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1 Pair Potentials and Cauchy Symmetry

Here are a few more details on why pair potentials lead to Cauchy symmetry. Consider the potential energy of the crystal at zero temperature

$$V_o(\boldsymbol{F}) = \frac{1}{2}\sum_{\substack{i,j\\ i\neq j}} \phi(\|\boldsymbol{x}_{ij}\|)\,, \tag{1}$$

where $\boldsymbol{x}_{ij} = \boldsymbol{x}_j - \boldsymbol{x}_i$ is the vector from atom i to atom j and $\phi(\cdot)$ is a given potential. Note that by the Cauchy-Born assumption

$$\|\boldsymbol{x}_{ij}\| = \sqrt{\boldsymbol{X}_{ij}\cdot 2\boldsymbol{E}\boldsymbol{X}_{ij} - \boldsymbol{X}_{ij}\cdot\boldsymbol{X}_{ij}} \tag{2}$$

for a simple lattice and that in the linearized case we can replace the Green-Lagrange strain by $\boldsymbol{\varepsilon}$, the small strain tensor. With this at hand,

$$\frac{\partial V_o}{\partial \boldsymbol{\varepsilon}} = \frac{1}{2}\sum_{\substack{i,j\\ i\neq j}} \phi' \frac{\partial\|\boldsymbol{x}_{ij}\|}{\partial\boldsymbol{\varepsilon}} = \frac{1}{2}\sum_{\substack{i,j\\ i\neq j}} \phi'\|\boldsymbol{x}_{ij}\|\boldsymbol{n}_{ij}\otimes\boldsymbol{n}_{ij}\,, \tag{3}$$

where $\boldsymbol{n}_{ij} = \boldsymbol{x}_{ij}/\|\boldsymbol{x}_{ij}\|$. The second derivative (the stiffness) yields:

$$\frac{\partial^2 V_o}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}} = \frac{1}{2}\sum_{\substack{i,j\\ i\neq j}} \left[\phi'' - \frac{\phi'}{\|\boldsymbol{x}_{ij}\|}\right]\|\boldsymbol{x}_{ij}\|^2\boldsymbol{n}_{ij}\otimes\boldsymbol{n}_{ij}\otimes\boldsymbol{n}_{ij}\otimes\boldsymbol{n}_{ij}\,. \tag{4}$$

This last expression clearly has minor, major, as well as Cauchy symmetries. This then produces some non-physical results. For example with an isotropic materials it requires $C_{1122} = C_{1212}$ – forcing $2\mu + \lambda = \mu$ and only one elastic constant. A better (crystollographic) example comes from the triclinic material. In general a triclinic material possesses no material symmetries and thus has 21 independent material constants (18 if you do not count the axes directions). With Cauchy symmetry one obtains 6 further inter-relations beyond those of major and minor symmetry resulting in only 15 material constants for a triclinic material (12 without axes) which is definitely wrong! In this situation the moduli in Voigt notation[1] (with Berkeley ordering $[11, 22, 33, 12, 23, 31]$) looks like:

$$\mathbb{C} \rightarrow \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{12} & C_{26} & C_{15} \\ & & & & C_{23} & C_{34} \\ & & & & & C_{13} \end{bmatrix}. \tag{5}$$

[1] In Voigt's original work he orders the index pairs as $[11, 22, 33, 23, 31, 12]$.