrm{q}} - m_{\mathrm{q}})} \left(\upsilon^{-(1+n_{\mathrm{q}}/3)} - \upsilon^{-(1+m_{\mathrm{q}}/3)} \right) . \quad (64)$$

The interatomic potential in (60) shows that the exponent in the repulsive part is $(n+1)$ times greater than that the attractive part. Since, $\mathrm{q} > 1$ (is a real number), the potential in (63) generalizes to a certain extent the Mie potential [1].

The Table II presents a map of equivalences for the n-q-*EoS* and some interatomic potentials and *EoS*s known in the literature. In particular, the second-order q-*EoS* entirely encompass the third-order Birch-Murnaghan *EoS*.

n	$\mathrm{q}^\star$	**Potential or EoS**
1	4/3	*Special Born-Mie*
1	5/3	*Birch's 2nd Order EoS*
1	3	*Lennard-Jones*
1	> 2	*Ulmann and Pan'kov*
2	$2\mathrm{q} - 1$	*Birch's 3rd Order EoS* [68]
2	4/3	*Bardeen EoS* [69]

TABLE II – The values for the order n and the parameter $\mathrm{q}^\star = n\mathrm{q} - (n-1)$, $(\mathrm{q} > 1)$, for some interatomic potentials and EoSs.

As can be seen, if one increases the order of the *EoS* then it will possibly encompasses other equations of state, since these equations can be put in the form of the q-deformed Mie potential.

As we comment at end of the section III, the expression for the interatomic potential in (60) shows that the order n changes the repulsive part in such a way that it becomes increasingly larger as n increases. Therefore, the order n determines how strong the contribution of the repulsive part is.

V. The Grüneisen Parameter and Its Relation with the Proposed n-q-*EoS*

Now, we discuss a connection between the q-*EoS* at order n with the Grüneisen parameter [70]. We focus on the approximation method from V.Y. Vashchenko and V.N. Zubarev [71], also known as *the Free-Volume Approximation*.

The inclusion of the temperature for a complete description of the solid in high pressures is an essential point, for example, in the description of geophysics of Earth interior. The Grüneisen parameter takes into account the contribution to pressure due to the energy of lattice vibrations, but implementing this has proven to be a complex task [72]-[87].

Here, we follow the ideas of Zharkov and Kalinin [76] and remember that the *quasi-harmonic approximation* yields so in high- as in low-temperatures the Mie-Grüneisen equation of state

$$\mathrm{P} = \Phi_{\mathrm{pot}}(V) + \gamma\,(E_{\mathrm{k}}/V)\,. \quad (65)$$

The first term in (65) takes into account the pressure due to the potential and depends only on the volume, while the second one comes up from the lattice vibrations and depends on the energy, E_{k}. Yet, this last contribution increases when the temperature increases, so the second term will compete in importance with the first one in the regime of high temperatures.

The pressure is entirely defined by the first contribution in the context of an isothermal *EoS* $(\mathrm{T} = 0)$. We use γ as a function of V [76] as obtained by Vashchenko and Zubarev [71] in the *Free-Volume Approximation* (vibrations of atoms in a spherically symmetrical field of their neighbors), so

$$\gamma^{vz} = -\frac{V}{2} \frac{\left[\partial^2 \left(\Phi_{\mathrm{pot}} V^{4/3}\right) / \partial V^2\right]}{\left[\partial \left(\Phi_{\mathrm{pot}} V^{4/3}\right) / \partial V\right]} . \quad (66)$$

Assuming that $\Phi_{\mathrm{pot}}(\upsilon)$ is given by (48), we get

$$\gamma^{vz} = -\frac{\upsilon}{2} \frac{\mathrm{d}}{\mathrm{d}\upsilon} \left\{ \ln \left[\upsilon^{1/3} \mathrm{B}_{\mathrm{T}}(\upsilon) \left(\frac{4}{3} \frac{\mathrm{P}(\upsilon)}{\mathrm{B}_{\mathrm{T}}} - 1 \right) \right] \right\} , \quad (67)$$

where we use the relation (49). Make a few manipulation in equation (67) we obtain for γ^{vz}

$$\gamma^{vz} = \frac{\frac{1}{2}\mathrm{B}'_{\mathrm{T}} - \frac{5}{6} - \frac{2}{9}(\mathrm{P}/\mathrm{B}_{\mathrm{T}})}{1 - \frac{4}{3}(\mathrm{P}/\mathrm{B}_{\mathrm{T}})} . \quad (68)$$

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Quantity	**Relationship with** q
n-q-*EoS*	$\mathrm{P}(\upsilon) = \mathrm{B}_0\upsilon^{-\mathrm{q}}(-\ln_{\mathrm{q}^\star}\upsilon)$
$\mathrm{B}_0'^{\,(n)}$	$(n+2)\,\mathrm{q} - n$
$\mathrm{B}_\infty'^{\,(n)}$	$n\,(\mathrm{q}-1) + \mathrm{q}$
$\mathrm{B}_0''^{\,(n)}$	$-\mathrm{q}\left(\mathrm{B}_\infty'^{\,(n)}/\mathrm{B}_0\right)$
$\gamma^{vz}(\mathrm{q},\mathrm{P})$	Equation (75)
$\gamma_0^{vz\,(n)}$	$(1/2)\,\mathrm{B}_0'^{\,(n)} - (5/6)$
$\gamma_\infty^{(n)}$	$(1/2)\,\mathrm{B}_\infty'^{\,(n)} - (1/6)$

TABLE III – The table summarizes all the relationships among the physical quantities calculated in this work and the q parameter. The parameter $\mathrm{q}^\star$ is defined by: $\mathrm{q}^\star = n\mathrm{q} - (n-1)$.

The expression in (68) shows that the q-*EoS* at order n maintains the known result for γ in the Free-Volume Approximation. Thus, the limits of γ^{vz} in (68) when $\mathrm{P}=0$ and $\mathrm{P}\to\infty$ stay valid

$$\gamma_0^{vz\,(n)} = (1/2)\,\mathrm{B}_0'^{\,(n)} - (5/6)\ , \qquad (69)$$
$$\gamma_\infty^{vz\,(n)} = \gamma_\infty^{(n)} = (1/2)\,\mathrm{B}_\infty'^{\,(n)} - (1/6)\ . \qquad (70)$$

Now, we bring the expression for γ^{vz} as an explicit function of q and υ to build a bridge with the equation proposed by Al'tshuler and Collaborators [18]. Developing equation (68) with the explicit υ dependence, we achieve

$$\gamma^{vz} = (1/6)\,(3\mathrm{q}-1) + (1/2)\,n\,(\mathrm{q}-1)\,\chi_n(\mathrm{q},\upsilon)\,, \qquad (71)$$

where the function $\chi(\mathrm{q},\upsilon)$ is given by

$$\chi_n(\mathrm{q},\upsilon) = \left[\eta_n/\mu_n(\mathrm{q},\upsilon)\right]\ , \qquad (72)$$
$$\eta_n = (n+1)\,\mathrm{q} - (n + (4/3))\,, \qquad (73)$$
$$\mu_n - \eta_n = \left[(4/3) - \mathrm{q}\right]\upsilon^{n(\mathrm{q}-1)}\ . \qquad (74)$$

From expression (71) we can fitting the behaviour for $\gamma(\mathrm{q},\upsilon)$ with the relative volume and compare this result with that obtained in [18]. To get this, first, we rewrite $\gamma(\mathrm{q},\upsilon)$ as below

$$\gamma^{vz}(\mathrm{q},\upsilon) = \gamma_\infty^{(n)} + (1/2)\,n\,(\mathrm{q}-1)\left[\chi_n(\mathrm{q},\upsilon) - 1\right], \qquad (75)$$

and using the relation

$$\left(\gamma_0^{vz\,(n)} - \gamma_\infty^{(n)}\right) = (1/2)\,\mathrm{q} + 2/3\ , \qquad (76)$$

we are led to the following expression

$$\gamma^{vz}(\mathrm{q},\upsilon) = \gamma_\infty^{(n)} + n\left[\left(\gamma_0^{vz\,(n)} - \gamma_\infty^{(n)}\right) + 1/6\right]\times \times\ \left[\chi_n(\mathrm{q},\upsilon) - 1\right]\ . \qquad (77)$$

Since the part that depends of the relative volume in (77) is entirely contained in the term $[\chi_n(\mathrm{q},\upsilon) - 1]$, the difference between the equation (77) and its correspondent expression from Al'tshuler and Collaborators [18] relies on the presence of the factors n and (1/6) in equation (77).

In the next section we carry on some tests for the q-*EoS* at order n, as given by equation (48).

VI. Comparision of the n-q-*EoS* with Other *EoS*s in the Literature

As a first task, we build a graphic comparison with certain equations of state: Murnaghan, third-order Birch-Murnaghan, and Vinet universal *EoS*. We can do it fitting from the known data for B_0 and B_0' in the literature, as well as we can building the curves of P versus υ from the accessible data in handbooks at the literature [88]-[90].

The fit in Figure 1 is based on the data available in the reference [63]. As we can see the q-*EoS* at order $n=2$ already presents the exact performance of the third-order Birch-Murnaghan *EoS*, but it is the q-*EoS*s at order $n \geq 3$ that exhibits a better performance than the latter. Since we can choose the best order in the q-*EoS* to describe a given material, we can do an optimization to find what the best order is for the better fit. This possibility, as far as we known is unique in the literature.

In turn, the Tables IV and V present for some chosen solids the values for the following parameters: $\mathrm{B}_0'^{\,(2)}$, $\mathrm{B}_\infty'^{\,(2)}$, $\mathrm{B}_0''^{\,(2)}$, $\gamma_0^{vz\,(2)}$ and $\gamma_\infty^{(2)}$, as functions of q and B_0.

VII. Some Final Considerations

The connection established between the general form of the strain and the parameter q, based on the mathematical approach of the Nonextensive Statistical Mechanics, allows us to build an isothermal equation of state, the q-*EoS*, that has showing a very proper performance in describes the behavior of solids when subjected to high pressures [1].

We advance in development and obtain a generalization of the previous formulation now with the q-*EoS* at order n. The latter is an equation of state now involving three parameters: q, B_0 and the order n. When the order is specified it turns into a q-*EoS* with two parameters $(\mathrm{B}_0, \mathrm{B}_0')$. The performance of this equation of state has been shown to be equivalent to that of third-order Birch-Murnaghan and outperforms the latter when $n \geq 3$ (see the right side of Figure 1).

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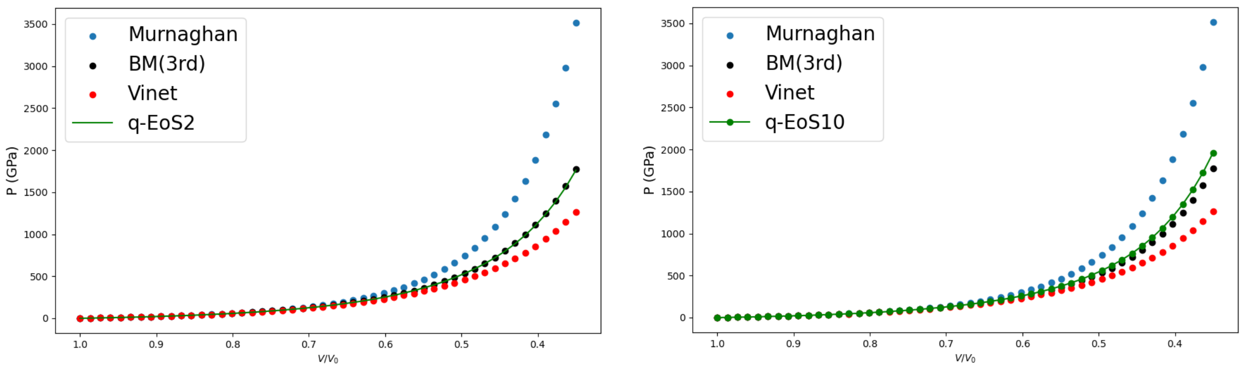

FIGURE 1 – A comparison of four equations of state for the metallic oxide *MgO*: Murnaghan (M), third-order Birch-Murnaghan (B-M(3rd)), Vinet (V), and the proposed q-*EoS* for the order $n = 2$, at left side, and for the order $n = 10$ at right side. The data are generated from the parameters B_0 and B'_0 [58].

Material	B_0	B'_0	q	$B'^{(2)}_\infty$	$B''^{(2)}_0$	$\gamma^{vz\,(2)}_0$	$\gamma^{(2)}_\infty$
MgO$^{(a)}$	160.64	4.35	1.59	2.76	−0.027	1.342	1.215
NaCl$^{(a)}$	23.70	5.14	1.78	3.35	−0.253	1.737	1.511
CaO$^{(b)}$	110.70	4.40	1.60	2.80	−0.040	1.367	1.233
Au$^{(a)}$	160.44	6.56	2.14	4.42	−0.059	2.447	2.043
Ar$^{(c)}$	2.86	7.20	2.30	4.90	−3.941	2.767	2.283
$\boldsymbol{Al_2O_3}^{(c)}$	254.40	4.28	1.57	2.71	−0.017	1.307	1.188

TABLE IV – The map of values for the parameters calculated from the knowledge of B_0 (GPa) and B'_0 using the q-*EoS* at order $n = 2$. The parameter B''_0 has unit of $(\text{GPa})^{-1}$. (*a*) T. Katsura, Y. Tange. Minerals **9**, (2019) [63]. (*b*) S. Speziale, S.R. Shieh, T.S. Duffy. J. Geophys. Research **111**, B02203 (2006). [56]. (*c*) T.J. Ahrens (Editor). Washington: American Geophysical Union (1995) [33].

Material	B_0	B'_0	q	$B'^{(10)}_\infty$	$B''^{(10)}_0$	$\gamma^{vz\,(10)}_0$	$\gamma^{(10)}_\infty$
MgO$^{(a)}$	160.64	4.35	1.20	3.15	−0.023	1.342	1.410
NaCl$^{(a)}$	23.70	5.14	1.26	3.88	−0.206	1.737	1.773
CaO$^{(b)}$	110.70	4.40	1.20	3.20	−0.035	1.367	1.433
Au$^{(a)}$	160.44	6.56	1.38	5.18	−0.045	2.447	2.423
Ar$^{(c)}$	2.86	7.20	1.43	5.77	−2.890	2.767	2.717
$\boldsymbol{Al_2O_3}^{(c)}$	254.40	4.28	1.19	3.09	−0.014	1.307	1.378

TABLE V – The map of values for the parameters calculated from the knowledge of B_0 (GPa) and B'_0 using the q-*EoS* at order $n = 10$. The parameter B''_0 has unit of $(\text{GPa})^{-1}$. (*a*) T. Katsura, Y. Tange. Minerals **9**, (2019) [63]. (*b*) S. Speziale, S.R. Shieh, T.S. Duffy. J. Geophys. Research **111**, B02203 (2006). [56]. (*c*) T.J. Ahrens (Editor). Washington: American Geophysical Union (1995) [33].

We need to extend the application of the n-q-*EoS* to the molecular and covalent crystals as well as to other types of materials to know its behavior at extreme pressures, but the tests carried out to date with the available pressure and volume data of solids have proven to be very promising [91].

From the disposal data at literature we believe that for a given order the n-q-*EoS* can provide an appropriate description for any solid, but this is a task for future works.

Besides, we also find the interatomic potential associated to the n-q-*EoS*. This n-q-deformed potential belongs to the class of the Mie interatomic potential and generalizes the purpose established in the first paper [1]. The n-q-deformed potential contains, as a special case, the q-deformed Lennard-Jones (L-J) potential which so generalizes the usual L-J potential, the latter is the cornerstone of modern developments in Molecular Dynamics (MD). We are still working on the consequences of this important result [92].

Another important point is to get an explicit form to the bulk modulus as a function of pressure, B (P) [93]. This will allows to develop a definitive comparison with the Stacey RKP equation [17] and at the same time a comparison with the several equations of state known at literature.

Finally, the performance of the n-q-*EoS* for a wide class of materials and for pressures as high as 1 TPa from *ab initio* calculations are works in progress. The latter will be reported shortly [94].

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