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Determination of Elastic Coefficients of Solids Using Pade Approximation Method

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Abstract

The present work employs the Pade Approximation, a technique widely applied across mathematics, physics and engineering to reduce complicated systems to a manageable form. Its wide acceptance rests on the fact that, in comparison with conventional methods, it reproduces complicated functions with markedly greater accuracy and numerical stability. Here an equation of state is obtained by examining the way energy, pressure and volume are interrelated and by applying the Pade Approximation to the pressure. The volume–pressure law was first treated theoretically by Lowdin and co-workers, who showed that it is accurate only in the low-pressure regime. To bring the description closer to the exact result they replaced the pressure power series by its Pade approximant.

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INTRODUCTION

The Pade approximation is used in a great variety of numerical tasks: solving differential equations, performing analytic continuation of power series, handling orthogonal polynomials and rational approximations, evaluating Gaussian quadratures, accelerating convergence, computing special functions, and locating the singularities, zeros, roots and poles of a series. A large proportion of the solutions of ordinary and partial differential equations appear as power series, since numerical treatment of such equations usually proceeds through approximation or truncation. These series are commonly represented by polynomials, yet polynomials are prone to oscillate and may thereby introduce sizeable errors, while their singular behaviour cannot be clearly discerned within a finite region of the plane [1]. An equation of state emerges once the interrelation between energy, pressure and volume is examined together with a Pade approximation for the pressure. Over a sequence of papers Borelius [2-7] has, across these works, empirically obtained an equation of state for solids that can be cast in reduced form

$$P_B = \frac{X}{1-X} \tag{1}$$

Where $P_B = \frac{P}{\alpha}$

and

$$X = \frac{\Delta V}{\beta}$$

Here P denotes the applied hydrostatic pressure, Δ V the accompanying change in volume, α and β are material constants of the solid, referred to respectively as its internal pressure and free volume.

A theoretical treatment of the volume–pressure law was given by Lowdin *et al*. [8] starting from the relations

$$E = f(V) \tag{2}$$

and

$$P = \frac{\partial E}{\partial V} \tag{3}$$

Writing both the energy and the pressure as infinite Taylor series in $\Delta V = V - V_0$ and keeping the (1,0) Pade approximant, which corresponds to the geometric-series form of the pressure series P, Lowdin *et al.* [8] obtained a volume–pressure law coinciding with the Borelius law [2]. This relation, however, holds only at low pressures. To improve agreement with the exact result they adopted the (1,1) Pade approximant for the pressure series, thereby introducing a third dimensionless parameter into the volume–pressure law, which in reduced form reads

$$P_B = X + \frac{X^2}{1-\gamma X} \tag{4}$$

This result is called the LCH law. For the particular value γ = 1, equation (4) reduces to the Borelius law of equation (1). Thakur [9] carried the Pade approximation one step further and proposed a modified volume–pressure law of the form.

$$P = X + X^2[1 - \ln(1-\gamma X)] \tag{5}$$

This form was found to describe the data better than either the Borelius law (1) or the LCH law (4).

Tiwari *et al*. [10] modified the above laws as follows –

Expanding the function (2) as a Taylor series in $\Delta V = V - V_0$ around the point $V = V_0$ one obtains

$$E = \sum_{n=0}^{\infty} \frac{{f_0}^{(n)}}{n} (\Delta V)^n \tag{6}$$

$$E = -\sum_{n=0}^{\infty} \frac{{f_0}^{(n+1)}}{n} (\Delta V)^n \tag{7}$$

Equation (7) is the exact form of the volume–pressure law. Since at equilibrium $f_0' = +0$, we introduce the further definitions

$$f_0'' = \frac{\alpha}{\beta} \tag{8}$$

$$f_0''' = \frac{2\alpha}{\beta^2}$$

The higher-order derivatives (n ≥ 2) may be generated from

$${f_0}^{(n)} = (-1)^n \gamma_n \frac{(n-1)!\alpha}{\beta^{n-1}} \tag{9}$$

in which the coefficients γ_n are dimensionless. In the special case one has $\gamma_2 = \gamma_3 = 1$, and in general

$$\gamma_n = \frac{2^{n-2} (f_0)^{n-3} f_0^n}{(n-1)!\,(f_0)^{n-2}} \tag{10}$$

Equation (8) then gives

$$\alpha = \frac{-2(f_0'')^2}{(f_0')} \text{ and } \beta = \frac{-2f_0''}{f_0'''} \tag{11}$$

Combining equations (7) and (9) leads to

$$P = \alpha \sum_{n=1}^{\infty} \gamma_{n+1} - (\frac{\Delta V}{\beta})^n \tag{12}$$

The power series (12) can be recast as

$$P_B = \frac{P}{\alpha} = X + X^2 + \gamma_4 X^3 + \gamma_5 X^3 \tag{13}$$

Applying the first Pade approximation, which requires

$$\gamma_4 = \gamma_5 = \text{----------} = \gamma_n \tag{14}$$

to equation (12) reproduces the Borelius law (1). Taking the second Pade approximation, for which

$$\begin{bmatrix} \gamma_n = \gamma \\ \gamma_5 = \gamma^2 \\ \gamma_6 = \gamma^3 \end{bmatrix} \quad (15)$$

in equation (12) yields the LCH law (4). Proceeding to the next Pade approximation, which requires

$$\begin{bmatrix} \gamma_4 = \gamma \\ \gamma_5 = \frac{\gamma^2}{2} \\ \gamma_6 = \frac{\gamma^3}{3} \end{bmatrix} \quad (16)$$

gives the modified law (5) of Thakur. The convergence of the modified law (5) improves as one moves successively through the Pade approximations (14) and (16).

The reduced Variables

It is helpful to work with dimensionless reduced variables. Following Lowdin *et al*. [8], the lattice energy $-E_0$ and equilibrium volume V_0 of the solid are adopted as the units of energy and volume, and are used throughout the treatment of the solid in its various forms. For the unit of pressure we introduce

$$P_r = -\frac{E_0}{V_0} \quad (17)$$

termed the reference pressure. The reduced variables, distinguished characterized by a subscript, are then defined as

$$\begin{bmatrix} E_1 = -\frac{E}{E_0} \\ P_1 = -\frac{P}{P_0} \\ \Delta V_1 = \frac{\Delta V}{V_0} \end{bmatrix} \quad (18)$$

The reduced compressibility K_1 is then given by

$$\frac{1}{K_1} = \frac{1}{KP_r} = -\frac{\partial P_1}{\partial V_1} \quad (19)$$

while the reduced Borelius parameters are defined by

$$\alpha_1 = \frac{\alpha}{P_r}$$

$$\beta_1 = \frac{\beta}{V_0}$$

From equations (6) and (9) we obtain

$$E_1 = -1 + \alpha_1\beta_1 \sum_{n=0}^{\infty} \frac{\gamma_n}{n} \left(-\frac{\Delta V_1}{\beta_1}\right)^n \quad (20)$$

Similarly for pressure

$$P_1 = \alpha_1 \sum_{n=1}^{\infty} \gamma_{n+1} \left(-\frac{\Delta V_1}{\beta_1}\right)^n \quad (21)$$

The link with the quantities introduced earlier is established through

$$P_B = \frac{P}{\alpha}$$

$$= \frac{P_1}{\alpha_1}$$

$$\Delta V_B = \frac{\Delta V}{\beta_1}$$

$$= \frac{\Delta V_1}{\beta_1}$$

$$= -X \quad (22)$$

Every one of the fundamental quantities can thus be written in dimensionless reduced form.

Determination of coefficient α, β and γ

The laws given by relations (1), (4) and (5) can reproduce high-pressure data with considerable accuracy once suitable values are assigned to the coefficients α, β and γ. These coefficients α, β and γ may be fixed in two ways: either by a least-squares fit to experimental data or by matching the equation of state to an appropriate interatomic potential model. The latter route is the one generally used to obtain the coefficients. The former is preferable in principle, since the very aim of the procedure is to dispense with empirical fitting. In the second approach the crystal volume is written as

$$V = CNa^3 \quad (23)$$

in which C is the crystal-structure parameter, N the Avogadro number and a the interionic inter ionic separation. The reduced separation is expressed in units of the equilibrium value a_0

$$a_1 = \frac{a}{a_0} \quad (24)$$

Which gives $V_1 = \frac{V}{V_0} = {a_1}^3$

$$V_1 = {a_1}^3 - 1$$

And

$$a_1 = (1 + \Delta V_1)^3$$

$$= \frac{\Delta V_1}{3} - \left[\frac{\Delta V_1}{3}\right]^2 + \frac{5}{3}\left[\frac{\Delta V_1}{3}\right]^3 - \frac{10}{3}\left[\frac{\Delta V_1}{3}\right]^4 \quad (25)$$

Consider an inter ionic potential model that gives the reduced energy E_1 as a function of the reduced separation a_1

$$E_1 = g_1(a_1) \quad (26)$$

which upon Taylor expansion gives

$$E_1 = \sum_{n=0}^{\infty} \frac{{g_1}^n}{n!} \Delta {a_1}^n \quad (27)$$

Matching equation (20) term by term with equation (27), together with equation (26), we obtain

$$\alpha_1 = \frac{2({g_1}'')^2}{3(6{g_1}'' - {g_1}''')} \quad (28)$$

$$\beta_1 = \frac{6{g_1}''}{6{g_1}'' - {g_1}'''} \quad (29)$$

$$\gamma = 4{g_1}'' \left(26{g_1}'' - 6{g_1}''' + \frac{{g_1}''''}{2}\right) \quad (30)$$

And

$$\frac{1}{K_1} = \frac{1}{9{g_1}''} \quad (31)$$

CONCLUSION

The numerical study reported here was carried out on the basis of the equations obtained above. The input parameters K_o, K^I_o, K^{II}_o and ξ for LiH and MgO were taken from the values quoted by Hama and Suito. The pressure P and the isothermal bulk modulus K_T predicted by the several equations of state were then compared for the two crystals. It is found that up to V/V_0 = 0.60 the Born–Mie, Brennan–Stacey and Shanker equations of state agree closely with the Hama–Suito results, whereas beyond V/V_0 = 0.60 the Brennan–Stacey values fall progressively below those of Hama and Suito. It is also noticed that for V/Vo below 0.60 the Hama–Suito results lie between those of the Born–Mie and Shanker equations. Taken over all values of V/V_0, the P and K_T from the Shanker equation match the Hama–Suito equation very closely for both LiH and MgO. By contrast, the remaining descriptions — the Born–Mie and Brennan–Stacey equations of state — beyond V/V_0 = 0.60 depart markedly from the Hama–Suito results for P and K_T. It is worth noting that the Hama–Suito equation of state closely reproduces the theoretical values obtained by the QSM and APW methods over the whole range of compression. Stacey [11] has stressed that examining how the quantity dK_T/dP changes with pressure furnishes a stringent test of any equation of state. Accordingly, dK_T/dP was evaluated as a function of P/K_T for the various equations of state. The figure shows that as the pressure rises K_T increases while dK_T/dP falls. In the limit of very high pressure, $V/V_0 \rightarrow 0$, $dK_T/dP \rightarrow 1/(P/K_T)$. This limiting value of dK_T/dP as $P \rightarrow \infty$ is written as K^I_∞. A first-principles QSM calculation gives $K^I_\infty = 5/3$ in the limit $V/V_0 \rightarrow 0$. A correct equation of state must therefore approach this end point under extreme compression, a requirement that the Hama–Suito equation of state meets very well.

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