Ferro-Teaser 1: solution

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I. QUESTION 1

If we write down, the lowest-order symmetry allowed terms in the Taylor expansion of the free energy (Landau would certainly approve of that), we find

$$F = AP^2 + BP^4 + C\eta^2 + DP\eta. \tag{1}$$

Here we used that F is a scalar, P changes sign under inversion, but not time reversal and η does not change sign under neither inversion nor time reversal. At the ferroelectric phase transition A changes sign resulting in a non-vanishing polarization P. From the coupling term it can be seen that a finite P acts just like an applied strain on η, resulting in a non-vanishing η as well. A ferroelectric transition therefore drives a corresponding ferroelastic transition.

II. QUESTION 2

First of all, we have to specify the domain of integration in the expression $\int_V dr\ \mathbf{r}\rho(\mathbf{r})/V$. For a finite system, we can always choose V large enough to contain all particles. Clearly, we cannot do that for an extended system. However, if we believe that P really is a bulk quantity it would make sense to integrate over one unit cell. Unfortunately, P then depends on the choice of unit cell. These difficulties are overcome by Vanderbilt's definition of the polarization in terms of a Berry phase.