Comments

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Comment on "Relationship between two-body interatomic potentials in a lattice model and elastic constants"

M. M. Shukla

Instituto de Física "Gleb Wataghin," Universidade Estadual de Campinas, C.P. 1170, 13100 Campinas, S.P., Brazil

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Thomas had considered the volume-dependent energy of metals, E_v, given by $E_v = (V/V_0)^n$, with $n = -2/3$. Johnson, on the other hand, shows $n = 1$. Correct interpretation of his results restores the value of n given by Thomas.

In the past, several attempts have been made to correlate the two-body pair potential in a solid with its elastic constants. The case of metals was more complicated as it has offered severe difficulties due to the presence and influence of conduction electrons. Fuch's[1] work on monovalent metals has demonstrated clearly that total interatomic interactions in metals could be divided into two parts, i.e., the central interaction (interionic) and the noncentral (volume-dependent) or electron-ion interaction. Fuchs's[1] work has been used invariably by subsequent workers in the lattice dynamics in metals.[2-4] Quite recently Thomas[5] and Johnson[6,7] have adapted a different way to express the volume-dependent part of the interatomic interaction. Thus they took

$$E_v = P\left(\frac{V}{V_0}\right)^n, \tag{1a}$$

where E_v is the potential energy describing electron-ion interaction, P is a constant, and V and V_0 are, respectively, the deformed and undeformed volume of the metal. While Thomas[5] has pointed out that the most probable value of n is $-\frac{2}{3}$, Johnson[6] has shown [his equation (25)] that $n=1$ is the best choice to reproduce the results given by Thomas[5] and others. As a matter of fact, $n=-\frac{2}{3}$ is the correct result on the model of Johnson[6] also. This is demonstrated here. To show our point, let us write the equation numbers (8b), (8c), and (8d) from the paper of Johnson[7] which are

$$C_{11} = \frac{1}{2V_0}\sum_s \psi''(x^s)^4 + n(n-2)P, \tag{1b}$$

$$C_{12} = \frac{1}{2V_0}\sum_s \psi_s''(x^s)^2(y^s)^2 + n^2P, \tag{1c}$$

$$C_{44} = \frac{1}{2V_0}\sum_s \psi_s''(x^s)^2(y^s)^2 - nP. \tag{1d}$$

In these equations, $\psi''(x^s)^2$ and $\psi''(x^s)^2(y^s)^2$ are the functions of the 1st and 2nd derivatives of the interionic potential of the metal. C_{ij} are the elastic constants of the metal.

These equations could be rewritten in a form suggested by Martin[8]:

$$C_{11} = (C_{11})^{sr} + p_e + k_e, \tag{2a}$$

$$C_{12} = (C_{12})^{sr} - p_e + k_e, \tag{2b}$$

$$C_{44} = (C_{44})^{sr} + p_e. \tag{2c}$$

In above equations $(C_{ij})^{sr}$ describe the values of the elastic constants calculated on short-range interaction, i.e., interionic interaction.

A direct comparison of the pairs of equations (1b) and (2a), (1c) and (2b), and (1d) and (2c) would give

$$p_e + k_e = n(n-2)P, \tag{3a}$$

$$-p_e + k_e = n^2P, \tag{3b}$$

$$p_e = -nP. \tag{3c}$$

Equations (3) give readily

$$k_e = n(n-1)P. \tag{3d}$$

Equations (3c) and (3d) are exactly the same relations as obtained by Thomas[5] by his equations (8) and (5). A look at Eq. (3c) and (3d) shows that

in order to determine the value of n, we must establish a relation between p_e and k_e. Following de Launay,[2] we have for a free-electron-gas metal

$$p_e = \tfrac{3}{5}k_e . \tag{4}$$

By substituting in Eq. (4), the relation (3c) and (3d) we have

$$-nP = \tfrac{3}{5}n(n-1)P \tag{5a}$$

or

$$n = -\tfrac{2}{3} . \tag{5b}$$

I would point out the most probable reason which led Johnson to choose $n=1$. From the set of Eqs. (1) and (2), we have apparently two different, but eventually the same, expressions for the Cauchy deviations, i.e.,

$$C_{12} - C_{44} = n(n+1)P , \tag{6a}$$

$$C_{12} - C_{44} = -2p_e + k_e . \tag{6b}$$

Johnson[6] was looking for a result [Eq. (9) of Thomas[5]]

$$C_{12} - C_{44} = 2P . \tag{7}$$

That is why he took $n=1$ in Eq. (6a).

He did not realize that P appearing in Eq. (6a) and (7) are different, i.e., P of Eq. (7) is actually equal to $\frac{1}{2}(-2p_e + k_e)$. I need not tell that the value of $n = -\frac{2}{3}$ is not the unique value of n for metals. It is commonly used in the literature.

Finally, I totally agree with Johnson[6,7] that more than one volume-dependent energy term should be considered in Eq. (1) for real solids. This point is elaborated for metals in the following. The total energy of electrons in a metal is given by[9]

$$E_v = \sum_{k<k_F}{}' \frac{\hbar^2 k^2}{2m} \frac{e^2 k_F}{\pi} \left(1 + \frac{k_f^2 - k^2}{2kk_F} \ln\left|\frac{k_F + k}{k_F - k}\right|\right). \tag{8}$$

Equation (8) can be written approximately

$$E_v = N\left(\frac{3}{5}\epsilon_F - \frac{3}{4}\frac{e^2 k_F}{4}\right). \tag{9}$$

Remembering that $r_s = (3V/4\pi N)^{1/3}$, $k_F = (9\pi/4)^{1/3} r_s^{-1}$, $\epsilon_F = \hbar^2 k_F / 2m$, Eq. (9) can be transformed to

$$E_v = P_1 \left(\frac{V}{V_0}\right)^{-2/3} + P_2 \left(\frac{V}{V_0}\right)^{-1/3} . \tag{10}$$

Comparison of Eqs. (1) and (10) tells that for the metals we must have at least two volume-dependent terms with $n_1 = -\frac{2}{3}$ and $n_2 = -\frac{1}{3}$. A more accurate expression for E_v from the work of Gell-Mann and Brueckner[10] would lead to one more value of n.

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