1 Formulation of Problem

$$\frac{\partial \Phi}{\partial u_{ij}} = 0 \rightarrow u_{ij}[P] \rightarrow \frac{\partial \Phi}{\partial P_i} = 0 \rightarrow P_i[T] \tag{1}$$

The Free Energy is given below using a sixth order expansion of the polarization order parameter.

$$\begin{gathered}
\Phi = a_1 \left(P_1^2 + P_2^2 + P_3^2\right) + a_{11} \left(P_1^4 + P_2^4 + P_3^4\right) + a_{12} \left(P_1^2 P_2^2 + P_3^2 P_2^2 + P_1^2 P_3^2\right) + \\
a_{111} \left(P_1^6 + P_2^6 + P_3^6\right) + a_{112} \left(P_1^4 \left(P_2^2 + P_3^2\right) + P_2^4 \left(P_1^2 + P_3^2\right) + P_3^4 \left(P_2^2 + P_1^2\right)\right) + \\
a_{123} P_1^2 P_2^2 P_3^2 + \\
\frac{1}{2} c_{11} \left(u_1^2 + u_2^2 + u_3^2\right) + c_{12} \left(u_1 u_2 + u_3 u_2 + u_1 u_3\right) + \frac{1}{2} c_{44} \left(u_4^2 + u_5^2 + u_6^2\right) - \\
q_{11} \left(P_1^2 u_1 + P_2^2 u_2 + P_3^2 u_3\right) - q_{12} \left(P_1^2 \left(u_2 + u_3\right) + P_3^2 \left(u_1 + u_2\right) + P_2^2 \left(u_1 + u_3\right)\right) - \\
q_{44} \left(P_2 P_3 u_4 + P_1 P_3 u_5 + P_1 P_2 u_6\right)
\end{gathered} \tag{2}$$

2 Strain Relations

The first derivative of the free energy gives the strain equilbrium conditions.

$$u_1 = Q_{11} P_1^2 + Q_{12}(P_2^2 + P_3^2) \tag{3}$$

$$u_2 = Q_{11} P_2^2 + Q_{12}(P_1^2 + P_3^2) \tag{4}$$

$$u_3 = Q_{11} P_3^2 + Q_{12}(P_1^2 + P_2^2) \tag{5}$$

$$u_4 = Q_{44} P_2 P_3, \quad u_5 = Q_{44} P_1 P_3, \quad u_6 = Q_{44} P_1 P_2 \tag{6}$$

The quadratic coefficients are then renormalized as:

$$a_{11} = a'_{11} - \left(\frac{q_{11} Q_{11}}{2} + q_{12} Q_{12}\right) \tag{7}$$

$$a_{12} = a'_{12} - \left(q_{12} Q_{11} + q_{11} Q_{12} + q_{12} Q_{12} + \frac{q_{44} Q_{44}}{2}\right) \tag{8}$$

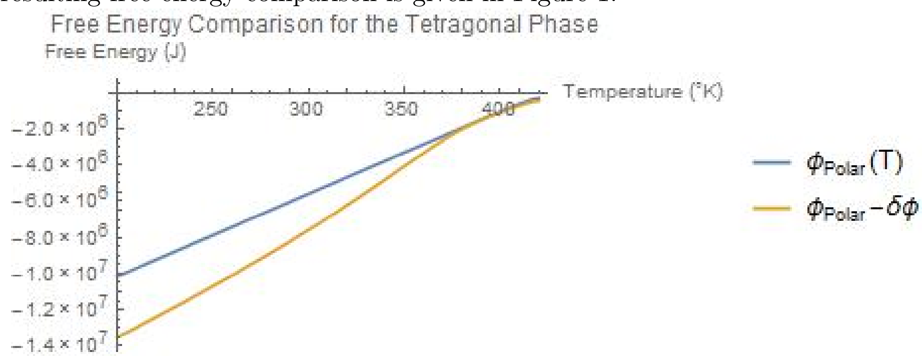
It is important to note that the coefficients given in papers are derived from experiments are analyzed using first principles to fit experimental observations. As such the parameters are already normalized to include the contribution from strain.

2.1 Tetragonal Phase

The free energy can be expressed as a polar component with some perturbation arising from the strain field.

$$\Phi_{Total} = \Phi_{Polar} - \delta\Phi|_{P=P_0} \tag{9}$$

Where P_0 is the normalized polarization solution within the strain field. The resulting free energy comparison is given in Figure 1.



The variation of the polarization in the tetragonal phase can be seen by comparing the solutions using a_{11} and a'_{11}. The "w/o strain" solution uses the a'_{11} coefficient whereas the "w/ strain" solution uses the normalized,a_{11}, coefficient. The phase transition starts to behave more as a second-order phase transition when the strain is not included, which is as expected since for temperatures close to $T_C$the coefficienta'_{11} has a different sign than a_{11}.