

THEOREM OF DIFFERENTIATION  
OF THE ENERGY OF A MULTIATOMIC  
SYSTEM WITH RESPECT TO ATOMIC  
COORDINATES (PART I)

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S u m m a r y

The theorem asserting that the arbitrary-order derivative of the average energy of a solid with respect to atomic coordinates equals the average value of the corresponding derivative of the potential energy operator with respect to atomic coordinates has been proved. This theorem is a generalization of the well-known Gell-Mann–Feynman theorem, which was proved only for the first derivative of the average energy with respect to atomic coordinates. A necessity in such a generalization is associated with the calculation of force constants in solids, which are the derivatives of the average energy with respect to atomic coordinates, and, maybe, other physical quantities.