Erratum

Many Body Interaction and Cauchy Relation for Elastic Constants

S. K. Sarkar and S. Sengupta

Z. Physik B **25**, 135–137 (1976)

In Equations (8) and (9) there is scope of some ambiguity in interpreting the summation procedure. To remove this let us rewrite Equation (6) as

$$\Phi = \sum_{(ij)} \phi^{(2)}(ij) + \sum_{(ijk)} \phi^{(3)}(ijk) + \dots$$

and define c.p.'s as

$$\begin{aligned} \Phi_1 \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix} \right) &= \sum_{(i'j')} \Phi_1^{(2)} \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix}, (i'j') \right) \\ &+ \sum_{(i'j'k')} \Phi_1^{(3)} \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix}, (i'j'k') \right) + \dots \\ \Phi_2 \left(\begin{smallmatrix} ij \\ \alpha\beta \end{smallmatrix} \right) &= \sum_{(i'j')} \Phi_2^{(2)} \left(\begin{smallmatrix} ij \\ \alpha\beta \end{smallmatrix}, (i'j') \right) \\ &+ \sum_{(i'j'k')} \Phi_2^{(3)} \left(\begin{smallmatrix} ij \\ \alpha\beta \end{smallmatrix}, (i'j'k') \right) + \dots \end{aligned}$$

where (ij) , (ijk) etc. mean pair, triplet etc. and $\sum_{(ij)}$ etc. mean summation over all pairs and triplets etc. Obviously

$$\Phi_1^{(2)} \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix}, (i'j') \right) \quad \text{and} \quad \Phi_1^{(3)} \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix}, (i'j'k') \right)$$

are meaningless unless i is equal to one of the symbols in $(i'j')$ and $(i'j'k')$. Similar consideration follows for $\Phi_2^{(2)}$ and $\Phi_2^{(3)}$. Then Equations (8) and (9) can be written as

$$\begin{aligned} c_{\alpha\gamma\beta\delta} &= -\frac{1}{2V} \sum_{(i'j')} \left[\sum_{ij} \Phi_2^{(2)} \left(\begin{smallmatrix} ij \\ \alpha\beta \end{smallmatrix}, (i'j') \right) R \left(\begin{smallmatrix} ij \\ \gamma \end{smallmatrix} \right) R \left(\begin{smallmatrix} ij \\ \delta \end{smallmatrix} \right) \right. \\ &\quad \left. + 2 \sum_i \Phi_1^{(2)} \left(\begin{smallmatrix} i \\ \gamma \end{smallmatrix}, (i'j') \right) R \left(\begin{smallmatrix} ij' \\ \delta \end{smallmatrix} \right) \delta_{\alpha\beta} \right] \\ &+ \frac{1}{V} \sum_{(i'j'k')} \left[\sum_{ij} \Phi_2^{(3)} \left(\begin{smallmatrix} ij \\ \alpha\beta \end{smallmatrix}, (i'j'k') \right) R \left(\begin{smallmatrix} ik' \\ \gamma \end{smallmatrix} \right) R \left(\begin{smallmatrix} ji \\ \delta \end{smallmatrix} \right) \right. \\ &\quad \left. - \sum_i \Phi_1^{(3)} \left(\begin{smallmatrix} i \\ \gamma \end{smallmatrix}, (i'j'k') \right) R \left(\begin{smallmatrix} ij' \\ \delta \end{smallmatrix} \right) \delta_{\alpha\beta} \right] + \dots \\ t_{\alpha\beta} &= \frac{1}{V} \sum_{(i'j')} \sum_i \Phi_1^{(2)} \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix}, (i'j') \right) R \left(\begin{smallmatrix} ij' \\ \beta \end{smallmatrix} \right) \\ &+ \frac{1}{V} \sum_{(i'j'k')} \sum_i \Phi_1^{(3)} \left(\begin{smallmatrix} i \\ \alpha \end{smallmatrix}, (i'j'k') \right) R \left(\begin{smallmatrix} ij' \\ \beta \end{smallmatrix} \right) + \dots \end{aligned}$$

S. K. Sarkar
S. Sengupta
Solid State Physics
Research Centre
Presidency College
Calcutta, India