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T3. Spontaneous ferroelectric polarization

Ferroelectric materials exhibit so-called **spontaneous polarization**, when their polarization P is different from zero even no external electric field is applied. Let's try to investigate this effect quantitatively. To do this, one must first determine how the internal energy per unit volume W depends on polarization P. The easiest way to do this is to expand this dependence into a Taylor series around $P = 0$. Terms with P in odd power get cancelled due to inversion symmetry, so:

$$W = \frac{1}{2}\alpha(T - T_0)P^2 + \frac{1}{4}\beta P^4 + \frac{1}{6}\gamma P^6. \tag{1}$$

Here $\alpha, \beta, \gamma > 0$, T is the temperature of the ferroelectric, and T_0 is the temperature at which the ferroelectric undergoes a phase transition changing its ability to spontaneously polarize.

In the equilibrium state, the energy must have a **local minimum**.

A1	Write down the conditions for a local energy minimum, if energy is given by equation (1). For which values of T the spontaneous polarization would be possible?

A2	Derive an equation for equilibrium values of spontaneous polarization, P_0.

A3	Expression from the previous task simplifies significantly in the limit $T \to T_0$. Find the values of P_0 in this limit. Express your answer in terms of α, β and $\Delta T = T_0 - T$.

Use the resulting expression later in this problem.

If an external electric field E is applied to a spontaneously polarized ferroelectric, its polarization will change slightly. It can be shown that for a sufficiently small external field this change can be considered linear, and one can define electric susceptibility as:

$$\chi \equiv \lim_{E \to 0} \frac{P_0(E) - P_0(0)}{E} \equiv \left. \frac{\partial P_0(E)}{\partial E} \right|_{E=0}.$$

B1	Derive an expression for the electric susceptibility of a spontaneously polarized ferroelectric.

T4. Ferroelectric hysteresis

Because of their spontaneous polarization, ferroelectrics exhibit **hysteresis properties**: their response to an external field (the dependence of the polarization P vs. the external electric field E) depends on their previous state.

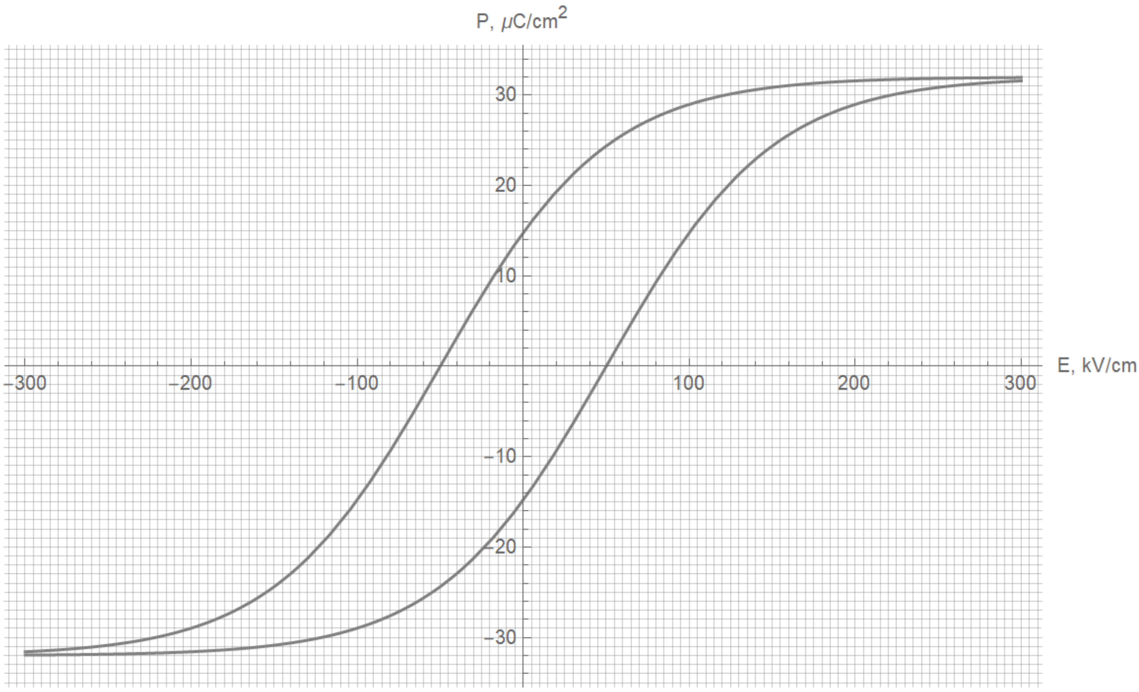
Consider a ferroelectric material that had polarization P_1 in an external electric field E_1 at the initial time. The field was then increased to E_2, and the polarization increased to P_2, following the law $P_{-}(E)$. Then the field was again reduced to E_1, and the polarization of the ferroelectric returned to its initial state following the law $P_{+}(E)$.

A1	Derive an expression for the elementary work δA that the external field has to do to change the polarization of a unit volume of ferroelectric by $\mathrm{d}P$.

A2	Derive an equation relating the heat δQ released inside the ferroelectric, the work δA done by external field and the change $\mathrm{d}U$ in ferroelectric internal energy.

A3	Express as some proper integral the total work A that the external field has to do to a unit volume of the material during the whole cycle of field's increase and decrease. By how much ΔU does the internal energy density changes during the cycle? How much heat Q is released in a unit volume?

Now consider a hysteresis loop of one of the most widely used ferroelectric materials, **barium titanate (BTO)**. The loop is plotted on a figure below.



On the horizontal axis is the external electric field strength in kV/cm, on the vertical axis is the polarization of the segnetoelectric in μC/cm^2.

Suppose a large (>300 V) negative voltage is applied to a thin BTO film of thickness $d = 10\ \mu$m and area $S = 1$ cm^2. Then it's changed to a large positive voltage and finally returned back.

B1	Calculate what amount of heat Q was released in the film.

Now suppose an alternating voltage with effective voltage $V_{\text{eff}} = 220$ V and frequency $\nu = 50$ Hz is applied to the film.

B2	Calculate the average thermal power $\dot{Q}$ released in the film.