Facultad de Ciencias

Estudio analítico de la formación de dominios de Kittel en nanoestructuras ferroeléctricas

(Analytical study of Kittel domain formation in ferroelectric nanostructures)

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Resumen

En los últimos años, ha habido un gran auge en el estudio de la polarizacion eléctrica en nanoestructuras ferroeléctricas, que forman patrones complejos con propiedades topológicas no triviales. Estas estructuras surgen debido al equilibrio entre las energías involucradas: eléctrica, elástica y de gradiente. Muchos de los trabajos publicados hasta ahora se fundamentan en simulaciones atomísticas a partir de primeros y segundos principios.

En este trabajo, analizaremos de manera analítica las expresiones de las tres energías que compiten: la energía de volumen, que resulta de polarizar un material ferroeléctrico y que toma una forma de doble pozo, la energía de gradiente debida a la formación de dominios y que supone que la polarización varía con la posición (tiene un gradiente); y la energía electrostática en ciertas configuraciones específicas (una lámina ferroeléctrica delgada aislada, una lámina ferroeléctrica sobre un sustrato y una superred formada por láminas ferroeléctricas y paraeléctricas) y sus condiciones de contorno. En este trabajo se va a realizar una derivación paso a paso de las mismas, detallando las diferentes aproximaciones utilizadas y su rango de validez.

Además, los resultados obtenidos se van a utilizar en modelos para evaluar la validez de la ley de Kittel y para compararlos con las predicciones de simulaciones atomísticas.

Palabras clave: polarización eléctrica, ferroeléctrico, dominios, energía, ley de Kittel.

Abstract

In recent years, there has been a significant surge in the study of electric polarization in ferroelectric nanostructures, which form complex patterns with non-trivial topological properties. These structures arise due to the balance between the involved energies: electrical, elastic, and gradient. Many of the works published so far are based on atomistic simulations from first and second principles.

In this work, we will analytically examine the expressions of the three competing energies: the volume energy, which results from polarizing a ferroelectric material and takes the form of a double well, the gradient energy, due to the formation of domains and which implies that the polarization varies with position (having a gradient); and the electrostatic energy in certain specific configurations (an isolated ferroelectric thin film, a ferroelectric film on top of a substrate, and a superlattice formed by a ferroelectric and paraeletric layers) and their boundary conditions. This work will provide a step-by-step derivation of these expressions, detailing the different approximations used and their range of validity.

Moreover, the obtained results will be used in models to evaluate the validity of the Kittel law and to compare them with the predictions of atomistic simulations.

Keywords: electric polarization, ferroelectric, domains, energy, Kittel law.

Glossary

- P_{S}: spontaneous polarization.
- χ_c: electronic contribution to the dielectric susceptibility normal to the film.
- χ_a: electronic contribution to the dielectric susceptibility parallel to the film.
- $\overleftrightarrow{\chi}$: electronic susceptibility tensor.
- W_+: width of the "up" domain.
- W_-: width of the "down" domain.
- $W = W_+ + W_-$: total width of the domain structure.
- d: thickness of the ferroelectric thin film.
- $A = \frac{W_+ - W_-}{W_+ + W_-} = \frac{W_+ - W_-}{W}$.
- Region 1: vacuum region on top of the ferroelectric thin film. It extends from $z = 0$ up to $z = +\infty$.
- Region 2: ferroelectric thin film. It extends from $z = 0$ to $z = -d$.
- Region 3: vacuum region below the ferroelectric thin film. It extends from $z = -\infty$ to $z = -d$.
- $\phi(x, z)$: electrostatic potential at each point in space.
- $\kappa_\alpha = 1 + \chi_\alpha$: electronic contribution to the dielectric constant.
- $k = \frac{2\pi}{W}$.
- $c = \sqrt{\frac{\kappa_a}{\kappa_c}}$.
- $R = \frac{\pi c d}{W}$.
- $g = c\kappa_c$.
- $\alpha = \frac{1}{4\pi\varepsilon_0}\left(\frac{8P_{\mathrm{S}}cd}{R}\right)$.
- $\beta_n = \frac{1}{\sinh(nR) + g\cosh(nR)}$.
- $\gamma_n = \frac{1}{1 + g\coth(nR)}$.
- $\delta_n = \frac{\sinh\left(cnk\frac{d_{\mathrm{P}}}{2}\right)}{\sinh\left(nk\frac{d_{\mathrm{S}}}{2}\right)}$.
- $\nu_n = \frac{4P_{\mathrm{S}}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)$.
- $\theta_n = \left[g\cosh\left(nkc\frac{d_{\mathrm{P}}}{2}\right) + \kappa_s\coth\left(nk\frac{d_{\mathrm{S}}}{2}\right)\sinh\left(cnk\frac{d_{\mathrm{P}}}{2}\right)\right]^{-1}$.
- $\mu_n = \{(g^2 + \kappa_{\mathrm{s}})\sinh(2nR) + g[1 + \kappa_{\mathrm{s}}\cosh(2nR) + 2\sinh^2(nR)]\}^{-1}$.
- D : Total thickness of one period of the ferroelectric/dielectric superlattice.
- d_{S}: thickness of the dielectric layer in the ferroelectric/dielectric superlattice.
- d_{P}: thickness of the ferroelectric layer in the ferroelectric/dielectric superlattice
- During the discussion of the Kittel law: $x = \frac{d}{\omega}$.
- During the discussion of the ferroelectric/paraelectric superlattice: $\alpha = d_{\mathrm{S}}/d_{\mathrm{P}}$
- In the isolated thin film section $\beta \approx \frac{16.829}{\pi^3(1+g)}$
- In the superlattice system $\beta(\kappa_s, \alpha) \approx \frac{16.829}{\pi^3(1+\alpha)(g+\kappa_s)}$
- In a ferroelectric on top of a substrate $\beta(\kappa_s) \approx \frac{8.414}{\pi^3}\frac{(g+\kappa_s)^2+\kappa_s(g+1)^2+2g^3+g\kappa_s^2+2g^2\kappa_s+g+2g^2}{[g^2+\kappa_s+g(\kappa_s+1)]^2}$

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1 Introduction

A ferroelectric material is an insulating system that satisfy two conditions. First, it has two or more stable polarization states in the absence of an electric field. Second, it must be possible to switch from one to another of these states by applying a sufficiently large electric field [1, 2].

The term "ferroelectricity" was coined after the many similarities in behaviour between ferroelectrics and ferromagnets. Ferroelectrics have an spontaneous electric polarization, P_{S}, in the absence of an external electric field, in the same way as ferromagnets do have an spontaneous magnetization in the absence of a magnetic field. This spontaneous property can be reoriented by an external field. This switching behaviour in both kind of materials display an hysteresis loop between the polarization (respectively magnetization) and the applied electric (respectively magnetic) field. This cycle describes the change in polarization or magnetization of the ferroic material, as observed in Fig. 1, where $\mathcal{E}_c$ is the coercive field that establishes a threshold value of the applied electric field for switching between spontaneous negative and positive polarization. Both ferromagnetic and ferroelectric polarization decrease with temperature, with a phase transition to an unpolarized paramagnetic or paraelectric phase, often occurring at high temperatures, typically called Curie temperature. Despite their similarities, the physical origin is very different: ferroelectrics have an asymmetry in charge, whereas ferromagnets have an asymmetry in electronic spin [3].

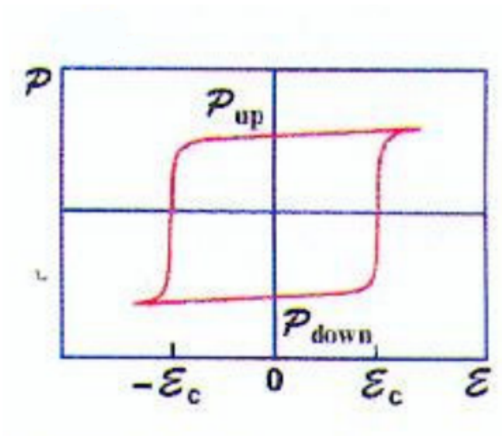


Figure 1: Hysteretic behavior of the polarization-electric field curve. Reprinted with premission from Ref. [4]

The hysteresis loops, like the one shown in Fig. 1, are the measurement of choice to demonstrate ferroelectricity experimentally. From a theoretical point of view, the existence of a double well shape for the energy (black line in Fig. 2) is usually considered as the fingerprint of a ferroelectric instability. The internal energy of the system can be represented as a Taylor expansion of the order parameter: a physical quantity that is zero in the high-symmetry phase and a finite value when the symmetry is decreased. For ferroelectric materials, the order parameter is the polarization. Only symmetry-compatible (even) terms are kept in the Taylor expansion. If the energy of the system is represented against the polarization for a temperature below the Curie temperature, which corresponds to the ferroelectric state, a double well shape is obtained. The two energy minima correspond to spontaneous positive and negative polarization. If the same representation is done for a temperature above the Curie temperature (red line in Fig. 2) , which corresponds to the paraelectric state, a single well is obtained with its minimum corresponding to a polarization equal to zero.

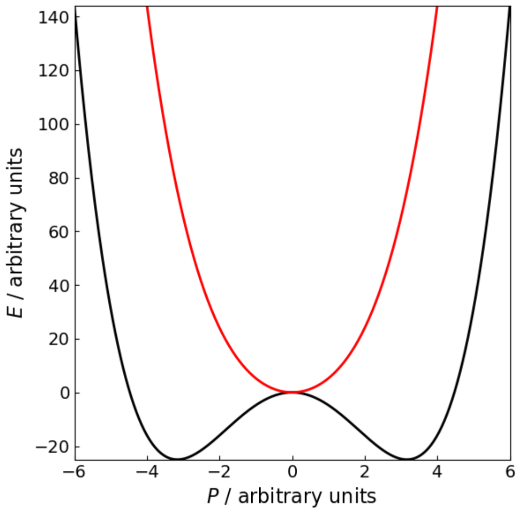
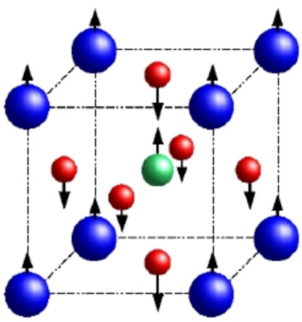


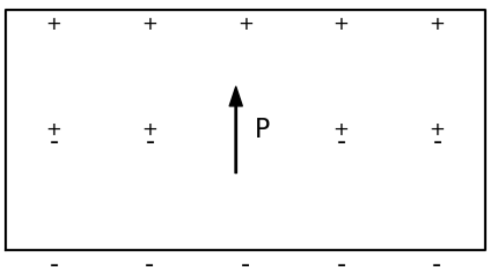
Figure 2: Energy as a function of polarization for a temperature below (solid black line) and above (solid red line) the Curie temperature.

Ferroelectrics are materials with a great applied interest. The fact that these materials have an spontaneous polarization in the absence of electric field makes them useful in the manufacture of Non-Volatile Random-Access Memory (NVFRAM) cells. Ferroelectrics are also piezoelectrics (electric charges appear at their surfaces when they are under mechanical strain, and vice versa) and pyroelectrics (their electrical dipole moment depends on the temperature), so they can be used in microactuators and infrared sensors. These type of materials posses a high electrical permittivity (especially close to the phase transition) which is the reason for their use in the fabrication of Dynamic Random Access Memory (DRAM) capacitors. In addition to these applications, these materials can be used in thermal infrared switches due to their electro-optic activity.

Due to the ongoing miniaturization of the electronic devices, the ferroelectric materials used in the design of these systems are grown under the form of thin films of a finite thickness. For a long time, the common belief was that ferroelectric properties were suppressed in thin films below a critical size. In a thin film, the cooperative atomic displacements associated with the ferroelectric phase transitions gives rise to a finite polarization with a component perpendicular to the surface (Fig. 3(a)). The normal component of this polarization has a discontinuity at the surface of the thin film which gives rise to bound polarization charges, $\sigma_{\text{bound}} = \mathbf{P} \cdot \hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is the unitary vector perpendicular to the surface [5] (Fig. 3(b)). These unscreened bound charges generate a depolarization field that goes from the positive charges to the negative ones and it is usually strong enough to suppress material's polarization completely. However, improvements in the late nineties of the XX-th century in the synthesis and characterization of ferroelectric thin films with a control at the atomic scale, have allowed the observation of ferroelectricity well below this critical thickness [6], challenging this long-accepted view. This brought the field to a high level of excitement and a huge research activity has been devoted to the understanding of the screening effects in ferroelectric thin films.



(a)



(b)

Figure 3: Atomic displacements that give rise to a finite polarization (a) and bound polarization charges generated by the discontinuity of the normal component of this polarization at the surface of the thin film (b).

If the polar state has to be preserved, it is interesting to explore different ways in which the depolarization field can be reduced (see Fig. 4). The first obvious one is to use free charges from metallic electrodes [7, 8, 9, 10]. By placing an electrode at each surface of the film, free charges of the electrode with opposite sign to those bound to the surface screen the polarization charges and reduce the depolarization field. However, with real metals (with a finite screening length), this cancellation is not perfect and a residual depolarization field is still present that destabilizes the ferroelectric phase below a critical thickness [11].

In many experimental situations, the thin films grown are not perfectly stechiometric and they might content vacancies. These defects (mostly oxygen vacancies [12, 13]) might act as source of extra doping charges as in standard extrinsic semiconductors. This surplus of mobile charges has been contemplated as an extra source of screening mechanism [14]. In other cases, we must take into account that the ferroelectric thin films are not grown in perfect vacuum. There are polar molecules in the environment that can be absorbed onto the surface of the thin film, reducing the bound charges and the depolarization field [15, 12]. Finally, other possibilities to maintain a *monodomain* configuration are the rotation of the polarization into the plane of the ferroelectric film (if allowed by the strain conditions), or the suppression of the polarization. In any of these cases there are no bound charges on the surfaces, and the depolarization field disappears.

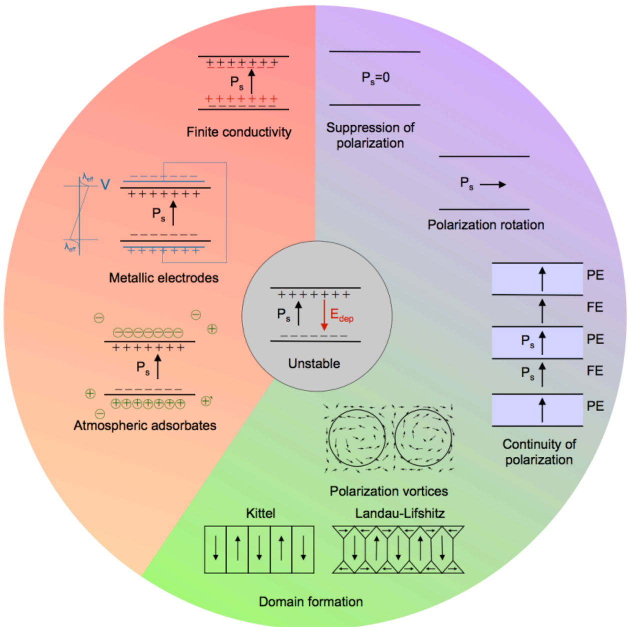


Figure 4: Different ways to screen the depolarization field created by unscreened bound charges on the surfaces of the ferroelectric. Reprinted with permission from Ref [2].

On the other hand, it is possible to reduce the depolarization field by forming a superlattice in which a ferroelectric is interleaved with a paraelectric. The ferroelectric tends to polarize, but the paraelectric does not. If the ferroelectric were to polarize slightly less than it does and the paraelectric were to polarize by another amount, bound charges would be reduced and, thus, depolarization field.

Last but not least, one of the possible (end very extended) mechanism to screen the depolarization fields is the formation of domains [16]. Those are small spatial regions with different polarizations separated by a boundary, referred to as the domain wall, than in ferroelectrics is very narrow. The orientations of the polarization formed in these types of domain structures result in the presence of charges of opposite sign on the surface of the ferroelectric, that are overall charge neutral, reducing the depolarization field and the associated electrostatic energy.

But the formation of the domains is not for free. The short-range interactions coming from the change of the dipole orientations when passing through a domain wall yields to an energy cost that is known as the "domain-wall energy". The delicate balance between the energy gain in the electrostatic energy due to the reduction of the depolarization fields and the energy cost of forming the domains determine the optimal domain size.

In this work, I shall analyze this subtle equilibrium between the different energy contributions that appear in ferroelectric thin films with different geometries (isolated slab and periodic dielectric/ferroelectric superlattices). Especial attention will be paid to the electrostatic energy and its implication on the accuracy of the Kittel law. The determination of the limit of validity of the approaches on top of which the computation of the electrostatic energy is done is crucial for a critical application and comparison on realistic systems. Although analytical expressions are given in some research papers [17] and textbooks (for instance, chapter 5 of Ref. [18]), its form is far from trivial, and its derivation contains some approximations that are usually overseen and whose application might not be as general as initially envisaged. Here, in particular, we shall follow the milestone work by Bennett *et al.* [17], bridging all the steps between the relevant equations. In order to make the approximations more prominent, and to have a clear catalogue and how they can affect the final conclusions, they will be highlighted in bold face in the present work.

This work combines topics coming from different courses undertaken during the degree, in particular Electromagnetism, Solid State Physics, Classical Mechanics, and Computation.

2 Kittel Law

As mentioned in Sec. 1, domain formation is a way to suppress the depolarization field. The structure and energy of domains in ferroic materials have been studied by Landau and Lifshitz [19], and time later by Kittel [20, 21] on ferromagnetic domains. The balance of the energy of domain walls, the magnetic field energy and the anisotropy energy in spin orientation determine the relationship between domain width ω and material thickness d. Adding these three energies and minimizing with respect to ω, a square-root dependence of domain width as a function of material thickness is obtained. This is known as the Landau-Kittel law, formulated as $\frac{\omega^2}{\delta} = Ad$, with A being a dimensionless constant of proportionality and δ indicating the thickness of the domain wall. While earlier studies presumed domain walls of negligible width, subsequent researches have revealed that the Kittel law is also true within the Ginzburg-Landau framework, where finite width domain walls may form [22].

This law was expanded to ferroelectric materials. The domain structure of Rochelle salt was studied with this square-root dependence [23] and it was further generalized to encompass specific periodicities and screening conditions in ultrathin ferroelectric films [24], as well as in superlattices containing paraelectric materials [17]. Aditionally, this concept was extended to ferroelastic thin films subjected to epitaxial strain [25]. Hence, it seems that the Landau-Kittel law is a general characteristic of all ferroic materials [16].

3 Isolated thin film

3.1 System geometry

The analysis of the functional form of the electrostatic energy will be carried out on ferroelectric nanostructures in different geometries. In this Section we shall deal with an isolated thin film, and in subsequent sections we will treat a paraelectric/ferroelectric periodic superlattice, or a ferroelectric thin film on top of a substrate.

The most simple case is a free-standing ferroelectric thin-film in vacuum, under open circuit boundary conditions, as shown in Fig. 5, where the full space is split into three different regions: the vacuum on top of the ferroelectric thin film (region 1), the thin film itself (region 2), and the vacuum below the ferroelectric thin film (region 3).

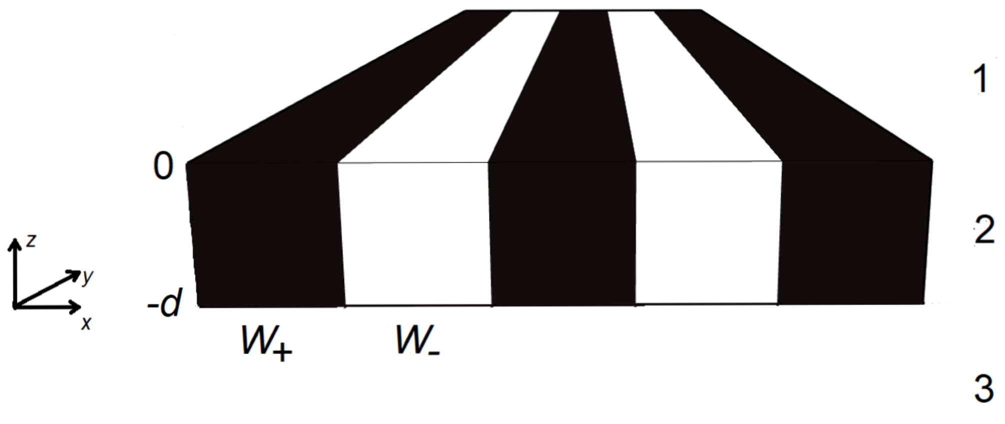


Figure 5: Geometry of the thin film in a vacuum, broken into domains. The black regions represent domains with positive spontaneous polarisation, $+P_S$, and the white regions represent domains with negative spontaneous polarisation, -P_S.

Significant approximations with respect the form of the polarization will be made. In particular:

- **The domain wall width will be neglected**. Here, we shall assume that the domain walls are infinitely thin. Indeed, in ferroelectric materials the typical width is of the order of a few lattice constants, much smaller than in the ferromagnetic case.

- **Surface or interface effects will be neglected.**

- **The total polarization field $\mathbf{P}(\mathbf{r})$ is taken to deviate from the spontaneous polarization only in linear response to the electric depolarization field**. The spontaneous polarization ($\pm P_{\rm S}$) will be assumed to have only a non-vanishing component along the z- direction. As we shall discuss at the end of the Sec. 3.2.1, this linear response treatment is equivalent to replace the double-well potential energy as a function of polarization of a typical proper ferroelectric at the bulk level (see black curve in Fig. 2) by a parabolic energy dependence of the polarization around the minima. The response will be governed by the dielectric susceptibilities normal (χ_c) and parallel (χ_a) to the film.

- **The behaviour of the system along the y-direction will be considered homogeneous**. Therefore, from now on we can focus on what is happening in a (x, z) plane.

- **The origin of the coordinate system will be chosen in such a way that the polarization profile is even**. That means that the origin of coordinates will be right at the center of one of the domains.

Within these approximations, the polarization is considered to be an even function with constant values of $+P_{\rm S}$ over a length of W_+ and $-P_{\rm S}$ over a length of W_- which is repeated periodically. Thus, the period of the polarization can be defined as $W = W_+ + W_-$.

Because the polarization function has a finite number of discontinuities and a finite number of extreme values (Dirichlet conditions), the spontaneous polarization function can be expressed as a Fourier series

$$P_{\rm S}(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi n}{W}x\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi n}{W}x\right), \tag{3.1}$$

where the coefficients of the Fourier expansion are given by

$$\begin{aligned} a_0 &= \frac{2}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} P_{\rm S}(t)dt \\ a_n &= \frac{2}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} P_{\rm S}(t)\cos\left(\frac{2\pi n}{W}t\right)dt \\ b_n &= \frac{2}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} P_{\rm S}(t)\sin\left(\frac{2\pi n}{W}t\right)dt. \end{aligned} \tag{3.2}$$

Every coefficient of the Fourier series is calculated in Appendix A. Taking the results for the coefficients a_0 [Eq. (A.1)] and a_n [Eq. (A.6)], and considering that all the b_n coefficients are zero by symmetry, than the spontaneous polarization under the presence of domains can be expressed as

$$P_{\rm S}(x) = P_{\rm S}A + \sum_{n=1}^{\infty} \frac{4P_{\rm S}}{n\pi}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx) \quad \text{with} \quad k = \frac{2\pi}{W}. \tag{3.3}$$

It is important to remark here how this spontaneous polarization inside the thin film is assumed to arise from the displacements of the ions following the soft-mode like the one displayed in Fig. 3(a), which we assume to be fixed, under zero applied field. In the remaining of this work, we shall compute the electric field that results from such a spontaneous polarization with the presence of a surface. Such electric field would induce a polarization, that added to the spontaneous one will give the total polarization. Going beyond this model would require a self-consistent procedure as the one carried out in more complex simulations, like the ones carried out by first-principles simulations.

3.2 Energy of the domains

In order to determine the static domain configuration of a ferroelectric, we have to minimize the total energy of the crystal [1]. In this total energy we must include:

- The internal energy, modeled by the double well energy described above.

- The domain wall energy.
- The electrostatic energy coming from the coupling between the polarization and the depolarization fields.

In the following subsections, we shall expand analytical expressions for the three of them, that will be later minimized in Sec. 3.2.6 to determine the validity of the Kittel law.

3.2.1 Internal double well energy

In the traditional phenomenological theory for ferroelectrics, the energy density (i.e. the energy per unit volume) is written in a very simple polynomial form, as a Taylor expansion around the reference prototype paraelectric phase with zero polarization. Due to symmetry contraints, only even powers appear in the expansion (so P is equivalent to $-P$). Here, for the sake of simplicity, we shall assume a uniaxial ferroelectric material, where the polarization can point only along the z-cartesian direction. Then, only one of the cartesian components of the polarization appears in the following expressions. Therefore, as typically done in Ginzburg-Landau functionals, we can write

$$E(P) = \frac{1}{2}a(T - T_{\mathrm{c}})P^2 + \frac{1}{4}bP^4 + \mathcal{O}(P^6), \tag{3.4}$$

where a and b are constants, T represents the temperature, and T_{c} is the critical temperature where the ferroelectric phase transition takes place. Assuming that b is positive (as corresponds to second-order phase transitions typical of ferroelectric thin films subject to epitaxial constraints [26]), nothing new is added by the 6-th order terms and beyond, which may be neglected,

$$E(P) = \frac{1}{2}a(T - T_{\mathrm{c}})P^2 + \frac{1}{4}bP^4. \tag{3.5}$$

The conjugate variable of the polarization is the electric field, $\mathcal{E}$, that can be defined as [27]

$$\mathcal{E} = \frac{dE}{dP}. \tag{3.6}$$

(In this Section, and to avoid confusion between the electric field and the energy density, we shall denote the electric field with calligraphic font, $\mathcal{E}$, while the energy will be denoted as E.)

The polarization for zero applied electric field (i.e. the spontaneous polarization) can then be obtained by a minimization of the energy functional given in Eq. (3.5)

$$\frac{dE(P)}{dP} = a(T - T_{\mathrm{c}})P + bP^3 = 0 \quad \Rightarrow \quad P\left[a(T - T_{\mathrm{c}}) + bP^2\right] = 0. \tag{3.7}$$

Therefore, the value of the polarization that minimizes the energy depends on the temperature. On the one hand, for $T \geq T_{\mathrm{c}}$, the only real root of Eq. (3.7) is $P = 0$ (remember that both a and b are positive). On the other hand, for $T < T_{\mathrm{c}}$, the minimum free energy is at $|P| = \sqrt{\frac{a(T_{\mathrm{c}}-T)}{b}}$. For the continuous second-order phase transitions that we are considering here, the critical temperature T_{c} is the Curie temperature. At the energy minimum, where the derivative of the energy with respect to the polarization (i.e. the electric field) vanishes, the value of P corresponds to the spontaneous polarization P_{S}.

In summary, the spontaneous polarization will increase with decreasing temperature from the point $T = T_{\mathrm{c}}$ as

$$P = 0 \quad \text{for} \quad T \geq T_{\mathrm{c}}, \tag{3.8}$$

$$P_{\mathrm{S}} = \pm\sqrt{\frac{a(T_{\mathrm{c}} - T)}{b}} \quad \text{for} \quad T < T_{\mathrm{c}}. \tag{3.9}$$

Taking the derivative of the energy density with respect to the polarization, we can get the expression for the electric field as a function of the polarization

$$\mathcal{E} = \frac{dE}{dP} = a(T - T_{\mathrm{c}})P + bP^3. \tag{3.10}$$

Differentiating again Eq. (3.10) with respect to the polarization we get the inverse of the electric susceptibility [1] ($\chi_c = 1/\varepsilon_0\, dP/d\mathcal{E}$; the subindex c refers to the fact that this is the susceptibility along the z-direction), also called the dielectric stiffness by some authors [28]

$$(\varepsilon_0\chi_c)^{-1} = \frac{d\mathcal{E}}{dP} = \frac{d^2E}{dP^2} = a(T-T_{\rm c}) + 3bP^2. \tag{3.11}$$

The dielectric stiffness can be evaluated for temperatures above and below the phase transition, just replacing the corresponding value of the spontaneous polarization

$$(\varepsilon_0\chi_c)^{-1} = a(T-T_{\rm c}) \quad \text{for} \quad T \geq T_{\rm c}, \tag{3.12}$$
$$(\varepsilon_0\chi_c)^{-1} = 2a(T_{\rm c}-T) \quad \text{for} \quad T < T_{\rm c}. \tag{3.13}$$

Rewriting Eq. (3.5) for $T < T_{\rm c}$

$$\begin{aligned} E(P) &= \frac{1}{2}a(T-T_{\rm c})P^2 + \frac{1}{4}bP^4 \\ &= \frac{1}{4}bP^4 - \frac{1}{2}a(T_{\rm c}-T)P^2 \\ &= b\left(\frac{1}{4}P^4 - \frac{1}{2}\frac{a}{b}(T_{\rm c}-T)P^2\right) \\ &= b\frac{a}{b}(T_{\rm c}-T)\left(\frac{P^4}{4\frac{a}{b}(T_{\rm c}-T)} - \frac{1}{2}P^2\right) \\ &= a(T_{\rm c}-T)\left(\frac{P^4}{4P_{\rm S}^2} - \frac{1}{2}P^2\right) \\ &= \frac{1}{2\varepsilon_0\chi_c}\left(\frac{P^4}{4P_{\rm S}^2} - \frac{1}{2}P^2\right). \end{aligned} \tag{3.14}$$

If we assume that the polarization of the ferroelectric will be the spontaneous value $P_{\rm S}$, except for small modifications induced by the electric depolarization field, then we can take the harmonic expansion about one of the minima of the double well,

$$\begin{aligned} E(P) &= E(P_{\rm S}) + \frac{dE}{dP}\Big|_{P=P_{\rm S}}(P-P_{\rm S}) + \frac{1}{2}\frac{d^2E}{dP^2}\Big|_{P=P_{\rm S}}(P-P_{\rm S})^2 + \dots \\ &\approx E(P_{\rm S}) + \frac{1}{2}\frac{d^2E}{dP^2}\Big|_{P=P_{\rm S}}(P-P_{\rm S})^2, \end{aligned} \tag{3.15}$$

where the first-order term vanishes because the energy functional is a minimum at $P = P_{\rm S}$ and we have cut the expansion in the harmonic term.

Now, assuming that in the vicinity of the minima our ferroelectric responds linearly to the electric field, with a dielectric susceptibility normal to the film χ_c, then

$$P = P_{\rm S} + \varepsilon_0\chi_c\mathcal{E} \qquad \Rightarrow \qquad \mathcal{E} = \frac{(P-P_{\rm S})}{\varepsilon_0\chi_c}. \tag{3.16}$$

Here we have again assumed that $P_{\rm S}$ is due to the lattice motion and is fixed, so the response to the field comes only from the electrons, i.e. χ_c is the electronic contribution to the electric susceptibility. Therefore,

$$\frac{d^2E}{dP^2} = \frac{d}{dP}\left(\frac{dE}{dP}\right) = \frac{d\mathcal{E}}{dP} = \frac{1}{\varepsilon_0\chi_c}. \tag{3.17}$$

Then, the harmonic expansion takes the final form

$$E(P) \approx E(P_{\rm S}) + \frac{(P-P_{\rm S})^2}{2\varepsilon_0\chi_c}, \tag{3.18}$$

that can be used to replace Eq. (3.14) if we are moving around one of the minima.

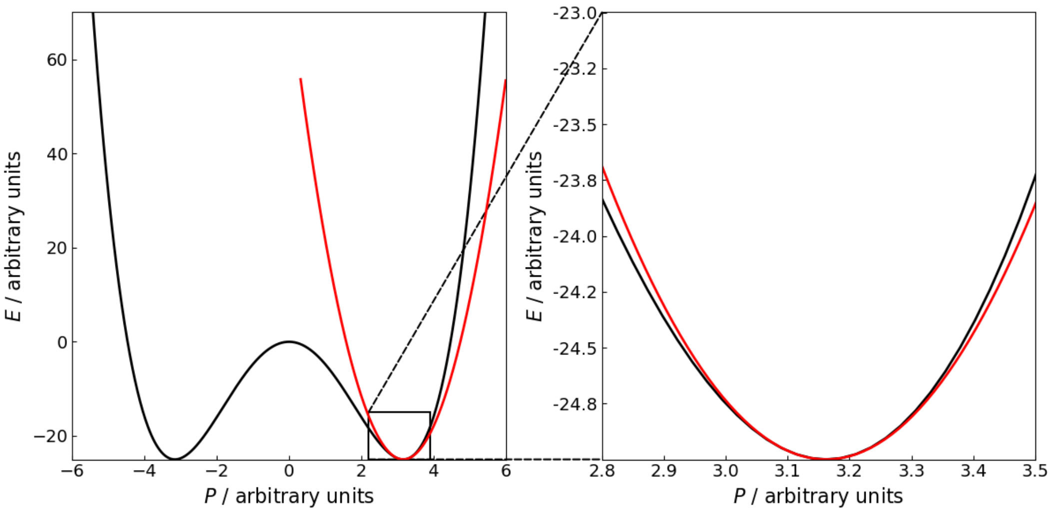


Figure 6: Double well energy of a ferroelectric represented by a solid black line [Eq. (3.5)] with a quadratic approximation about one of the minima represented by a solid red line [Eq. (3.18)].

3.2.2 Domain wall energy

Let us call the energy per unit area of a domain wall as Σ. Then, the energy per domain wall will be Σ times the area of the domain wall, that using the notation of Fig. 5 is d (the thickness of the ferroelectric film) times the length of the sample along the y-direction, L_y. In this work, we shall be interested in comparing energies per unit volume. Therefore, for this purpose we must divide the previous energy by the volume of a domain period. Taking into account that in one of these periods we have two domains, the domain wall energy per unit volume will amount to

$$U_{\mathrm{W}} = \frac{2\Sigma d L_y}{d L_y W} = \frac{2\Sigma}{W} = \frac{2\Sigma}{2\omega} = \frac{\Sigma}{\omega}, \tag{3.19}$$

where we have assumed that $W_+ = W_- \equiv \omega$, and $W = W_+ + W_- = 2\omega$.

3.2.3 Electrostatic potential

Now, the goal is to find the electrostatic potential at each point of space, $\phi(x,z)$, and relate it with the parameters describing the polarization (such as the spontaneous polarization, or the width of the domains) and the response to external stimuli (such as the electrical permittivity). For the sake of simplicity, we shall assume here the simplest case of an isolated thin film. Although the derivation might be a little bit verbose, we believe it is convenient to demonstrate it in a step by step basis, underlining all the approximations that are used in between. These will determine at the end the limit of validity of the expressions that will be found for the electrostatic potentials and fields. More complicated geometries (thin film on top of a substrate or ferroelectric/dielectric superlattices) are left for subsequent chapters.

In order to cope with these tasks, we shall presume the following **assumptions**

- There is **no free charge in the structures**, $\rho_{\mathrm{free}}(x,z) = 0$.
- The **geometry of the ferroelectric is tetragonal**. That means that the tensors that will be discussed below are diagonal. Here we shall be interested on the values along the x- and z-directions.

From the first of the previous hypothesis, we know that the divergence of the electric displacement $\mathbf{D}$ vanishes. Since $\mathbf{D} = \varepsilon_0 \boldsymbol{\mathcal{E}} + \mathbf{P}$, where $\boldsymbol{\mathcal{E}}$ is the electric field generated by the spontaneous polarization $\mathbf{P}_{\mathrm{S}}$ that arises from the displacement of the ions, which we assume to be fix. Then

$$\nabla \cdot \mathbf{D} = \nabla \cdot (\varepsilon_0 \boldsymbol{\mathcal{E}} + \mathbf{P}) = 0. \tag{3.20}$$

The total polarization under the presence of a field, $\mathbf{P}$, is equal to the spontaneous polarization plus the polarization induced by the field,

$$\mathbf{P} = \mathbf{P}_{\mathrm{S}} + \varepsilon_0 \overleftrightarrow{\chi} \boldsymbol{\mathcal{E}}, \tag{3.21}$$

where $\overleftrightarrow{\chi}$ is the electronic susceptibility tensor. In the vacuum regions (where there is no material), the total polarization vanishes. Inside the ferroelectric thin film, assuming a tetragonal symmetry, the electronic susceptibility tensor is diagonal, with different values along the $x-$ and the $z-$ direction (χ_a and χ_c, respectively). Replacing these in Eq. (3.20), we arrive to the conclusion that, in the vacuum regions (1 and 3),

$$\nabla \cdot \mathbf{D} = \nabla \cdot (\varepsilon_0 \boldsymbol{\mathcal{E}}) = \varepsilon_0 \nabla \cdot \boldsymbol{\mathcal{E}} = \varepsilon_0 \left[\nabla \cdot (-\nabla\phi)\right] = -\varepsilon_0 \nabla^2 \phi = 0, \tag{3.22}$$

where the electric field is written as minus the gradient of the electrostatic potential, $\boldsymbol{\mathcal{E}} = -\nabla\phi$.

In the same way, within the ferroelectric thin film,

$$\begin{aligned}
\nabla \cdot \mathbf{D} &= \nabla \cdot (\varepsilon_0 \boldsymbol{\mathcal{E}} + \mathbf{P}_\mathrm{S} + \varepsilon_0 \overleftrightarrow{\chi} \boldsymbol{\mathcal{E}}) = \nabla \cdot (\varepsilon_0 (1 + \overleftrightarrow{\chi}) \boldsymbol{\mathcal{E}}) \\
&= \left(\frac{\partial \left[\varepsilon_0 (1+\chi_a) \mathcal{E}_x\right]}{\partial x} + \frac{\partial \left[\varepsilon_0 (1+\chi_c) \mathcal{E}_z\right]}{\partial z} \right), \\
&= - \left(\kappa_a \frac{\partial^2 \phi}{\partial x^2} + \kappa_c \frac{\partial^2 \phi}{\partial z^2} \right) = 0,
\end{aligned} \tag{3.23}$$

where the electronic dielectric constant component along a given cartesian direction κ_α has been defined as $\kappa_\alpha = 1 + \chi_\alpha$, with α = a, c. Since the spontaneous polarization is aligned with the z-direction in our tetragonal-symmetry structure, $\mathbf{P}_\mathrm{S}$ changes from $(0, 0, P_{\mathrm{S},z})$ to $(0, 0, -P_{\mathrm{S},z})$ when crossing the domain wall along x. In other words, $\frac{\partial P_{\mathrm{S},z}}{\partial x} \neq 0$ but $\frac{\partial P_{\mathrm{S},z}}{\partial z} = 0$, so

$$\nabla \cdot \mathbf{P}_\mathrm{S} = \frac{\partial P_{\mathrm{S},x}}{\partial x} + \frac{\partial P_{\mathrm{S},y}}{\partial y} + \frac{\partial P_{\mathrm{S},z}}{\partial z} = 0. \tag{3.24}$$

In conclusion, and from the results obtained in Eq. (3.22) for vacuum and Eq. (3.23) within the thin film, the electrostatic potential ϕ satisfies the following Laplace equations in the three regions of space

$$\nabla^2 \phi_1 = \nabla^2 \phi_3 = 0, \tag{3.25}$$

$$\kappa_a \frac{\partial^2 \phi_2}{\partial x^2} + \kappa_c \frac{\partial^2 \phi_2}{\partial z^2} = 0 \tag{3.26}$$

These differential equations are linear. If we find different solutions [$\phi_i^n(x,z)$, where i = (1,2,3) identifies the three regions in space] of these equations, labeled by an index n, then the general solution will be the sum of all of them,

$$\phi_i(x,z) = \sum_n \phi_i^n(x,z). \tag{3.27}$$

To find these solutions $\phi_i^n(x,z)$, we will use the method of separation of variables. To illustrate the procedure, we shall first concentrate on region 1. There, the potential can be defined as

$$\phi_1^n(x,z) = F_1^n(x) G_1^n(z). \tag{3.28}$$

Replacing this into Eq. (3.25)

$$\frac{\mathrm{d}^2 F_1^n(x)}{\mathrm{d}x^2} G_1^n(z) + F_1^n(x) \frac{\mathrm{d}^2 G_1^n(z)}{\mathrm{d}z^2} = 0. \tag{3.29}$$

The trivial solution is discarded and it is assumed that $F_1^n(x) \neq 0$ and $G_1^n(z) \neq 0$. From Eq. (3.29)

$$-\frac{1}{F_1^n(x)} \frac{\mathrm{d}^2 F_1^n(x)}{\mathrm{d}x^2} = \frac{1}{G_1^n(z)} \frac{\mathrm{d}^2 G_1^n(z)}{\mathrm{d}z^2} \tag{3.30}$$

The left side of this equation is a function only of x, and the right side is a function only of z. For that to be true, each side must be constant (let us call it λ_n^2). In this way, the only thing to do is to solve the two ordinary differential equations with constant coefficients

$$\frac{\mathrm{d}^2 F_1^n(x)}{\mathrm{d}x^2} = -\lambda_n^2 F_1^n(x), \tag{3.31}$$

$$\frac{\mathrm{d}^2 G_1^n(z)}{\mathrm{d}z^2} = \lambda_n^2 G_1^n(z). \tag{3.32}$$

The general solutions of Eq. (3.31) and Eq. (3.32) are

$$F_1^n(x) = a_n^{(1)} e^{i\lambda_n x} + b_n^{(1)} e^{-i\lambda_n x}, \tag{3.33}$$

and

$$G_1^n(z) = c_n^{(1)} e^{\lambda_n z} + d_n^{(1)} e^{-\lambda_n z}. \tag{3.34}$$

Since the potentials must be periodic in x, with the periodicity of the domain structure W, then the constants λ_n must be equal to the different harmonics $2\pi n/W$. To simplify the notation, we can define

$$k = \frac{2\pi}{W}, \tag{3.35}$$

where $W = W_+ + W_-$, and then $\lambda_n = nk$. Thus introducing Eq. (3.33) and Eq. (3.34) into Eq. (3.28), and then summing over all the harmonics as shown in Eq. (3.27),

$$\phi_1(x,z) = \sum_{n=0}^{\infty} \left(a_n^{(1)} e^{inkx} + b_n^{(1)} e^{-inkx} \right) \left(c_n^{(1)} e^{nkz} + d_n^{(1)} e^{-nkz} \right). \tag{3.36}$$

In the previous sum, we can particularize and take out of the sum the solution with $n = 0$, that would correspond to $\lambda_{n=0} = 0$. In this particular case, two possible solutions of Eq. (3.31) and Eq. (3.32) are possible. Since $\lambda = 0$ and considering that always $F(x)$ must be periodic with the periodicity of the domains, then we can take $F_1^{n=0}(x)$ as a constant. In this case, Eq. (3.31) trivially verifies. Then, for $G_1^{n=0}(z)$ two possible solutions might satisfy Eq. (3.32): $G_1^{n=0}(z)$ constant, or $G_1^{n=0}(z)$ linearly dependent with z. Which solution is the most appropriate for every region will be discussed below. Thus, calling to this generic solution $a_0^{(1)}(z)$,

$$\phi_1(x,z) = a_0^{(1)}(z) + \sum_{n=1}^{\infty} \left(a_n^{(1)} e^{inkx} + b_n^{(1)} e^{-inkx} \right) \left(c_n^{(1)} e^{nkz} + d_n^{(1)} e^{-nkz} \right). \tag{3.37}$$

In region 3, the potential has the same shape as in region 1 but with different coefficients and constant

$$\phi_3(x,z) = a_0^{(3)}(z) + \sum_{n=1}^{\infty} (a_n^{(3)} e^{inkx} + b_n^{(3)} e^{-inkx})(c_n^{(3)} e^{nkz} + d_n^{(3)} e^{-nkz}). \tag{3.38}$$

In region 2, substituting the proposed solution into the Laplace equation [Eq. (3.26)] for this region

$$\begin{gathered} \left(\kappa_a \frac{\partial^2}{\partial x^2} + \kappa_c \frac{\partial^2}{\partial z^2} \right) \phi_2 = 0 \\ \kappa_a \frac{d^2 F_2^n(x)}{dx^2} G_2^n(z) + \kappa_c F_2^n \frac{d^2 G_2^n(z)}{dz^2} = 0. \end{gathered} \tag{3.39}$$

Rewriting Eq. (3.39)

$$-\kappa_a \frac{1}{F_2^n(x)} \frac{d^2 F_2^n(x)}{dx^2} = \kappa_c \frac{1}{G_2^n(z)} \frac{d^2 G_2^n(z)}{dz^2}, \tag{3.40}$$

and, as in the previous case, Eq. (3.40) has solution only if the two terms are equal to a constant λ_n^2.

$$\begin{gathered} -\kappa_a \frac{d^2 F_2^n(x)}{dx^2} = \lambda_n^2 F_2^n(x), \\ \kappa_c \frac{d^2 G_2^n(z)}{dz^2} = \lambda_n^2 G_2^n(z). \end{gathered} \tag{3.41}$$

In this case, and following the same procedure used to obtain the potential as we did for region 1, it is found that

$$\phi_2(x,z) = a_0^{(2)}(z) + \sum_{n=1}^{\infty} (a_n^{(2)} e^{i\frac{\lambda_n}{\sqrt{\kappa_a}}x} + b_n^{(2)} e^{-i\frac{\lambda_n}{\sqrt{\kappa_a}}x})(c_n^{(2)} e^{\frac{\lambda_n}{\sqrt{\kappa_c}}z} + d_n^{(2)} e^{-\frac{\lambda_n}{\sqrt{\kappa_c}}z}) \tag{3.42}$$

Again, since the polarization is an even function, periodic along the $x-$ direction [see Eq. (3.3)], we expect that the potential along x must be also periodic with the same periodicity. Therefore, for region 2

$$\frac{\lambda_n}{\sqrt{\kappa_a}} = n\frac{2\pi}{W} = nk, \tag{3.43}$$

and

$$\phi_2(x,z) = a_0^{(2)}(z) + \sum_{n=1}^{\infty}(a_n^{(2)}e^{inkx} + b_n^{(2)}e^{-inkx})(c_n^{(2)}e^{nkcz} + d_n^{(2)}e^{-nkcz}), \tag{3.44}$$

where we have introduced the factor $c = \sqrt{\frac{\kappa_a}{\kappa_c}}$.

Besides, the even parity condition implies that the following relationship between the coefficients $a_n^{(1)} = b_n^{(1)}$, $a_n^{(2)} = b_n^{(2)}$, and $a_n^{(3)} = b_n^{(3)}$ must be complied, so the solutions of the potentials for the x direction can be replaced by even and periodic cosine functions.

Under these conditions,

$$\begin{aligned}
\phi_1(x,z) &= a_0^{(1)}(z) + \sum_{n=1}^{\infty} 2a_n^{(1)}\cos(nkx)(c_n^{(1)}e^{nkz} + d_n^{(1)}e^{-nkz}), \\
\phi_2(x,z) &= a_0^{(2)}(z) + \sum_{n=1}^{\infty} 2a_n^{(2)}\cos(nkx)(c_n^{(2)}e^{nkcz} + d_n^{(2)}e^{-nkcz}), \\
\phi_3(x,z) &= a_0^{(3)}(z) + \sum_{n=1}^{\infty} 2a_n^{(3)}\cos(nkx)(c_n^{(3)}e^{nkz} + d_n^{(3)}e^{-nkz}),
\end{aligned} \tag{3.45}$$

The prefactors $2 \times a_n^{(i)}$ for the corresponding regions 1, 2, and 3 can be absorbed into the coefficients $c_n^{(i)}$ and $d_n^{(i)}$, defining new coefficients $c_n'^{(i)} = 2a_n^{(i)}c_n^{(i)}$, and $d_n'^{(i)} = 2a_n^{(i)}d_n^{(i)}$

$$\begin{aligned}
\phi_1(x,z) &= a_0^{(1)}(z) + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(1)}e^{nkz} + d_n'^{(1)}e^{-nkz}), \\
\phi_2(x,z) &= a_0^{(2)}(z) + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(2)}e^{nkcz} + d_n'^{(2)}e^{-nkcz}), \\
\phi_3(x,z) &= a_0^{(3)}(z) + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(3)}e^{nkz} + d_n'^{(3)}e^{-nkz}).
\end{aligned} \tag{3.46}$$

The next step is to find values for the coefficients $c_n'^{(i)}$ and $d_n'^{(i)}$ for the three regions. For that, we shall make use of our **boundary conditions**

- The field in the vacuum regions 1 and 3 must vanish when $z \to +\infty$, and $z \to -\infty$, respectively. This provides the following two constraints
$$c_n'^{(1)} = d_n'^{(3)} = 0. \tag{3.47}$$

- The potentials must be equal at the interfaces of the thin films with the vacuum, providing another two constraints
$$\begin{aligned}
\phi_2(x, z=0) &= \phi_1(x, z=0), \\
\phi_2(x, z=-d) &= \phi_3(x, z=-d),
\end{aligned} \tag{3.48}$$
for any value of x. Since the potentials at the interface are the same at the two sides of the interface, the in-plane components of their gradient (i.e. the in-plane components of the field) must be equal. Therefore, the boundary conditions for the tangential components of the electric field at the interface [29] are automatically satisfied.

- Since we are assuming the absence of free charges, the normal components (i.e. along the z-direction) of the displacement fields must also be preserved. This condition implies the two following constraints, one for each surface of the ferroelectric layer

$$(\mathbf{D}_1 - \mathbf{D}_2) \cdot \hat{\boldsymbol{n}} = 0 \Rightarrow D_{1,z} = D_{2,z}, \tag{3.49}$$
$$(\mathbf{D}_2 - \mathbf{D}_3) \cdot \hat{\boldsymbol{n}} = 0 \Rightarrow D_{2,z} = D_{3,z}, \tag{3.50}$$

where $\hat{\boldsymbol{n}}$ is a unitary vector field normal to the surface. Since $\mathbf{D} = \varepsilon_0 \boldsymbol{\mathcal{E}} + \mathbf{P}$, and there is no polarization in the vacuum regions, then

$$\begin{aligned} &\mathbf{D}_1 = \varepsilon_0 \boldsymbol{\mathcal{E}}_1, \\ &\mathbf{D}_2 = \varepsilon_0 \boldsymbol{\mathcal{E}}_2 + \mathbf{P} = \varepsilon_0 \boldsymbol{\mathcal{E}}_2 + (\mathbf{P}_\mathrm{S} + \varepsilon_0 \overleftrightarrow{\chi} \boldsymbol{\mathcal{E}}_2) = \varepsilon_0 \overleftrightarrow{\kappa} \boldsymbol{\mathcal{E}}_2 + \mathbf{P}_\mathrm{S} = \varepsilon_0 \kappa_a \mathcal{E}_x^{(2)} \mathbf{u}_x + (\varepsilon_0 \kappa_c \mathcal{E}_z^{(2)} + P_\mathrm{S}(x)) \mathbf{u}_z, \\ &\mathbf{D}_3 = \varepsilon_0 \boldsymbol{\mathcal{E}}_3. \end{aligned} \tag{3.51}$$

In the previous equation, the double arrow on top of susceptibility or dielectric permittivity indicates that they are tensors with different values along the x and z directions.

Now, knowing the electric fields can be written as gradients of the potentials, $\boldsymbol{\mathcal{E}} = -\nabla \phi$,

$$\begin{aligned} \mathbf{D}_1 &= -\varepsilon_0 \nabla \phi_1 = -\varepsilon_0 \frac{\partial \phi_1}{\partial x} \mathbf{u}_x - \varepsilon_0 \frac{\partial \phi_1}{\partial z} \mathbf{u}_z, \\ \mathbf{D}_2 &= -\varepsilon_0 \kappa_a \frac{\partial \phi_2}{\partial x} \mathbf{u}_x + \left[-\varepsilon_0 \kappa_c \frac{\partial \phi_2}{\partial z} + P_S(x) \right] \mathbf{u}_z, \\ \mathbf{D}_3 &= -\varepsilon_0 \nabla \phi_3 = -\varepsilon_0 \frac{\partial \phi_3}{\partial x} \mathbf{u}_x - \varepsilon_0 \frac{\partial \phi_3}{\partial z} \mathbf{u}_z. \end{aligned} \tag{3.52}$$

From the continuity condition expressed in Eq. (3.49) at the interface between the regions 1 and 2, located at $z = 0$,

$$-\varepsilon_0 \left. \frac{\partial \phi_1}{\partial z} \right|_{z=0} = -\varepsilon_0 \kappa_c \left. \frac{\partial \phi_2}{\partial z} \right|_{z=0} + P_\mathrm{S}(x) \Rightarrow \kappa_c \left. \frac{\partial \phi_2}{\partial z} \right|_{z=0} - \left. \frac{\partial \phi_1}{\partial z} \right|_{z=0} = \frac{1}{\varepsilon_0} P_\mathrm{S}(x). \tag{3.53}$$

From the continuity condition expressed in Eq. (3.50) at the interface between the regions 2 and 3, located at $z = -d$,

$$-\varepsilon_0 \left. \frac{\partial \phi_3}{\partial z} \right|_{z=-d} = -\varepsilon_0 \kappa_c \left. \frac{\partial \phi_2}{\partial z} \right|_{z=-d} + P_\mathrm{S}(x, z=0) \Rightarrow \kappa_c \left. \frac{\partial \phi_2}{\partial z} \right|_{z=-d} - \left. \frac{\partial \phi_3}{\partial z} \right|_{z=-d} = \frac{1}{\varepsilon_0} P_\mathrm{S}(x, z=-d). \tag{3.54}$$

Besides, we can obtain the $n = 0$ terms from the conditions imposed above. From Eq. (3.49) and Eq. (3.50), the normal component of the displacement vector field along z must be preserved everywhere. In vacuum, there is no polarization and, from the first condition above the electric field also vanishes. Therefore, $D_{1,z} = D_{2,z} = D_{3,z} = 0$, and

$$D_{2,z} = -\varepsilon_0 \kappa_c \frac{\partial \phi_2}{\partial z} + P_\mathrm{S}(x) = 0. \tag{3.55}$$

Both ϕ_2 [Eq. (3.46)] and P_S [Eq. (3.3)] are expressed as a linear combination of periodic functions with different harmonics. Every harmonic is linearly independent of the others. Therefore, we can apply Eq. (3.55) to each of them. Doing so for the zero-th order term ($n = 0$),

$$\begin{aligned} &-\varepsilon_0 \kappa_c \frac{d a_0^{(2)}}{dz} + A P_\mathrm{S} = 0, \\ &\frac{d a_0^{(2)}}{dz} = \frac{1}{\varepsilon_0 \kappa_c} A P_\mathrm{S}, \\ &a_0^{(2)} = \frac{A P_\mathrm{S}}{\varepsilon_0 \kappa_c} z + C, \end{aligned} \tag{3.56}$$

where C is an integration constant. This can be solved assuming the electrostatic potential in the vacuum region 1 is flat (no electric field) and setting the value of this potential to 0. Then, according to the continuity condition for the normal component of the displacement field at $z = 0$ between regions 1 and 2, $C = 0$. Once this is solved, from the continuity of $\mathbf{D}$ at the other surface between regions 2 and 3 at $z = -d$, we can conclude that

$$
\begin{aligned}
a_0^{(1)} &= 0, \\
a_0^{(2)} &= \frac{AP_\text{S}}{\varepsilon_0 \kappa_c} z, \\
a_0^{(3)} &= -\frac{AP_\text{S}}{\varepsilon_0 \kappa_c} d.
\end{aligned} \tag{3.57}
$$

If we take into account the value for the first term of each of the series and the fact that the electric fields in the vacuum regions cancel out at infinity [Eq. (3.47)], the potentials given in Eq. (3.46) can be written as follows

$$
\begin{aligned}
\phi_1(x,z) &= \sum_{n=1}^{\infty} d_n'^{(1)} \cos(nkx) e^{-nkz}, \\
\phi_2(x,z) &= \frac{AP_\text{S}}{\varepsilon_0 \kappa_c} z + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(2)} e^{nkcz} + d_n'^{(2)} e^{-nkcz}), \\
\phi_3(x,z) &= -\frac{AP_\text{S}}{\varepsilon_0 \kappa_c} d + \sum_{n=1}^{\infty} c_n'^{(3)} \cos(nkx) e^{nkz}.
\end{aligned} \tag{3.58}
$$

In order to obtain the expression for the remaining unknown coefficients in Eq. (3.58), the fact that the potentials and the normal component of the displacement vectors must be equal on the surfaces of the film can be used. In this way, applying the second condition stated above

$$
\phi_1(x, z=0) = \phi_2(x, z=0) \Rightarrow \sum_{n=1}^{\infty} d_n'^{(1)} \cos(nkx) = \sum_{n=1}^{\infty} (c_n'^{(2)} + d_n'^{(2)}) \cos(nkx) \Rightarrow d_n'^{(1)} = c_n'^{(2)} + d_n'^{(2)} \tag{3.59}
$$

$$
\begin{aligned}
\phi_2(x, z=-d) = \phi_3(x, z=-d) \Rightarrow -\frac{AP_\text{S}}{\varepsilon_0 \kappa_c} d + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(2)} e^{-nkcd} + d_n'^{(2)} e^{nkcd}) = -\frac{AP_\text{S}}{\varepsilon_0 \kappa_c} d + \sum_{n=1}^{\infty} c_n'^{(3)} \cos(nkx) e^{-nkd} \\
\Rightarrow c_n'^{(3)} e^{-nkd} = c_n'^{(2)} e^{-nkcd} + d_n'^{(2)} e^{nkcd}
\end{aligned} \tag{3.60}
$$

If we unify in a single variable, R, the thickness of the ferroelectric thin film, d, the width of the domains, W, and the relation between the dielectric permittivity in-plane (along x) and out-of-plane (along z), $c = \sqrt{\kappa_a / \kappa_c}$,

$$
\begin{aligned}
R &= \frac{\pi c d}{W}, \\
nkcd &= n \frac{2\pi}{W} cd = 2n \frac{\pi c d}{W} = 2nR,
\end{aligned} \tag{3.61}
$$

then Eq. (3.60)

$$
\phi_2(x, z=-d) = \phi_3(x, z=-d) \quad \Rightarrow \quad c_n'^{(3)} e^{-nkd} = c_n'^{(2)} e^{-2nR} + d_n'^{(2)} e^{2nR}. \tag{3.62}
$$

From the third condition with respect to the continuity of the normal component of the displacement vector between the regions 1 and 2, Eq. (3.53), and the expressions of the potentials in Eq. (3.58),

$$
\begin{aligned}
&\kappa_c \left. \frac{\partial \phi_2}{\partial z} \right|_{z=0} - \left. \frac{\partial \phi_1}{\partial z} \right|_{z=0} = \frac{1}{\varepsilon_0} P_\text{S}(x), \\
&\kappa_c \left. \left(\frac{AP_\text{S}}{\varepsilon_0 \kappa_c} + \sum_{n=1}^{\infty} nkc \cdot \cos(nkx)(c_n'^{(2)} e^{nkcz} - d_n'^{(2)} e^{-nkcz}) \right) \right|_{z=0} + \sum_{n=1}^{\infty} nk d_n'^{(1)} \cos(nkx) e^{-nkz} \Big|_{z=0} = \frac{P_\text{S}(x)}{\varepsilon_0}, \\
&\frac{AP_\text{S}}{\varepsilon_0} + \sum_{n=1}^{\infty} nkc\kappa_c \cdot \cos(nkx)(c_n'^{(2)} - d_n'^{(2)}) + \sum_{n=1}^{\infty} nk d_n'^{(1)} \cos(nkx) = \frac{P_\text{S}(x)}{\varepsilon_0}.
\end{aligned} \tag{3.63}
$$

Replacing the value of the polarization given in Eq. (3.3)

$$\frac{AP_{\mathrm{S}}}{\varepsilon_0} + \sum_{n=1}^{\infty} nkc\kappa_c \cos(nkx)(c_n'^{(2)} - d_n'^{(2)}) + \sum_{n=1}^{\infty} nkd_n'^{(1)} \cos(nkx) = \frac{AP_{\mathrm{S}}}{\varepsilon_0} + \sum_{n=1}^{\infty} \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx),$$

$$\sum_{n=1}^{\infty} nkc\kappa_c \cos(nkx)(c_n'^{(2)} - d_n'^{(2)}) + \sum_{n=1}^{\infty} nkd_n'^{(1)} \cos(nkx) = \sum_{n=1}^{\infty} \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx),$$

$$nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + nkd_n'^{(1)} = \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right). \tag{3.64}$$

From the third condition with respect to the continuity of the normal component of the displacement vector between the regions 2 and 3, Eq. (3.54), and the expressions of the potentials in Eq. (3.58),

$$\kappa_c \left.\frac{\partial \phi_2}{\partial z}\right|_{z=-d} - \left.\frac{\partial \phi_3}{\partial z}\right|_{z=-d} = \frac{1}{\varepsilon_0} P_{\mathrm{S}}(x),$$

$$\kappa_c \left(\frac{AP_{\mathrm{S}}}{\varepsilon_0 \kappa_c} + \sum_{n=1}^{\infty} nkc \cdot \cos(nkx)(c_n'^{(2)} e^{nkcz} - d_n'^{(2)} e^{-nkcz})\right)\Bigg|_{z=-d} - \sum_{n=1}^{\infty} nkc_n'^{(3)} \cos(nkx) e^{nkz}\Big|_{z=-d} = \frac{P_{\mathrm{S}}(x)}{\varepsilon_0},$$

$$\frac{AP_{\mathrm{S}}}{\varepsilon_0} + \sum_{n=1}^{\infty} nkc\kappa_c \cos(nkx)(c_n'^{(2)} e^{-nkcd} - d_n'^{(2)} e^{nkcd}) - \sum_{n=1}^{\infty} nkc_n'^{(3)} \cos(nkx) e^{-nkd} = \frac{P_S(x)}{\varepsilon_0}. \tag{3.65}$$

Again, replacing the value of the polarization given in Eq. (3.3)

$$\frac{AP_{\mathrm{S}}}{\varepsilon_0} + \sum_{n=1}^{\infty} nkc\kappa_c \cos(nkx)(c_n'^{(2)} e^{-nkcd} - d_n'^{(2)} e^{nkcd}) - \sum_{n=1}^{\infty} nkc_n'^{(3)} \cos(nkx) e^{-nkd} = \frac{AP_{\mathrm{S}}}{\varepsilon_0} + \sum_{n=1}^{\infty} \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx),$$

$$\sum_{n=1}^{\infty} nkc\kappa_c \cos(nkx)(c_n'^{(2)} e^{-nkcd} - d_n'^{(2)} e^{nkcd}) - \sum_{n=1}^{\infty} nkc_n'^{(3)} \cos(nkx) e^{-nkd} = \sum_{n=1}^{\infty} \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx),$$

$$nkc\kappa_c(c_n'^{(2)} e^{-nkcd} - d_n'^{(2)} e^{nkcd}) - nkc_n'^{(3)} e^{-nkd} = \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right),$$

$$nkc\kappa_c(c_n'^{(2)} e^{-2nR} - d_n'^{(2)} e^{2nR}) - nkc_n'^{(3)} e^{-nkd} = \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right). \tag{3.66}$$

Now, it is time to recap the four relationships between the different coefficients that we have obtained after applying the boundary conditions at the two surfaces

$$d_n'^{(1)} = c_n'^{(2)} + d_n'^{(2)}, \tag{3.67}$$

$$c_n'^{(3)} e^{-nkd} = c_n'^{(2)} e^{-2nR} + d_n'^{(2)} e^{2nR}, \tag{3.68}$$

$$nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + nkd_n'^{(1)} = \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right), \tag{3.69}$$

$$nkc\kappa_c(c_n'^{(2)} e^{-2nR} - d_n'^{(2)} e^{2nR}) - nkc_n'^{(3)} e^{-nkd} = \frac{4P_{\mathrm{S}}}{n\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \tag{3.70}$$

Since the right-hand side of Eq. (3.69) is equal to the right-hand side of Eq. (3.70)

$$nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + nkd_n'^{(1)} = nkc\kappa_c(c_n'^{(2)} e^{-2nR} - d_n'^{(2)} e^{2nR}) - nkc_n'^{(3)} e^{-nkd} \tag{3.71}$$

Now, replacing Eq. (3.68) into Eq. (3.71),

$$
\begin{aligned}
nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + nkd_n'^{(1)} &= nkc\kappa_c(c_n'^{(2)}e^{-2nR} - d_n'^{(2)}e^{2nR}) - nkc_n'^{(2)}e^{-2nR} - nkd_n'^{(2)}e^{2nR},\\
c\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + d_n'^{(1)} &= c\kappa_c(c_n'^{(2)}e^{-2nR} - d_n'^{(2)}e^{2nR}) - c_n'^{(2)}e^{-2nR} - d_n'^{(2)}e^{2nR}.
\end{aligned}
\tag{3.72}
$$

Finally, replacing Eq. (3.67) into Eq. (3.72),

$$
c\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + c_n'^{(2)} + d_n'^{(2)} = c\kappa_c(c_n'^{(2)}e^{-2nR} - d_n'^{(2)}e^{2nR}) - c_n'^{(2)}e^{-2nR} - d_n'^{(2)}e^{2nR}. \tag{3.73}
$$

Within Eq. (3.73), the terms in which an exponential appears will be joined on one side of the equality and on the other side those which do not have an exponential

$$
(c\kappa_c - 1)c_n'^{(2)}e^{-2nR} - (c\kappa_c + 1)d_n'^{(2)}e^{2nR} = (c\kappa_c + 1)c_n'^{(2)} + (1 - c\kappa_c)d_n'^{(2)}, \tag{3.74}
$$

and, putting together the terms with $c\kappa_c - 1$ and the terms with $c\kappa_c + 1$

$$
(c\kappa_c - 1)(c_n'^{(2)}e^{-2nR} + d_n'^{(2)}) = (c\kappa_c + 1)(c_n'^{(2)} + d_n'^{(2)}e^{2nR}). \tag{3.75}
$$

In an standard ferroelectric, such as $PbTiO_3$, $\kappa_c = 34$ and $\kappa_a = 185$, so $c = \sqrt{\kappa_a/\kappa_c} = 2.33$, and $c\kappa_c = 79.31$, almost two orders of magnitude larger than the unity. Therefore, we can take **the approach, based on these material parameters,** of $c\kappa_c + 1 \approx c\kappa_c$, and $c\kappa_c - 1 \approx c\kappa_c$. With this in mind, Eq. (3.75) reduces to

$$
c_n'^{(2)}e^{-2nR} + d_n'^{(2)} = c_n'^{(2)} + d_n'^{(2)}e^{2nR}. \tag{3.76}
$$

This equation can be rewritten as

$$
\begin{aligned}
c_n'^{(2)}e^{-2nR} + d_n'^{(2)} - c_n'^{(2)} - d_n'^{(2)}e^{2nR} = 0 \quad &\Rightarrow \quad (e^{-2nR} - 1)c_n'^{(2)} + (1 - e^{2nR})d_n'^{(2)} = 0\\
&\Rightarrow \quad d_n'^{(2)} = \frac{e^{-2nR} - 1}{e^{2nR} - 1}c_n'^{(2)}\\
&\Rightarrow \quad d_n'^{(2)} = -\frac{1 - e^{2nR}}{(1 - e^{2nR})e^{2nR}}c_n'^{(2)}\\
&\Rightarrow \quad d_n'^{(2)} = -c_n'^{(2)}e^{-2nR}.
\end{aligned}
\tag{3.77}
$$

Since the relation between $d_n'^{(2)}$ and $c_n'^{(2)}$ has already been obtained in Eq. (3.77), the ratio of all other coefficients with $c_n'^{(2)}$ can be found. For instance, from Eq. (3.67),

$$
\begin{aligned}
d_n'^{(1)} &= c_n'^{(2)} + d_n'^{(2)}\\
&= c_n'^{(2)} - c_n'^{(2)}e^{-2nR}\\
&= c_n'^{(2)}(1 - e^{-2nR})\\
&= c_n'^{(2)}e^{-2nR}(e^{2nR} - 1)\\
&= c_n'^{(2)}e^{-nR}(e^{nR} - e^{-nR})\\
&= 2c_n'^{(2)}e^{-nR}\sinh(nR).
\end{aligned}
\tag{3.78}
$$

And from Eq. (3.68)

$$
\begin{aligned}
c_n'^{(3)}e^{-nkd} &= c_n'^{(2)}e^{-2nR} + d_n'^{(2)}e^{2nR}\\
&= c_n'^{(2)}e^{-2nR} - c_n'^{(2)}\\
&= -c_n'^{(2)}e^{-nR}(e^{nR} - e^{-nR})\\
&= -2c_n'^{(2)}e^{-nR}\sinh(nR).
\end{aligned}
\tag{3.79}
$$

From Eq. (3.69), Eq. (3.77), and Eq. (3.78)

$$
\begin{aligned}
\frac{4P_\mathrm{S}}{n\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right) &= nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + nkd_n'^{(1)} \\
&= nkc\kappa_c(c_n'^{(2)} + c_n'^{(2)}e^{-2nR}) + nk2c_n'^{(2)}e^{-nR}\sinh(nR) \\
&= nk[c\kappa_c(1+e^{-2nR}) + 2e^{-nR}\sinh(nR)]c_n'^{(2)} \\
&= nk[c\kappa_c e^{-nR}(e^{nR}+e^{-nR}) + 2e^{-nR}\sinh(nR)]c_n'^{(2)} \\
&= nk[2c\kappa_c e^{-nR}\cosh(nR) + 2e^{-nR}\sinh(nR)]c_n'^{(2)} \\
&= 2nke^{-nR}[g\ \cosh(nR) + \sinh(nR)]c_n'^{(2)},
\end{aligned} \tag{3.80}
$$

where we have introduced $g = c\kappa_c$. Therefore, the value of $c_n'^{(2)}$ can be written as

$$
c_n'^{(2)} = \frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{2e^{-nR}[g\ \ \cosh(nR)+\sinh(nR)]}. \tag{3.81}
$$

Then, from Eq. (3.77)

$$
\begin{aligned}
d_n'^{(2)} &= -c_n'^{(2)}e^{-2nR} \\
&= -\frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{e^{-2nR}}{2e^{-nR}[g\cosh(nR)+\sinh(nR)]} \\
&= -\frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{e^{-nR}}{2[g\ \cosh(nR)+\sinh(nR)]},
\end{aligned} \tag{3.82}
$$

and from Eq. (3.78),

$$
\begin{aligned}
d_n'^{(1)} &= 2c_n'^{(2)}e^{-nR}\sinh(nR) \\
&= 2\frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{e^{-nR}\sinh(nR)}{2e^{-nR}[g\cosh(nR)+\sinh(nR)]} \\
&= \frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\sinh(nR)}{g\cosh(nR)+\sinh(nR)} \\
&= \frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{1+g\ \coth(nR)}.
\end{aligned} \tag{3.83}
$$

Finally, from Eq. (3.79)

$$
\begin{aligned}
c_n'^{(3)} &= -2c_n'^{(2)}e^{-nR}e^{nkd}\sinh(nR) \\
&= -2\frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{e^{-nR}e^{nkd}\sinh(nR)}{2e^{-nR}[g\ \cosh(nR)+\sinh(nR)]} \\
&= -\frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{e^{nkd}\sinh(nR)}{g\ \cosh(nR)+\sinh(nR)} \\
&= -\frac{4P_\mathrm{S}}{n^2k\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{e^{nkd}}{1+g\ \coth(nR)}.
\end{aligned} \tag{3.84}
$$

We have arrived to the point where all the coefficients that appear in Eq. (3.58) are known. Replacing them, we get the final expressions for the potentials in the three regions

$$
\begin{aligned}
\phi_1(x,z) &= \sum_{n=1}^{\infty} d_n'^{(1)} \cos(nkx) e^{-nkz} \\
&= \sum_{n=1}^{\infty} \left[\frac{4P_\mathrm{S}}{n^2 k\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{1}{1+g\ \coth(nR)} \right] \cos(nkx) e^{-nkz} \\
&= \frac{1}{4\pi\epsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} 16 P_\mathrm{S} \frac{W}{2\pi} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \frac{e^{-nkz}}{1+g\ \coth(nR)} \\
&= \frac{1}{4\pi\epsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} 8 P_\mathrm{S} \frac{\pi cd}{\pi R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \frac{e^{-nkz}}{1+g\ \coth(nR)} \\
&= \frac{1}{4\pi\epsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{8 P_\mathrm{S} cd}{R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \frac{e^{-nkz}}{1+g\ \coth(nR)},
\end{aligned} \tag{3.85}
$$

where we have used the previously introduced definitions for $k = 2\pi/W$, and $R = \pi cd/W$.

For the potential in the region 2, we have

$$
\begin{aligned}
\phi_2(x,z) &= \frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} z + \sum_{n=1}^{\infty} \cos(nkx) (c_n'^{(2)} e^{nkcz} + d_n'^{(2)} e^{-nkcz}) \\
&= \frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} z + \sum_{n=1}^{\infty} \cos(nkx) \left[\left(\frac{4P_\mathrm{S}}{n^2 k\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{1}{2e^{-nR}[g\ \cosh(nR)+\sinh(nR)]} \right) e^{nkcz} + \right. \\
&\qquad \left. + \left(-\frac{4P_\mathrm{S}}{n^2 k\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{e^{-nR}}{2[g\ \cosh(nR)+\sinh(nR)]} e^{-nkcz} \right) \right] \\
&= \frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} z + \frac{1}{\pi\varepsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} 4P_\mathrm{S} \frac{W}{2\pi} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \left[\frac{e^{nkcz}}{2e^{-nR}[g\ \cosh(nR)+\sinh(nR)]} - \right. \\
&\qquad \left. - \frac{e^{-nR} e^{-nkcz}}{2[g\ \cosh(nR)+\sinh(nR)]} \right] \\
&= \frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} z + \frac{1}{4\pi\varepsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} 16P_\mathrm{S} \frac{\pi cd}{2\pi R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \left[\frac{e^{nR} e^{nkcz}}{2[g\ \cosh(nR)+\sinh(nR)]} - \right. \\
&\qquad \left. - \frac{e^{-nR} e^{-nkcz}}{2[g\ \cosh(nR)+\sinh(nR)]} \right] \\
&= \frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} z + \frac{1}{4\pi\varepsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} 16P_\mathrm{S} \frac{cd}{2R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \left[\frac{e^{nR} e^{nkcz} - e^{-nR} e^{-nkcz}}{2[g\ \cosh(nR)+\sinh(nR)]} \right] \\
&= \frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} z + \frac{1}{4\pi\varepsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{8P_\mathrm{S} cd}{R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \left[\frac{\sinh(nR + cnkz)}{[g\ \cosh(nR)+\sinh(nR)]} \right].
\end{aligned} \tag{3.86}
$$

Finally, for the potential in the third region,

$$
\begin{aligned}
\phi_3(x,z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} d + \sum_{n=1}^{\infty} c_n'^{(3)} \cos(nkx) e^{nkz} \\
&= -\frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} d + \sum_{n=1}^{\infty} \left[-\frac{4P_\mathrm{S}}{n^2 k\pi\varepsilon_0} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{e^{nkd}}{1+g\ \coth(nR)} \right] \cos(nkx) e^{nkz} \\
&= -\frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} d + \frac{1}{\pi\varepsilon_0} \sum_{n=1}^{\infty} \left[-\frac{4P_\mathrm{S}}{n^2} \frac{W}{2\pi} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{e^{nk(d+z)}}{1+g\ \coth(nR)} \right] \cos(nkx) \\
&= -\frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} d - \frac{1}{4\pi\varepsilon_0} \sum_{n=1}^{\infty} \frac{16P_\mathrm{S}}{n^2} \frac{\pi cd}{2\pi R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \frac{e^{nk(d+z)}}{1+g\ \coth(nR)} \\
&= -\frac{AP_\mathrm{S}}{\varepsilon_0\kappa_c} d - \frac{1}{4\pi\varepsilon_0} \sum_{n=1}^{\infty} \frac{1}{n^2} \frac{8P_\mathrm{S} cd}{R} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) \frac{e^{nk(d+z)}}{1+g\ \coth(nR)}
\end{aligned} \tag{3.87}
$$

To simplify the notation, some constants of the potentials of the Eqs. (3.85)-(3.87) will be renamed as follows

$$\begin{aligned}\alpha &= \frac{1}{4\pi\varepsilon_0}\left(\frac{8P_{\mathrm{S}}cd}{R}\right)\\ \beta_n &= \frac{1}{\sinh(nR)+g\cosh(nR)}\\ \gamma_n &= \frac{1}{1+g\coth(nR)}\end{aligned} \tag{3.88}$$

so that the expressions of the potentials are

$$\phi_1(x,z) = \alpha\sum_{n=1}^{\infty}\frac{\gamma_n}{n^2}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx)e^{-nkz}, \tag{3.89}$$

$$\phi_2(x,z) = \frac{AP_S}{\varepsilon_0\kappa_c}z+\alpha\sum_{n=1}^{\infty}\frac{\beta_n}{n^2}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx)\sinh(nR+cnkz), \tag{3.90}$$

$$\phi_3(x,z) = -\frac{AP_S}{\varepsilon_0\kappa_c}d-\alpha\sum_{n=1}^{\infty}\frac{\gamma_n}{n^2}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx)e^{nk(z+d)}. \tag{3.91}$$

These potentials are written (with some typos) in Eq.(5.2.15a)-(5.2.15c) in Ref. [18]. But, as shown before, its derivation is far from trivial.

Taking into account the above potentials, we can obtain a figure with the equipotential lines in a $(x,\, z)$ plane (see Fig. 7)

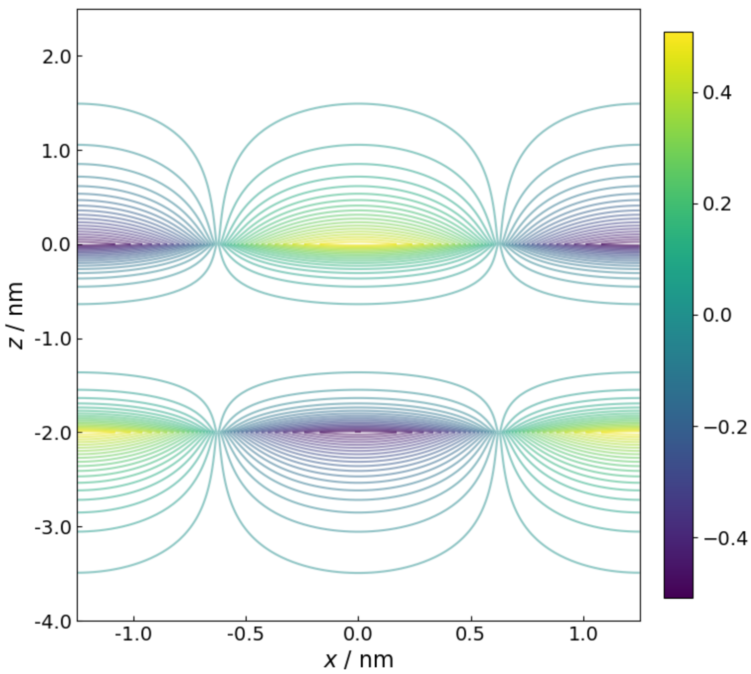


Figure 7: Equipotential lines in a $(x,\, z)$ plane for a ferroelectric thin film thickness of $d = 2$ nm. In this figure, the color of the lines represents the value of the potential according to the color bar on the right. The parameters used to create this figure are: $P_{\mathrm{S}} = 0.78$ C·m^{-2}, $\kappa_a = 185$, $\kappa_c = 34$, $W = 2.5$ nm and $A = 0$.

3.2.4 Electric fields

Once the electrostatic potentials for the three regions in space are known, we can compute the corresponding electric fields applying in each region $\boldsymbol{\mathcal{E}} = -\nabla\phi$. Therefore, for region 1, taking the gradient of the potential written in Eq. (3.89),

$$\mathcal{E}_x^{(1)} = -\frac{\partial \phi_1}{\partial x} = \alpha \sum_{n=1}^{\infty} \frac{\gamma_n}{n^2} \sin\left(\frac{n\pi}{2}(A+1)\right) nk \sin(nkx) e^{-nkz}$$
$$= \alpha k \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \sin(nkx)\gamma_n e^{-nkz}, \tag{3.92}$$
$$\mathcal{E}_z^{(1)} = -\frac{\partial \phi_1}{\partial z} = -\alpha \sum_{n=1}^{\infty} \frac{\gamma_n}{n^2} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx)(-nk) e^{-nkz}$$
$$= \alpha k \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \cos(nkx)\gamma_n e^{-nkz}. \tag{3.93}$$

For region 2, taking the gradient of Eq. (3.90),

$$\mathcal{E}_x^{(2)} = -\frac{\partial \phi_2}{\partial x} = \alpha \sum_{n=1}^{\infty} \frac{\beta_n}{n^2} \sin\left(\frac{n\pi}{2}(A+1)\right) nk \sin(nkx) \sinh(nR + cnkz)$$
$$= \alpha k \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \sin(nkx)\beta_n \sinh(nR + cnkz), \tag{3.94}$$
$$\mathcal{E}_z^{(2)} = -\frac{\partial \phi_2}{\partial z} = -\frac{AP_{\mathrm{S}}}{\varepsilon_0 \kappa_c} - \alpha \sum_{n=1}^{\infty} \frac{\beta_n}{n^2} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) cnk \cosh(nR + cnkz)$$
$$= -\frac{AP_{\mathrm{S}}}{\varepsilon_0 \kappa_c} - \alpha kc \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \cos(nkx)\beta_n \cosh(nR + cnkz). \tag{3.95}$$

Finally, for region 3, starting from the potential given in Eq. (3.91)

$$\mathcal{E}_x^{(3)} = -\frac{\partial \phi_3}{\partial x} = \alpha \sum_{n=1}^{\infty} \frac{\gamma_n}{n^2} \sin\left(\frac{n\pi}{2}(A+1)\right) (-nk) \sin(nkx) e^{nk(z+d)}$$
$$= -\alpha k \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \sin(nkx)\gamma_n e^{nk(z+d)}, \tag{3.96}$$
$$\mathcal{E}_z^{(3)} = -\frac{\partial \phi_3}{\partial z} = \alpha \sum_{n=1}^{\infty} \frac{\gamma_n}{n^2} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx)(nk) e^{nk(z+d)}$$
$$= \alpha k \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \cos(nkx)\gamma_n e^{nk(z+d)}. \tag{3.97}$$

One important approximation in this model is that, although there is an in-plane component of the field along x, and the in-plane electronic susceptibility of the ferroelectric thin film does not vanish, **the model does not consider the development of an in-plane polarization.**

Considering the components of the electric field for each region obtained above, we can create a figure that represents the electric field in a $(x,\, z)$ plane (see Fig. 8)

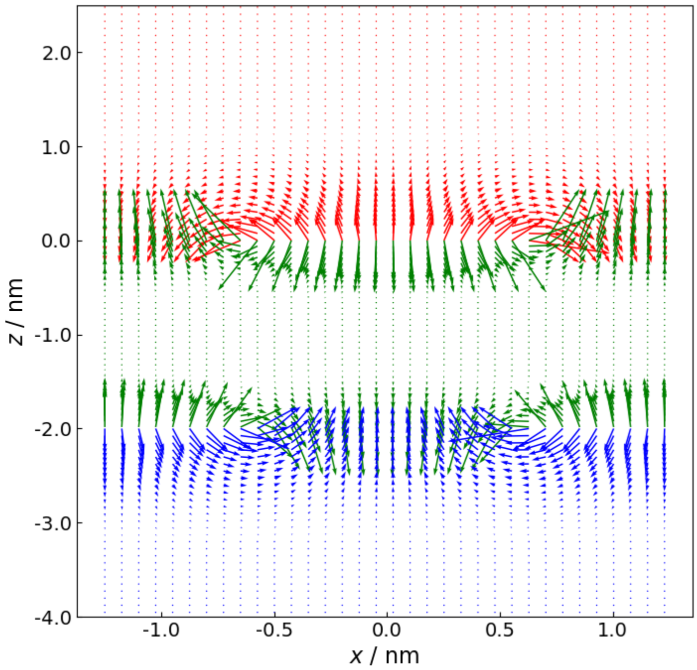


Figure 8: Electric field in a (x,z) plane for a ferroelectric thin film thickness of $d = 2$ nm. The electric field in region 1 is identified by red vectors, in region 2 by green vectors and in region 3 by blue vectors. The length of each vector indicates the intensity of the electric field at that point in the plane. The parameters used to create this figure are: $P_{\rm S} = 0.78$ C·m^{-2}, $\kappa_a = 185$, $\kappa_c = 34$, $W = 2.5$ nm and $A = 0$.

3.2.5 Electrostatic energy

In the vacuum regions, the total electrostatic energy can be written as [30]

$$U^{\rm elec}_{\rm vacuum} = \frac{\varepsilon_0}{2} \int \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{E}} \; dV, \tag{3.98}$$

where the integral is taken over the corresponding vacuum regions.

Within the ferroelectric layer, the total electrostatic energy is given by [29]

$$U^{\rm elec}_{\rm ferro} = \frac{\varepsilon_0}{2} \int \boldsymbol{\mathcal{E}} \cdot \mathbf{D} \; dV. \tag{3.99}$$

where the integral is taken over the volume of the ferroelectric thin film. The units of both $U^{\rm elec}_{\rm vacuum}$, and $U^{\rm elec}_{\rm ferro}$ are Joules in the international system.

Let us compute the electrostatic energy stored in the vacuum region 1. Again, in this section we are going to present an step by step derivation of the different expressions. Although it is very verbose, it will help to speed up the later computation in more complex systems (like the ferroelectric/dielectric superlattices or the ferroelectric thin films on top of a substrate). Without any doubt, such derivations will guide future students and newcomers in the field. The square of the electric fields given by Eq. (3.92) and Eq. (3.93) are

$$\begin{aligned}
\mathcal{E}_x^{(1)2} &= (\alpha k)^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\gamma_n}{n} \sin\left(\frac{n\pi}{2}(A+1)\right) \sin(nkx) e^{-nkz} \frac{\gamma_m}{m} \sin\left(\frac{m\pi}{2}(A+1)\right) \sin(mkx) e^{-mkz}, \\
\mathcal{E}_z^{(1)2} &= (\alpha k)^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\gamma_n}{n} \sin\left(\frac{n\pi}{2}(A+1)\right) \cos(nkx) e^{-nkz} \frac{\gamma_m}{m} \sin\left(\frac{m\pi}{2}(A+1)\right) \cos(mkx) e^{-mkz}
\end{aligned} \tag{3.100}$$

Taking these expressions into account, $U^{\rm elec}_{\rm vacuum(1)}$ can be calculated from Eq. (3.98). Since we have assumed that all the physical magnitudes are periodic along the y-direction, we can integrate only in the (x,z) plane to obtain the energy per unit length along y.

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{vacuum(1)}}}{L_y} &= \int \frac{\varepsilon_0}{2}\left[\mathcal{E}_x^{(1)2}+\mathcal{E}_z^{(1)2}\right]dxdz \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2\int\Bigg[\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{\gamma_n}{n}\sin\left(\frac{n\pi}{2}(A+1)\right)\sin(nkx)e^{-nkz}\frac{\gamma_m}{m}\sin\left(\frac{m\pi}{2}(A+1)\right)\sin(mkx)e^{-mkz}+ \\
&\quad +\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{\gamma_n}{n}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx)e^{-nkz}\frac{\gamma_m}{m}\sin\left(\frac{m\pi}{2}(A+1)\right)\cos(mkx)e^{-mkz}\Bigg]dxdz.
\end{aligned} \tag{3.101}$$

Let us integrate this electrostatic energy over one period of length W along the x direction, and over all the extension of the vacuum region on top of the film (z ranging between 0 and ∞). If the result is divided by the domain width, the electrostatic energy will be given in units of energy/domain area.

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{vacuum(1)}}}{L_yW} = \frac{\varepsilon_0}{2W}(\alpha k)^2\sum_{n=1}^{\infty}\frac{\gamma_n^2}{n^2}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\Bigg[&\int_{-W/2}^{W/2}\sin^2(nkx)dx\int_0^{\infty}e^{-2nkz}dz+ \\
&+\int_{-W/2}^{W/2}\cos^2(nkx)dx\int_0^{\infty}e^{-2nkz}dz\Bigg],
\end{aligned} \tag{3.102}$$

where we have applied the orthogonality relations of sines and cosines

$$\int_{-W/2}^{W/2}\sin(nkx)\sin(mkx)dx \text{ and } \int_{-W/2}^{W/2}\cos(nkx)\cos(mkx)dx \begin{cases}=0 & \text{if } n\neq m\\ \neq 0 & \text{if } n=m\end{cases}, \quad n>0 \tag{3.103}$$

Now, using this property

$$\begin{aligned}
\int_{-\frac{W}{2}}^{\frac{W}{2}}\cos^2(nkx)dx &= \int_{-\frac{W}{2}}^{\frac{W}{2}}\frac{\cos(2nkx)+1}{2}dx \\
&= \frac{1}{4nk}\sin(2nkx)\Big|_{-\frac{W}{2}}^{\frac{W}{2}}+\frac{1}{2}\left(\frac{W}{2}+\frac{W}{2}\right) \\
&= \frac{1}{4nk}2\sin(2n\pi)+\frac{W}{2} \\
&= \frac{W}{2},
\end{aligned} \tag{3.104}$$

and

$$\begin{aligned}
\int_{-\frac{W}{2}}^{\frac{W}{2}}\sin^2(nkx)dx &= \int_{-\frac{W}{2}}^{\frac{W}{2}}\frac{1-\cos(2nkx)}{2}dx \\
&= \frac{1}{2}\left(\frac{W}{2}+\frac{W}{2}\right)-\frac{1}{4nk}\sin(2nkx)\Big|_{-\frac{W}{2}}^{\frac{W}{2}} \\
&= \frac{W}{2}-\frac{1}{4nk}2\sin(2n\pi) \\
&= \frac{W}{2},
\end{aligned} \tag{3.105}$$

then

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{vacuum}(1)}}{L_y W} &= \frac{\varepsilon_0}{2W}(\alpha k)^2 \sum_{n=1}^{\infty} \frac{\gamma_n^2}{n^2} \sin^2\left(\frac{n\pi}{2}(A+1)\right) \left[\frac{W}{2}\int_0^{\infty} e^{-2nkz} dz + \frac{W}{2}\int_0^{\infty} e^{-2nkz} dz\right] \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty} \frac{\gamma_n^2}{n^2} \sin^2\left(\frac{n\pi}{2}(A+1)\right) \left[\frac{1}{2}\left(-\frac{1}{2nk} e^{-2nkz}\Big|_0^{\infty}\right) + \frac{1}{2}\left(-\frac{1}{2nk} e^{-2nkz}\Big|_0^{\infty}\right)\right] \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty} \frac{\gamma_n^2}{n^2} \sin^2\left(\frac{n\pi}{2}(A+1)\right) \left(\frac{1}{2}\frac{1}{2nk} + \frac{1}{2}\frac{1}{2nk}\right) \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty} \frac{\gamma_n^2}{n^2} \sin^2\left(\frac{n\pi}{2}(A+1)\right) \frac{1}{2nk} \\
&= \frac{\varepsilon_0}{4}\alpha^2 k \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2 \\
&= \frac{\varepsilon_0}{4}\frac{1}{16\pi^2\varepsilon_0^2}\left(\frac{8P_{\rm S}cd}{R}\right)^2 k \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2 \\
&= \frac{1}{4}\frac{4P_{\rm S}^2c^2d^2}{\pi^2\varepsilon_0 R^2} k \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2 \\
&= \frac{1}{4}\frac{4P_{\rm S}^2c^2d^2}{\pi^2\varepsilon_0 R\frac{\pi cd}{W}} \frac{2\pi}{W} \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2 \\
&= \frac{1}{4}\frac{8P_{\rm S}^2cd}{\pi^2\varepsilon_0 R} \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2 \\
&= \frac{1}{4}\frac{8P_{\rm S}^2gd}{\pi^2\varepsilon_0 R\kappa_c} \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2,
\end{aligned} \tag{3.106}
$$

where we have made use again of the fact that $g = c\kappa_c$, and some of the expressions written in Eq. (3.61) and Eq. (3.88).

Following the same recipe, we can compute the electrostatic energy stored in the vacuum region 3. The square of the electric fields given by Eq. (3.96) and Eq. (3.97) are

$$
\begin{aligned}
\mathcal{E}_x^{(3)2} &= (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\gamma_n}{n}\sin\left(\frac{n\pi}{2}(A+1)\right)\sin(nkx)e^{nk(z+d)}\frac{\gamma_m}{m}\sin\left(\frac{m\pi}{2}(A+1)\right)\sin(mkx)e^{mk(z+d)}, \\
\mathcal{E}_z^{(3)2} &= (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\gamma_n}{n}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx)e^{nk(z+d)}\frac{\gamma_m}{m}\sin\left(\frac{m\pi}{2}(A+1)\right)\cos(mkx)e^{mk(z+d)}.
\end{aligned} \tag{3.107}
$$

Then $U^{\text{elec}}_{\text{vacuum}(3)}$ can be calculated again from Eq. (3.98). Integrating only in the $(x,\ z)$ plane, we obtain $U^{\text{elec}}_{\text{vacuum}(3)}$ per unit length along y

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{vacuum}(3)}}{L_y} &= \int \frac{\varepsilon_0}{2}\left[\mathcal{E}_x^{(3)2} + \mathcal{E}_z^{(3)2}\right] dxdz \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2 \int \Bigg[\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\gamma_n}{n}\sin\left(\frac{n\pi}{2}(A+1)\right)\sin(nkx)e^{nk(z+d)}\frac{\gamma_m}{m}\sin\left(\frac{m\pi}{2}(A+1)\right)\sin(mkx)e^{mk(z+d)} + \\
&\qquad + \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\gamma_n}{n}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx)e^{nk(z+d)}\frac{\gamma_m}{m}\sin\left(\frac{m\pi}{2}(A+1)\right)\cos(mkx)e^{mk(z+d)}\Bigg] dxdz
\end{aligned} \tag{3.108}
$$

Doing the same as in the previous region but, in this case, integrating in z from $-\infty$ to $-d$, the electrostatic energy of the region 3 will be given in units of energy/domain area as well

$$\frac{U^{\rm elec}_{\rm vacuum(3)}}{L_yW} = \frac{\varepsilon_0}{2}(\alpha k)^2\sum_{n=1}^{\infty}\frac{\gamma_n^2}{n^2}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{W}\left[\int_{-W/2}^{W/2}\sin^2(nkx)dx\int_{-\infty}^{-d}e^{2nk(z+d)}dz+ \right.$$
$$\left. +\int_{-W/2}^{W/2}\cos^2(nkx)dx\int_{-\infty}^{-d}e^{2nk(z+d)}dz\right] \tag{3.109}$$

also due to the orthogonality relations of sines and cosines. Using the Eq. (3.104) and the Eq. (3.105)

$$\begin{aligned}
\frac{U^{\rm elec}_{\rm vacuum(3)}}{L_yW} &= \frac{1}{2}\varepsilon_0(\alpha k)^2\sum_{n=1}^{\infty}\frac{\gamma_n^2}{n^2}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\left[\frac{1}{2}\left(\frac{1}{2nk}e^{2nk(z+d)}\Big|_{-\infty}^{-d}\right)+\frac{1}{2}\left(\frac{1}{2nk}e^{2nk(z+d)}\Big|_{-\infty}^{-d}\right)\right]\\
&= \frac{1}{2}\varepsilon_0(\alpha k)^2\sum_{n=1}^{\infty}\frac{\gamma_n^2}{n^2}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\left(\frac{1}{2}\frac{1}{2nk}+\frac{1}{2}\frac{1}{2nk}\right)\\
&= \frac{1}{2}\varepsilon_0(\alpha k)^2\sum_{n=1}^{\infty}\frac{\gamma_n^2}{n^2}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{2nk}\\
&= \frac{1}{4}\varepsilon_0\alpha^2k\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\\
&= \frac{1}{4}\varepsilon_0\frac{1}{16\pi^2\varepsilon_0^2}\left(\frac{8P_{\rm S}cd}{R}\right)^2k\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\\
&= \frac{1}{4}\frac{4P_{\rm S}^2c^2d^2}{\pi^2\varepsilon_0R^2}k\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\\
&= \frac{1}{4}\frac{4P_{\rm S}^2c^2d^2}{\pi^2\varepsilon_0R\frac{\pi cd}{W}}\frac{2\pi}{W}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\\
&= \frac{1}{4}\frac{8P_{\rm S}^2cd}{\pi^2\varepsilon_0R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\\
&= \frac{1}{4}\frac{8P_{\rm S}^2gd}{\pi^2\varepsilon_0R\kappa_c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2.
\end{aligned} \tag{3.110}$$

Within the ferroelectric region 2, taking the squares of the electric field in Eq. (3.94) and Eq. (3.95),

$$\begin{aligned}
\mathcal{E}_x^{(2)2} &= (\alpha k)^2\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n}\sin(nkx)\beta_n\sinh(nR+cnkz)\frac{\sin\left(\frac{m\pi}{2}(A+1)\right)}{m}\sin(mkx)\beta_m\sinh(mR+cmkz),\\
\mathcal{E}_z^{(2)2} &= \left(\frac{AP_{\rm S}}{\varepsilon_0\kappa_c}\right)^2+2\frac{AP_{\rm S}}{\varepsilon_0\kappa_c}\alpha kc\sum_{n=1}^{\infty}\frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n}\cos(nkx)\beta_n\cosh(nR+cnkz)+\\
&+(\alpha kc)^2\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n}\cos(nkx)\beta_n\cosh(nR+cnkz)\frac{\sin\left(\frac{m\pi}{2}(A+1)\right)}{m}\cos(mkx)\beta_m\cosh(mR+cmkz),
\end{aligned} \tag{3.111}$$

then the electrostatic energy within the ferroelectric layer can be computed from the Eq. (3.99). Doing the same as before, we can obtain this electrostatic energy per unit length along y

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y} = \int \frac{\varepsilon_0}{2} \Bigg\{ & \kappa_a (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \sin(nkx)\beta_n \sinh(nR+cnkz)\cdot \\
& \cdot \frac{\sin\left(\frac{m\pi}{2}(A+1)\right)}{m} \sin(mkx)\beta_m \sinh(mR+cmkz)+ \\
& + \kappa_c \Bigg[\left(\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\right)^2 + 2\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\alpha kc \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \cos(nkx)\beta_n \cosh(nR+cnkz)+ \\
& + (\alpha kc)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n} \cos(nkx)\beta_n \cosh(nR+cnkz)\cdot \\
& \cdot \frac{\sin\left(\frac{m\pi}{2}(A+1)\right)}{m} \cos(mkx)\beta_m \cosh(mR+cmkz) \Bigg] \Bigg\} dxdz
\end{aligned}
\tag{3.112}
$$

Doing the same as before, but integrating over all the thickness of the ferroelectric layer along z, we obtain the elctrostatic energy in units of energy/domain area

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} = & \frac{\varepsilon_0}{2}\kappa_a(\alpha k)^2 \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2 \frac{1}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} \sin^2(nkx)dx \int_{-d}^{0} \sinh^2(nR+cnkz)dz+ \\
& + \frac{\varepsilon_0}{2}\kappa_c \int_{-d}^{0} dz \frac{1}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} \left(\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\right)^2 dx+ \\
& + AP_{\text{S}}\alpha kc \sum_{n=1}^{\infty} \frac{\sin\left(\frac{n\pi}{2}(A+1)\right)}{n}\beta_n \frac{1}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} \cos(nkx)dx \int_{-d}^{0} \cosh(nR+cnkz)dz+ \\
& + \frac{\varepsilon_0}{2}\kappa_c(\alpha kc)^2 \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2 \frac{1}{W}\int_{-\frac{W}{2}}^{\frac{W}{2}} \cos^2(nkx)dx \int_{-d}^{0} \cosh^2(nR+cnkz)dz,
\end{aligned}
\tag{3.113}
$$

where we have applied again the orthogonality relations of sines and cosines. Now we use again the Eq.(3.104) and the Eq.(3.105) and we perform the other integrals over x that have not been solved yet. The integral of the constants in one period over x is then trivially solved

$$
\begin{aligned}
\int_{-\frac{W}{2}}^{\frac{W}{2}} \left(\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\right)^2 dx &= \left(\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\right)^2 \left(\frac{W}{2}+\frac{W}{2}\right) \\
&= \left(\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\right)^2 W.
\end{aligned}
\tag{3.114}
$$

Finally,

$$
\int_{-\frac{W}{2}}^{\frac{W}{2}} \cos(nkx)dx = 0. \tag{3.115}
$$

If the results of these integrals are taken into account, the depolarization energy per unit area in region 2 becomes

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} = & \frac{\varepsilon_0}{4}\kappa_a(\alpha k)^2 \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2 \int_{-d}^{0} \sinh^2(nR+cnkz)dz+ \\
& + \frac{\varepsilon_0}{2}\kappa_c \left(\frac{AP_{\text{S}}}{\varepsilon_0\kappa_c}\right)^2 \int_{-d}^{0} dz+ \\
& + \frac{\varepsilon_0}{4}\kappa_c(\alpha kc)^2 \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2 \int_{-d}^{0} \cosh^2(nR+cnkz)dz
\end{aligned}
\tag{3.116}
$$

Solving for the second integral on the right-hand side of Eq. (3.116),

$$\frac{U_{\mathrm{ferro}(2)}^{\mathrm{elec}}}{L_y W} = \frac{\varepsilon_0}{2}\kappa_c d\left(\frac{AP_{\mathrm{S}}}{\varepsilon_0\kappa_c}\right)^2 + \frac{\varepsilon_0}{4}\alpha^2 k^2\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2\int_{-d}^{0}[\kappa_c c^2\cosh^2(nR+cnkz)+\kappa_a\sinh^2(nR+cnkz)]dz. \tag{3.117}$$

The last integral is then solved until the final expression of the depolarization energy in region 2 is obtained. Remembering that $c^2 = \kappa_a/\kappa_c$,

$$\begin{aligned}\frac{U_{\mathrm{ferro}(2)}^{\mathrm{elec}}}{L_y W} &= \frac{\varepsilon_0}{2}\kappa_c d\left(\frac{AP_{\mathrm{S}}}{\varepsilon_0\kappa_c}\right)^2 + \frac{\varepsilon_0}{4}\kappa_a\alpha^2 k^2\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2\int_{-d}^{0}[\cosh^2(nR+cnkz)+\sinh^2(nR+cnkz)]dz\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{4}\kappa_a\alpha^2 k^2\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2\int_{-d}^{0}\cosh[2(nR+cnkz)]dz,\end{aligned} \tag{3.118}$$

where we have applied $\cosh(2x) = \cosh^2(x) + \sinh^2(x)$. Then, since $\int\cosh(ax)dx = 1/a\sinh(ax)$,

$$\begin{aligned}\frac{U_{\mathrm{ferro}(2)}^{\mathrm{elec}}}{L_y W} &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{4}\kappa_a\alpha^2 k^2\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2\frac{1}{2nkc}\sinh[2(nR+cnkz)]\Big|_{-d}^{0}\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{4}\kappa_a\alpha^2 k^2\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2\frac{1}{2nkc}\{\sinh(2nR)-\sinh[2(nR-cnkd)]\}\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{4}\kappa_a\alpha^2 k^2\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^2}\beta_n^2\frac{1}{2nkc}[\sinh(2nR)-\sinh(-2nR)]\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{4}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\beta_n^2\sinh(2nR),\end{aligned} \tag{3.119}$$

where we have made use of the fact that $R = \pi cd/W$ [Eq. (3.61)] and $k = 2\pi/W$, so

$$\begin{aligned}2(nR-cnkd) = 2&\left(n\frac{\pi cd}{W}-cn\frac{2\pi}{W}d\right)\\ 2&\left(-\frac{n\pi cd}{W}\right)\\ -&\,2nR.\end{aligned} \tag{3.120}$$

Then, from Eq. (3.88), $\beta_n = \frac{1}{\sinh(nR)+g\cosh(nR)}$ and $\sinh(2x) = 2\sinh(x)\cosh(x)$

$$\begin{aligned}\frac{U_{\mathrm{ferro}(2)}^{\mathrm{elec}}}{L_y W} &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{4}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\frac{2\cosh(nR)\sinh(nR)}{[\sinh(nR)+g\cosh(nR)]^2}\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{2}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\frac{\cosh(nR)\sinh(nR)}{\sinh^2(nR)+g^2\cosh^2(nR)+2\sinh(nR)g\cosh(nR)}\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{2}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\frac{\frac{\cosh(nR)}{\sinh(nR)}}{1+g^2\frac{\cosh^2(nR)}{\sinh^2(nR)}+2g\frac{\cosh(nR)}{\sinh(nR)}}\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{2}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\frac{\coth(nR)}{1+g^2\coth^2(nR)+2g\coth(nR)}\\ &= \frac{1}{2}\frac{A^2P_{\mathrm{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{2}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\frac{\coth(nR)}{(1+g\coth(nR))^2}.\end{aligned} \tag{3.121}$$

Again, making use of Eq. (3.88), $\gamma_n = \frac{1}{1+g\coth(nR)}$, and $\alpha = \frac{1}{4\pi\varepsilon_0}\left(\frac{8P_{\mathrm{S}}cd}{R}\right)$

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_yW} &= \frac{1}{2}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{2}\kappa_a\alpha^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\coth(nR) \\
&= \frac{1}{2}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\kappa_c}d + \frac{\varepsilon_0}{2}\kappa_a\frac{1}{16\pi^2\varepsilon_0^2}\left(\frac{8P_{\text{S}}cd}{R}\right)^2\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\coth(nR) \\
&= \frac{1}{2}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\kappa_c}d + \frac{1}{2}\frac{4\kappa_aP_{\text{S}}^2c^2d^2}{\pi^2\varepsilon_0R^2}\frac{k}{c}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\coth(nR) \\
&= \frac{1}{2}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\kappa_c}d + \frac{1}{2}\frac{P_{\text{S}}^2}{\pi^2\varepsilon_0}\frac{4\kappa_acd^2}{R^2}\frac{2R}{cd}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\coth(nR) \\
&= \frac{1}{2}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\kappa_c}d + \frac{1}{2}\frac{P_{\text{S}}^2}{\pi^2\varepsilon_0}\frac{8\kappa_ad}{R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2\coth(nR) \\
&= \frac{1}{2}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\kappa_c}d + \frac{1}{2}\frac{P_{\text{S}}^2d}{\varepsilon_0\kappa_c}\frac{8g}{\pi^2R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2g\coth(nR). \qquad (3.122)
\end{aligned}
$$

Adding the Eq.(3.106), Eq.(3.110) and Eq.(3.122) together, it is obtained the total depolarization energy per unit area

$$
\begin{aligned}
\frac{U_{\text{elec}}}{L_yW} &= \frac{1}{2}\frac{P_{\text{S}}^2A^2}{\varepsilon_0\kappa_c}d + \frac{1}{2}\frac{P_{\text{S}}^2d}{\varepsilon_0\kappa_c}\frac{8g}{\pi^2R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2g\coth(nR) + \frac{1}{2}\frac{P_{\text{S}}^2d}{\varepsilon_0\kappa_c}\frac{8g}{\pi^2R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2 \\
&= \frac{1}{2}\frac{P_{\text{S}}^2d}{\varepsilon_0\kappa_c}\left\{A^2 + \frac{8g}{\pi^2R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\gamma_n^2[g\coth(nR)+1]\right\} \\
&= \frac{1}{2}\frac{P_{\text{S}}^2d}{\varepsilon_0\kappa_c}\left[A^2 + \frac{8g}{\pi^2R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\frac{1}{1+g\coth(nR)}\right]. \qquad (3.123)
\end{aligned}
$$

This energy per unit area is written in Eq.(5.2.16) in Ref. [18].

In the following, **we shall consider $W_+ = W_- = \omega$, which leads to $W = 2\omega$, and $A = \frac{W_+ - W_-}{W_+ + W_-} = 0$**. In addition, the electrostatic energy is divided by d to obtain the depolarization energy per unit volume. Under these assumptions, this energy simplifies to

$$
\frac{U_{\text{elec}}}{L_yWd} = \frac{U_{\text{elec}}}{V} = \frac{1}{2}\frac{P_{\text{S}}^2}{\varepsilon_0\kappa_c}\frac{8g}{\pi^2R}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\frac{1}{1+g\coth(nR)} \qquad (3.124)
$$

It is wanted to write the energy of the Eq. (3.124) in terms of the ratio x of the thickness to width,

$$
x = \frac{d}{\omega}, \qquad (3.125)
$$

so that

$$
\begin{aligned}
\frac{U_{\text{elec}}}{V} &= \frac{1}{2}\frac{P_{\text{S}}^2}{\varepsilon_0\kappa_c}\frac{8g}{\pi^2\frac{\pi cd}{2\omega}}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\frac{1}{1+g\ \coth(n\frac{\pi cd}{2\omega})} \\
&= \frac{P_{\text{S}}^2}{2\varepsilon_0\kappa_c}\frac{16g}{\pi^3c}\frac{1}{x}\sum_{n=1}^{\infty}\frac{1}{n^3}\sin^2\left(\frac{n\pi}{2}\right)\frac{1}{1+g\ \coth\left(\frac{n\pi}{2}cx\right)}. \qquad (3.126)
\end{aligned}
$$

This expression is written in Eq.(2.4) in Ref. [17] and should be valid, within the range of approximations discussed throughout the present section, for any value of x. However, its analytical form is very complex. In many calculations, simplified expressions are used to make the problem tractable. That is the case of (i) the limit of a monodomain configuration (when the thickness of the domains $\omega \to \infty$ and therefore $x \to 0$); and (ii) in the so-called Kittel limit where many domains are formed to screen the depolarization energy (so $\omega \to 0$ and $x \to \infty$).

The electrostatic energy in the monodomain limit $\frac{U_{\text{elec}}^{\text{mono}}}{V}$ is obtained when $x \to 0$

$$
\lim_{x\to 0}\frac{1}{x\left[1+g\ \coth\left(\frac{n\pi}{2}cx\right)\right]} = \lim_{x\to 0}\frac{\left[1+g\ \coth\left(\frac{n\pi}{2}cx\right)\right]^{-1}}{x}. \qquad (3.127)
$$

Expanding the function of the numerator to first order and solving the limit

$$
\begin{aligned}
\lim_{x\to 0} \frac{\left[1+g\ \coth\left(\frac{n\pi}{2}cx\right)\right]^{-1}}{x} &= \lim_{x\to 0} \frac{\left[1+\frac{2g}{n\pi cx}+\frac{gn\pi cx}{6}\right]^{-1}}{x} \\
&= \lim_{x\to 0} \frac{\left[\frac{6n\pi cx+12g+g(n\pi cx)^2}{6n\pi cx}\right]^{-1}}{x} \\
&= \lim_{x\to 0} \frac{6n\pi c}{6n\pi cx+12g+g(n\pi cx)^2} \\
&= \frac{n\pi c}{2g},
\end{aligned}
\tag{3.128}
$$

that yields to

$$
\lim_{x\to 0} \frac{U_{\text{elec}}}{V} = \frac{P_{\text{S}}^2}{2\varepsilon_0\kappa_c}\frac{8}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\sin^2\left(\frac{n\pi}{2}\right). \tag{3.129}
$$

The infinite sum converges to

$$
\begin{aligned}
\sum_{n=1}^{\infty}\frac{1}{n^2}\sin^2\left(\frac{n\pi}{2}\right) &= \sum_{n=\text{impar}}\frac{1}{n^2}+\sum_{n=\text{par}}\frac{1}{n^2}-\sum_{n=\text{par}}\frac{1}{n^2} \\
&= \frac{\pi^2}{6}-\sum_{n=\text{par}}\frac{1}{n^2} \\
&= \frac{\pi^2}{6}-\sum_{n=1}\frac{1}{(2n)^2} \\
&= \frac{\pi^2}{6}-\frac{1}{4}\sum_{n=1}\frac{1}{n^2} \\
&= \frac{\pi^2}{6}-\frac{1}{4}\frac{\pi^2}{6} \\
&= \frac{\pi^2}{8},
\end{aligned}
\tag{3.130}
$$

where it has been used the result from the serie of the Basel problem [31]. Thus the monodomain limit obtained when $x \to 0$ is

$$
\frac{U_{\text{elec}}^{\text{mono}}}{V} = \frac{P_{\text{S}}^2}{2\varepsilon_0\kappa_c}. \tag{3.131}
$$

On the other hand, the electrostatic in the Kittel limit, $\frac{U_{\text{elec}}^{\text{Kittel}}}{V}$, i. e. when $d >> w$ and $x \to \infty$, can be also approximated using

$$
\lim_{x\to\infty} \coth\left(\frac{n\pi}{2}cx\right) = 1, \tag{3.132}
$$

so we can obtain

$$
\lim_{x\to\infty} \frac{U_{\text{elec}}}{V} = \frac{P_{\text{S}}^2}{2\varepsilon_0}\frac{16}{\pi^3(1+g)}\frac{1}{x}\sum_{n=1}^{\infty}\frac{1}{n^3}\sin^2\left(\frac{n\pi}{2}\right). \tag{3.133}
$$

The infinite series is given by

$$
\begin{aligned}
\sum_{n=1}^{\infty} \frac{1}{n^3} \sin^2\left(\frac{n\pi}{2}\right) &= \sum_{n=\text{impar}} \frac{1}{n^3} + \sum_{n=\text{par}} \frac{1}{n^3} - \sum_{n=\text{par}} \frac{1}{n^3} \\
&= \zeta(3) - \sum_{n=\text{par}} \frac{1}{n^3} \\
&= \zeta(3) - \sum_{n=1}^{\infty} \frac{1}{(2n)^3} \\
&= \zeta(3) - \frac{1}{8}\sum_{n=1}^{\infty} \frac{1}{n^3} \\
&= \zeta(3) - \frac{1}{8}\zeta(3) \\
&= \frac{7}{8}\zeta(3) \\
&\approx 1.0518,
\end{aligned} \tag{3.134}
$$

where $\zeta(z)$ is the Riemann Zeta function and it is used the definition of the $\zeta(3)$ [32]. So a Kittel-like expression is obtained in the limit $x \to \infty$,

$$
\frac{U_{\text{elec}}^{\text{Kittel}}}{V} \approx \frac{P_{\text{S}}^2}{2\varepsilon_0} \beta \frac{1}{x}, \tag{3.135}
$$

where

$$
\beta = \frac{16}{\pi^3(1+g)} \sum_{n=1}^{\infty} \frac{1}{n^3} \sin^2\left(\frac{n\pi}{2}\right) \approx \frac{16.829}{\pi^3(1+g)}. \tag{3.136}
$$

The full expression for the electrostatic energy [Eq. (3.126)] is compared with the monodomain expression [Eq. (3.131)] in Fig. 9, and with the Kittel limit [Eq. (3.135)] in Fig. 10

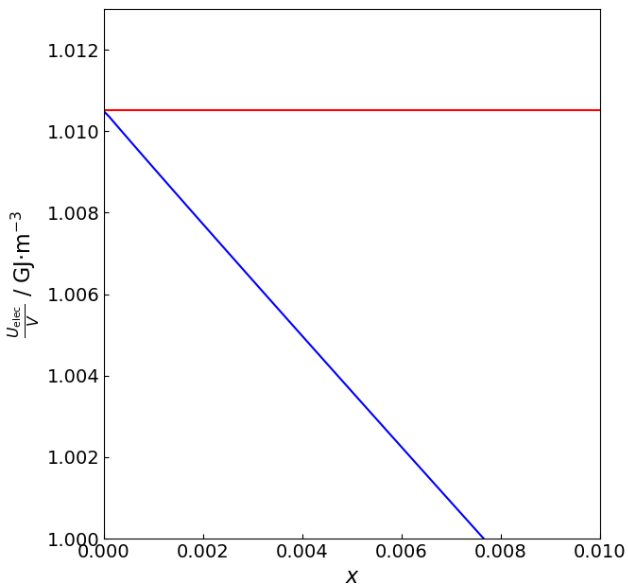


Figure 9: Electrostatic energy in the monodomain limit as a function of x. Eq.(3.131) has been used to obtain the solid red line and Eq.(3.126) to obtain the solid blue line taking into account the first 8000 odd terms of the series. The parameters used to create this figure are: $P_{\text{S}} = 0.78$ C·m^{-2}, $\kappa_a = 185$ and $\kappa_c = 34$.

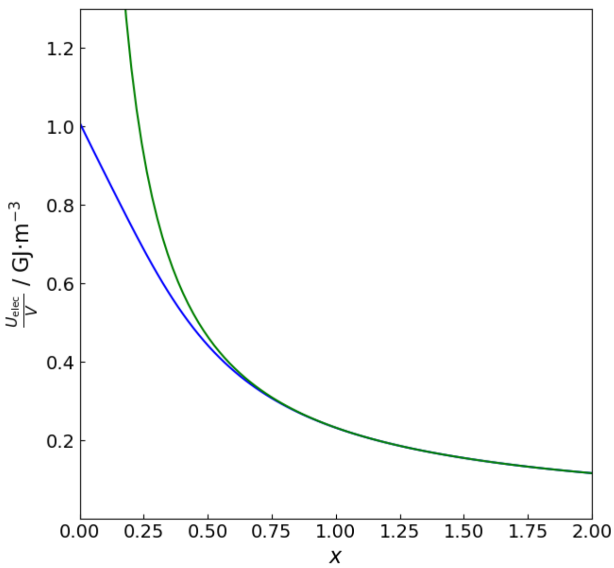


Figure 10: Electrostatic energy in the Kittel limit as a function of x. Eq.(3.135) has been used to create the solid green line and Eq.(3.126) to create the solid blue line taking into account the first 8000 odd terms of the series. The parameters used to create this figure are: $P_{\rm S} = 0.78$ C·m^{-2}, $\kappa_a = 185$ and $\kappa_c = 34$.

We can see how the approximations works well when $x < 0.008$ (errors of the orden of 1% in Fig. 9), and when $x > 0.95$ (green and blue line essentialy overlap in Fig. 10). It is remarkable how the Kittel approximation deviates from the more accurate result for small values of x, giving values for the electrostatic energy that diverge when $x \to 0$, in contrast with the computed electrostatic energy provided in Eq, (3.126), that tends to the monodomain value. This will have important consequences at the time of validiting of the Kittel law in this ultrathin limit, as we shall discuss in the following Section.

3.2.6 Kittel law

As described at the beginning of Sec 3.2, to determine the optimal width of the domains for a given thickness of the isolated thin film we have to: (i) write the total expression of the energy including all the contributions (internal energy, domain wall energy, and electrostatic energy); and (ii) minimize this expression with respect to the domain width, ω.

Due to the complexity of the electrostatic energy [Eq. (3.126)], many authors have replaced this expression by the simplified function in the Kittel limit, given in Eq. (3.135). Within this approach, valid for $d >> \omega$ as shown in Fig. 10, the total energy per unit volume is given by

$$U = \frac{(P - P_{\rm S})^2}{2\varepsilon_0 \chi_c} + \frac{P_{\rm S}^2}{2\varepsilon_0}\beta\frac{\omega}{d} + \frac{\Sigma}{\omega}. \tag{3.137}$$

where we have used the harmonic expansion about one of the minima of the double well energy, because we are assuming small variations with respect to the spontaneous polarization, and we have set the origin of energy to this point. Minimizing the total energy per unit volume with respect ω

$$\frac{\partial U}{\partial \omega} = \frac{P_{\rm S}^2}{2\varepsilon_0}\beta\frac{1}{d} - \frac{\Sigma}{\omega^2} = 0, \tag{3.138}$$

then the well accepted Kittel law is obtained, with

$$\omega = \sqrt{l_k d}, \tag{3.139}$$

where

$$l_k = \frac{2\varepsilon_0 \Sigma}{P_{\rm S}^2 \beta} \tag{3.140}$$

is the Kittel length, which defines a characteristic length scale of the system.

Scaling both the domain width and the thickness of the thin film by this Kittel length, in order to have adimensional units, an universal relationship can be plotted (see black line in Fig. 11).

The dependency of ω with d shown before is taken as the common wisdom, but we cannot forget that the electrostatic energy has been approximated during the derivation. Therefore, a sensible question is whether such a functional form remains valid when the electrostatic energy is replaced by the more exact value [Eq. (3.126)]. Using the complicate expression for the electrostatic energy given in Eq. (3.126) has the advantage of getting more realistic results but the disadvantage of losing the analytical power to analyze the results. The minimization of the total energy per unit volume must be done numerically. We have implemented a code in python to perform this task (available in `https://personales.unican.es/junqueraj/Python_codes.zip`) that is fully documented and ready to use by any user. The results are shown in the red curve of Fig. 11. Several conclusions can be drawn for this Figure. (i) For large enough values of d/l_k (marked with d_1 in Fig. 11), the results are essentially identical. (ii) The domain width, ω/l_k, decreases with the thickness, d/l_k, up to a minimum value, obtained for a critical thickness d_{m}. For thinner films, (d_3), the domain widths sharply increase and tend to a monodomain configuration. Indeed, the domain width diverges at d_∞.

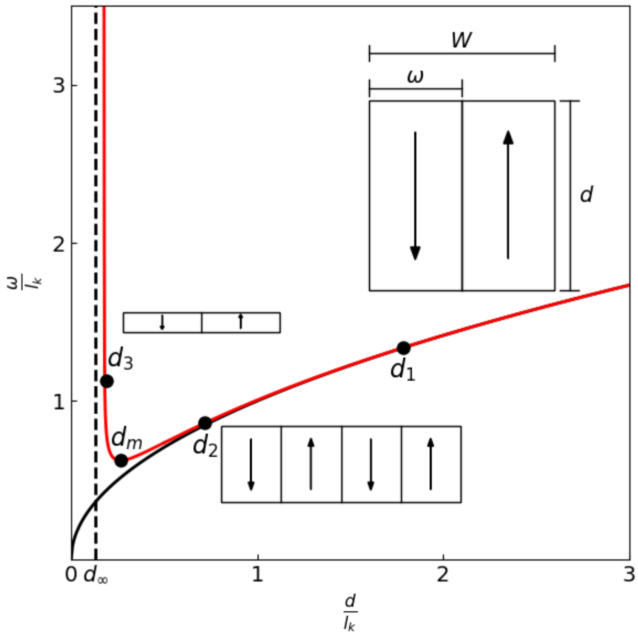


Figure 11: Domain width that minimizes the total energy per unit volume of the ferroelectric thin film for different thicknesses. Both magnitudes are given in adimensional units, dividing them by the Kittel length. The solid black line is obtained with the Kittel expression for the electrostatic energy [Eq. (3.139)]. The red line is obtained for the more exact expression for the electrostatic energy, Eq.(3.126), taking into account the first 100 terms of the series. Cartoons, that are made in scale, represent the corresponding domain configuration in d_1, d_2 and d_3.

Fig. 11 is telling us that the Kittel law breaks below a given thickness of the isolated thin film. However, the results are somehow hindered by the use of adimensional units. A pertinent question is whether for a standard material, such as $PbTiO_3$, this breaking of the domain wall should be observed. Taking the material parameters, we obtain that the minimum width should be obtained for a thickness $d_{\mathrm{m}} \approx 0.148$ nm, smaller than one unit cell of the material. Since the thickness of a real thin film cannot be made smaller than one unit cell, this theoretical behaviour cannot be observed experimentally. Nevertheless, there is an open question: would there be another material for which this thickness should be in a sensible and experimentally accesible range? This remains an open question for future research.

4 Superlattice

4.1 System geometry

Another case of interest is a superlattice formed by ferroelectric thin films interleaved with paraelectric layers, under open circuit boundary conditions, as shown in Fig. 12, where the study area has a length of $D = d_{\mathrm{P}} + d_{\mathrm{S}}$ in the z-direction (d_P is the thickness of the ferroelectric film and d_S is the thickness of the paraelectric layer). This area is split in three different regions: half of the paraelectric layer on top of the ferroelectric thin film (region 1), the thin film itself (region 2), and half of the paraelectric layer below the ferroelectric thin film (region 3). This case has been intensively studied in the literature, both from the theoretical and experimental perspective [5], because non-trivial topological texture with novel and exotic properties might appear in superlattices like $PbTiO_3/SrTiO_3$.

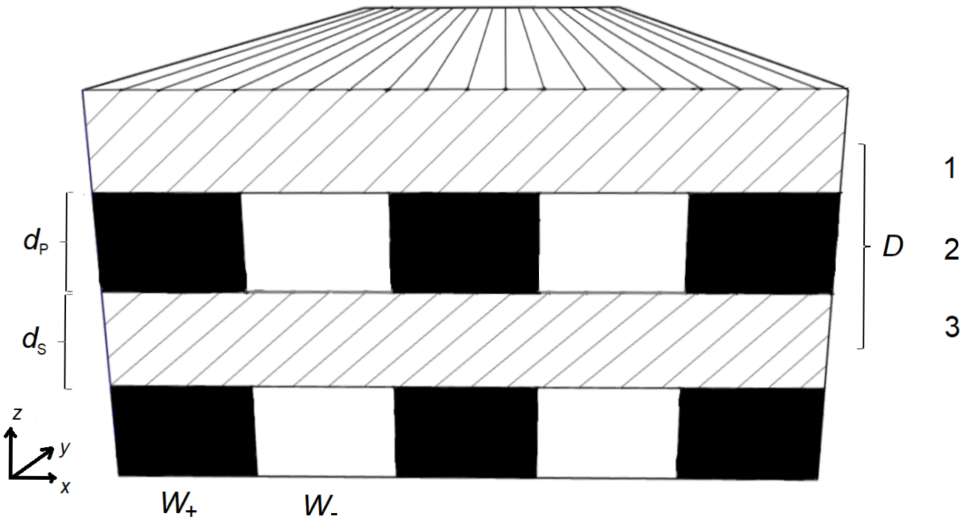


Figure 12: Geometry of the superlattice, formed by a ferroelectric thin film interleaved with a paraelectric layer. Ferroelectric thin films are broken into domains. The black regions represent domains with positive spontaneous polarisation, $+P_\mathrm{S}$, and the white regions represent domains with negative spontaneous polarisation, -P_S. Paraelectric layers are represented by diagonal lines inside them. d_P represents the thickness of the ferroelectric films, while d_S indicates the thickness of the paraelectric layers.

In this case, the origin of the coordinate system will be chosen in the same way as in the isolated thin film, changing its z position from the surface of the ferroelectric to the center of the domain.

4.2 Electrostatic potential

In this case, the potential will be obtained using the same **assumptions** as in Sec. 3.2.3 and applying the following **boundary conditions**

- The potentials must be equal at the ferroelectric/paraelectric interfaces, providing two constraints

$$\begin{aligned} \phi_2(x, z = d_\mathrm{P}/2) &= \phi_1(x, z = d_\mathrm{P}/2) \\ \phi_2(x, z = -d_\mathrm{P}/2) &= \phi_3(x, z = -d_\mathrm{P}/2) \end{aligned} \tag{4.1}$$

  for any value of x. As detailed earlier, under this condition, the tangential components of the electric field at the interfaces are automatically satisfied.

- The potentials must be equal at the limits in z of the study area due to the periodicity of the system, which means

$$\phi_1(x, z = D/2) = \phi_3(x, z = -D/2) \tag{4.2}$$

  for any value of x.

- Since we are assuming the absence of free charges (as in the isolated thin film), the normal components of the displacement fields must also be preserved. This condition implies

$$(\mathbf{D}_1 - \mathbf{D}_2) \cdot \hat{\boldsymbol{n}} = 0 \Rightarrow D_{1,z} = D_{2,z}, \tag{4.3}$$

$$(\mathbf{D}_2 - \mathbf{D}_3) \cdot \hat{\boldsymbol{n}} = 0 \Rightarrow D_{2,z} = D_{3,z}, \tag{4.4}$$

where $\hat{\boldsymbol{n}}$ is a unitary vector field normal to the surface. Since $\mathbf{D} = \varepsilon_0 \boldsymbol{\mathcal{E}} + \mathbf{P}$ and there is no spontaneous polarisation in the paraelectric film

$$\begin{aligned}
&\mathbf{D}_1 = \varepsilon_0 \boldsymbol{\mathcal{E}}_1 + \mathbf{P}_1 = \varepsilon_0 \boldsymbol{\mathcal{E}}_1 + \varepsilon_0 \overleftrightarrow{\chi_s} \boldsymbol{\mathcal{E}}_1 = \varepsilon_0 \overleftrightarrow{\kappa_s} \boldsymbol{\mathcal{E}}_1 = \varepsilon_0 \kappa_s \mathcal{E}_x^{(1)} \mathbf{u}_x + \varepsilon_0 \kappa_s \mathcal{E}_z^{(1)} \mathbf{u}_z, \\
&\mathbf{D}_2 = \varepsilon_0 \boldsymbol{\mathcal{E}}_2 + \mathbf{P}_2 = \varepsilon_0 \boldsymbol{\mathcal{E}}_2 + (\mathbf{P}_\mathrm{S} + \varepsilon_0 \overleftrightarrow{\chi} \boldsymbol{\mathcal{E}}_2) = \varepsilon_0 \overleftrightarrow{\kappa} \boldsymbol{\mathcal{E}}_2 + \mathbf{P}_\mathrm{S} = \varepsilon_0 \kappa_a \mathcal{E}_x^{(2)} \mathbf{u}_x + (\varepsilon_0 \kappa_c \mathcal{E}_z^{(2)} + P_\mathrm{S}(x)) \mathbf{u}_z, \\
&\mathbf{D}_3 = \varepsilon_0 \boldsymbol{\mathcal{E}}_3 + \mathbf{P}_3 = \varepsilon_0 \boldsymbol{\mathcal{E}}_3 + \varepsilon_0 \overleftrightarrow{\chi_s} \boldsymbol{\mathcal{E}}_3 = \varepsilon_0 \overleftrightarrow{\kappa_s} \boldsymbol{\mathcal{E}}_3 = \varepsilon_0 \kappa_s \mathcal{E}_x^{(3)} \mathbf{u}_x + \varepsilon_0 \kappa_s \mathcal{E}_z^{(3)} \mathbf{u}_z.
\end{aligned} \tag{4.5}$$

In these equations, we have used $\overleftrightarrow{\chi_s}$ and $\overleftrightarrow{\kappa_s}$, which are the electronic susceptibility tensor and the electronic dielectric constant tensor, respectively. The paraelectric material is assumed to be isotropic, so these tensors have the same value in the x and z directions of space. Now, knowing $\boldsymbol{\mathcal{E}} = -\nabla \phi$

$$\begin{aligned}
\mathbf{D}_1 &= -\varepsilon_0 \kappa_s \frac{\partial \phi_1}{\partial x} \mathbf{u}_x - \varepsilon_0 \kappa_s \frac{\partial \phi_1}{\partial z} \mathbf{u}_z, \\
\mathbf{D}_2 &= -\varepsilon_0 \kappa_a \frac{\partial \phi_2}{\partial x} \mathbf{u}_x + \left[-\varepsilon_0 \kappa_c \frac{\partial \phi_2}{\partial z} + P_\mathrm{S}(x) \right] \mathbf{u}_z, \\
\mathbf{D}_3 &= -\varepsilon_0 \kappa_s \frac{\partial \phi_3}{\partial x} \mathbf{u}_x - \varepsilon_0 \kappa_s \frac{\partial \phi_3}{\partial z} \mathbf{u}_z.
\end{aligned} \tag{4.6}$$

- The system has a symmetry under $z \to -z$, which leads to

$$\phi_1(x, z) = -\phi_3(x, -z) \tag{4.7}$$

  for any value of x and z.

If these boundary conditions are taken into account and the same procedure as in Sec. 3.2.3 is followed, as shown in Appendix B, the potential in each region of the study area is

$$\phi_1(x, z) = -\frac{A P_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}} \right) d_\mathrm{S}} \left(z - \frac{D}{2} \right) - \sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) \sinh \left[nk \left(z - \frac{D}{2} \right) \right], \tag{4.8}$$

$$\phi_2(x, z) = \frac{A P_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}} \right) d_\mathrm{P}} z + \sum_{n=1}^{\infty} \nu_n \theta_n \cos(nkx) \sinh(nkcz), \tag{4.9}$$

$$\phi_3(x, z) = -\frac{A P_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}} \right) d_\mathrm{S}} \left(z + \frac{D}{2} \right) - \sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) \sinh \left[nk \left(z + \frac{D}{2} \right) \right], \tag{4.10}$$

where

$$\delta_n = \frac{\sinh\left(cnk \frac{d_\mathrm{P}}{2} \right)}{\sinh\left(nk \frac{d_\mathrm{S}}{2} \right)}, \tag{4.11}$$

$$\nu_n = \frac{4 P_\mathrm{S}}{n^2 \pi \varepsilon_0 k} \sin\left(\frac{n\pi}{2} (A+1) \right), \tag{4.12}$$

$$\theta_n = \left[g \cosh\left(nkc \frac{d_\mathrm{P}}{2} \right) + \kappa_s \coth\left(nk \frac{d_\mathrm{S}}{2} \right) \sinh\left(cnk \frac{d_\mathrm{P}}{2} \right) \right]^{-1}. \tag{4.13}$$

These potentials are witten in Eq.(A7) in Ref. [17].

4.3 Electric fields

Once the electrostatic potentials for the three regions are known, we can compute the corresponding electric fields applying in each region $\boldsymbol{\mathcal{E}} = -\nabla \phi$. Therefore, for region 1, taking the gradient of the potential written in Eq. (4.8),

$$\mathcal{E}_x^{(1)} = -\frac{\partial \phi_1}{\partial x} = -\sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \sin(nkx) nk \sinh \left[nk \left(z - \frac{D}{2} \right) \right] \tag{4.14}$$

$$\mathcal{E}_z^{(1)} = -\frac{\partial \phi_1}{\partial z} = \frac{A P_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}} \right) d_\mathrm{S}} + \sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) nk \cosh \left[nk \left(z - \frac{D}{2} \right) \right] \tag{4.15}$$

For region 2, taking the gradient of Eq. (4.9),

$$\mathcal{E}_x^{(2)} = -\frac{\partial \phi_2}{\partial x} = \sum_{n=1}^{\infty} \nu_n \theta_n \sin(nkx) nk \sinh(nkcz) \tag{4.16}$$

$$\mathcal{E}_z^{(2)} = -\frac{\partial \phi_2}{\partial z} = -\frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{P}} - \sum_{n=1}^{\infty} \nu_n \theta_n \cos(nkx) nkc \cosh(nkcz) \tag{4.17}$$

Finally, for region 3, starting from the potential given in Eq. (4.10)

$$\mathcal{E}_x^{(3)} = -\frac{\partial \phi_3}{\partial x} = -\sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \sin(nkx) nk \sinh\left[nk\left(z + \frac{D}{2}\right)\right] \tag{4.18}$$

$$\mathcal{E}_z^{(3)} = -\frac{\partial \phi_3}{\partial z} = \frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{S}} + \sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) nk \cosh\left[nk\left(z + \frac{D}{2}\right)\right] \tag{4.19}$$

4.4 Electrostatic energy

If the same procedure as in Sec. 3.2.5 is carried out, as outline in Appendix C, the depolarization energy per unit volume **doing the approach of $d = d_\mathrm{P}$, $d_\mathrm{S} = \frac{d_\mathrm{S}}{d} d = \alpha d$ and considering $W_+ = W_- = \omega$, which leads to $W = 2\omega$, and $A = \frac{W_+ - W_-}{W_+ + W_-} = 0$** is

$$\frac{U_\mathrm{elec}}{V} = \frac{8P_\mathrm{S}^2}{\pi^3 \varepsilon_0 (1+\alpha)} \frac{1}{x} \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{1}{g \coth\left(\frac{n\pi c}{2} x\right) + \kappa_s \coth\left(\frac{n\pi}{2} \alpha x\right)}. \tag{4.20}$$

This expression is written in Eq.(A15) in Ref. [17]. Considering Eq. (4.20), the energy per unit volume of the superlattice repetition can be obtained when $x \to 0$ (monodomain) and $x \to \infty$ (Kittel-like expression). These two limit expressions are achieved following the same procedure as in Sec. 3.2.5 and the detailed derivation can be found in Appendix C. The monodomain limit is

$$\frac{U_\mathrm{elec}^\mathrm{mono}}{V} = \frac{P_\mathrm{S}^2}{2\varepsilon_0 (1+\alpha)(\kappa_c + \alpha^{-1}\kappa_s)}, \tag{4.21}$$

and the Kittel-like expression

$$\frac{U_\mathrm{elec}^\mathrm{Kittel}}{V} \approx \frac{P_\mathrm{S}^2}{2\varepsilon_0} \beta(\kappa_s.\alpha) \frac{1}{x}, \tag{4.22}$$

where

$$\beta(\kappa_s, \alpha) \approx \frac{16.829}{\pi^3 (1+\alpha)(g + \kappa_s)}. \tag{4.23}$$

4.5 Kittel law

Following the procedure used in Sec. 3.2.6 for an isolated ferroelectric film, the Kittel law for a superlattice system has been obtained in Appendix D, assuming the electrostatic energy per unit volume in the Kittel limit as given in Eq. (4.22), minimizing the total energy per unit volume with respect to ω when $d >> \omega$. The Kittel law found is

$$\omega = \sqrt{l_k(\kappa_s, \alpha) d}, \tag{4.24}$$

where

$$l_k(\kappa_s, \alpha) = \frac{2\varepsilon_0 \Sigma}{P_\mathrm{S}^2 \beta(\kappa_s, \alpha)} \tag{4.25}$$

is the new Kittel length for the ferroelectric/paraelectric, which defines a characteristic length scale of the system. This Kittel law is plotted in black solid lines in Fig. 13.

Also, following the spirit of Sec. 3.2.6, we minimize numerically the total energy per unit volume for the complete electrostatic energy. Results are shown in Fig. 13 for different ratios of the ferroelectric/paraelectric volume, where we have scaled the domain width and the thickness of the thin film by this new Kittel length defined before, in order to have adimensional units. Several conclusions can be obtained from this Figure. (i) There will always be a critical thickness for which the domain size is minimum. This thickness will depend on the proportion of ferroelectric and paraelectric material, i.e. it will depend on α and the dielectric constant of the paraelectric material κ_s. (ii) The

Kittel law obtained with the approximated electrostatic energy is a good approximation from a certain value of d, which is smaller the larger α. (iii) There is a critical value of α for which the Kittel law is independent of κ_s. This value is $\alpha = 2.33$. (iv) As α decreases, i.e. as the paraelectric thickness decreases, the paraelectric material will tend to polarize by a certain amount. Consequently, the bound charges of the surfaces that separate the ferroelectric and paraelectric layers decrease, leading to a reduction of the depolarization field. This entails an increase of the domain width. If we also take into account a high dielectric constant of the paraelectric material, which indicates a high ability of the material to polarize in the presence of an electric field, the domain width will be even larger.

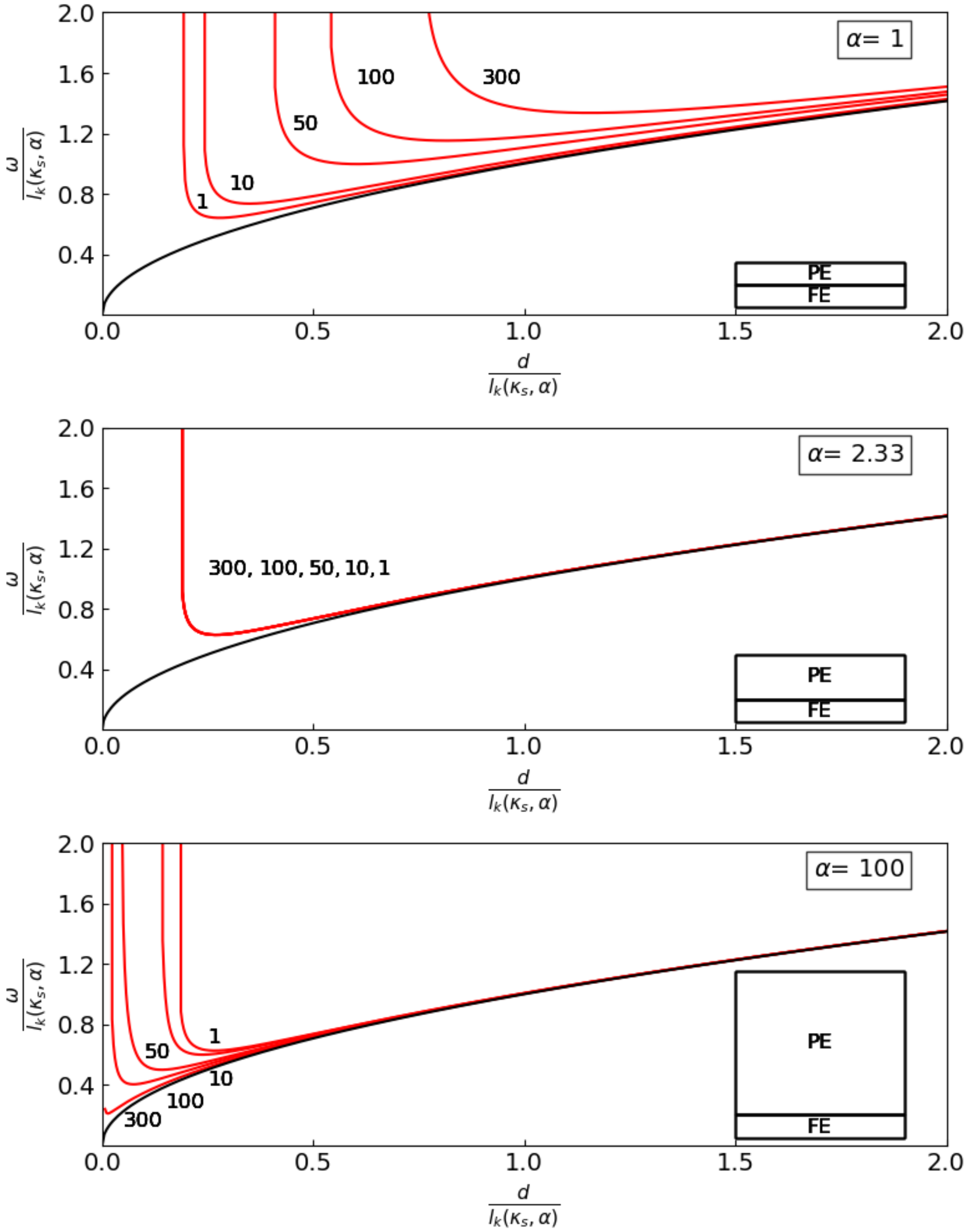


Figure 13: Domain width that minimizes the total energy per unit volume of the superlattice system for different thicknesses of this layer. Each magnitude is normalized by the Kittel length for that value of κ_s. For the top figure, $\alpha = 1$ has been used, for the middel one $\alpha = 2.33$, and for the bottom one $\alpha = 100$. The solid black line of each plot is the Kittel law for $\kappa_s = 300$ and for each of the solid red lines, different values of κ_s have been used along with Eq. (4.20), taking into account the first ten terms of the series (the value of κ_s used in the solid red lines is written next to them). Cartoons represent the proportion between the thickness of the paraelectric layer (PE) and the ferroelectric film (FE) used in each plot. These cartoons ar not made in scale.

We can explore a realistic $PbTiO_3/SrTiO_3$ system, which is the most studied both theoretically and experimentally [5]. Setting realistic values for the parameters, we can plot ω against d in physical units (see Fig. 14).

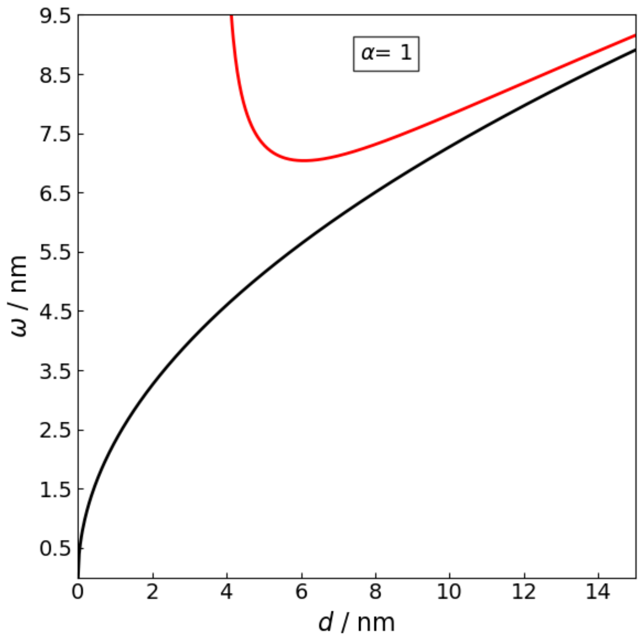


Figure 14: Domain width that minimizes the total energy per unit volume of the superlattice system for different thicknesses of the ferroelectric thin film that are at the Kittel limit. The solid black line is the Kittel law and for the solid red line Eq.(4.20) has been used, taking into account the first 100 terms of the series. We have used $\alpha = 1$.

This can be compared with second-principles calculations carried out by Fernando Gómez *et al.* In these simulations, it was confirmed that the Kittel law holds at least for thicknesses greater than 3.2 nm. As shown in Fig. 14, the minimization of the total energy per unit volume is in good agreement with the traditional Kittel law for ferroelectric thicknesses above 6 nm.

5 Substrate

5.1 System geometry

Finally, another case is a ferroelectric thin-film on top of a dielectric, isotropic, semi-infinite substrate, under open circuit boundary conditions, too. This scenario is reflected in Fig. 15, where the full space is split into three different regions: the vacuum on top of the ferroelectric thin film (region 1), the thin film itself (region 2), and the substrate below the ferroelectric thin film (region 3). In this situation, we have kept the same position of the origin of the coordinate system as in the isolated thin film.

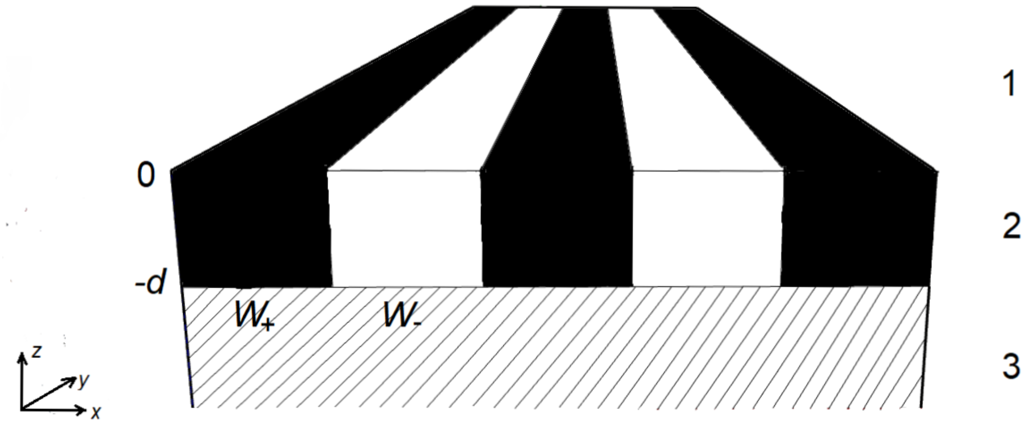


Figure 15: Geometry of the thin film, broken into domains, on a substrate. The black regions represent domains with positive spontaneous polarisation, $+P_{\mathrm{S}}$, and the white regions represent domains with negative spontaneous polarisation, -P_{S}. The substrate is represented by diagonal lines inside it.

5.2 Electrostatic potential

In this case, the potential of the three regions of space will be obtained using the same **assumptions** and **boundary conditions** as in Sec. 3.2.3. The expression of the displacement vector in each region of space is different compared to the case of the isolated ferroelectric film because we are considering a distinct system. Therefore, in order to satisfy the boundary condition for the continuity of the normal component of this vector at surfaces of the thin film, we need to use the following expressions

$$\begin{aligned}
&\mathbf{D}_1 = \varepsilon_0 \boldsymbol{\mathcal{E}}_1,\\
&\mathbf{D}_2 = \varepsilon_0 \boldsymbol{\mathcal{E}} + \mathbf{P}_2 = \varepsilon_0 \boldsymbol{\mathcal{E}}_2 + (\mathbf{P}_{\mathrm{S}} + \varepsilon_0 \overleftrightarrow{\chi} \boldsymbol{\mathcal{E}}_2) = \varepsilon_0 \overleftrightarrow{\kappa} \boldsymbol{\mathcal{E}}_2 + \mathbf{P}_{\mathrm{S}} = \varepsilon_0 \kappa_a \mathcal{E}_x^{(2)} \mathbf{u}_x + (\varepsilon_0 \kappa_c \mathcal{E}_z^{(2)} + P_{\mathrm{S}}(x)) \mathbf{u}_z,\\
&\mathbf{D}_3 = \varepsilon_0 \boldsymbol{\mathcal{E}}_3 + \mathbf{P}_3 = \varepsilon_0 \boldsymbol{\mathcal{E}}_3 + \varepsilon_0 \overleftrightarrow{\chi_s} \boldsymbol{\mathcal{E}}_3 = \varepsilon_0 \overleftrightarrow{\kappa_s} \boldsymbol{\mathcal{E}}_3 = \varepsilon_0 \kappa_s \mathcal{E}_x^{(3)} \mathbf{u}_x + \varepsilon_0 \kappa_s \mathcal{E}_z^{(3)} \mathbf{u}_z.
\end{aligned} \tag{5.1}$$

Now, knowing the electric fields can be written as gradients of the potentials, $\boldsymbol{\mathcal{E}} = -\nabla \phi$,

$$\begin{aligned}
&\mathbf{D}_1 = -\varepsilon_0 \frac{\partial \phi_1}{\partial x} \mathbf{u}_x - \varepsilon_0 \frac{\partial \phi_1}{\partial z} \mathbf{u}_z,\\
&\mathbf{D}_2 = -\varepsilon_0 \kappa_a \frac{\partial \phi_2}{\partial x} \mathbf{u}_x + \left[-\varepsilon_0 \kappa_c \frac{\partial \phi_2}{\partial z} + P_{\mathrm{S}}(x) \right] \mathbf{u}_z,\\
&\mathbf{D}_3 = -\varepsilon_0 \kappa_{\mathrm{s}} \frac{\partial \phi_3}{\partial x} \mathbf{u}_x - \varepsilon_0 \kappa_{\mathrm{s}} \frac{\partial \phi_3}{\partial z} \mathbf{u}_z.
\end{aligned} \tag{5.2}$$

If these boundary conditions are taken into account and the same procedure as in Sec. 3.2.3 is followed, as explained in Appendix E, the potential in each region of space is

$$\phi_1(x,z) = \sum_{n=1}^{\infty} \alpha \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{1}{n^2} [2g \sinh^2(nR) + \kappa_{\mathrm{s}} \sinh(2nR)] \mu_n \cos(nkx) e^{-nkz} \tag{5.3}$$

$$\begin{aligned}
\phi_2(x,z) = \frac{P_S A}{\varepsilon_0 \kappa_c} z + \sum_{n=1}^{\infty} \cos(nkx) \alpha \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} [2g \sinh(nR) \sinh(nR + nkcz) + \kappa_{\mathrm{s}} \sinh(2nR + nkcz) +\\
+ \sinh(nkcz)]
\end{aligned} \tag{5.4}$$

$$\phi_3(x,z) = -\frac{P_S A}{\varepsilon_0 \kappa_c} d - \sum_{n=1}^{\infty} \alpha \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{1}{n^2} [2g \sinh^2(nR) + \sinh(2nR)] \mu_n \cos(nkx) e^{nk(z+d)} \tag{5.5}$$

where

$$\mu_n = \{(g^2 + \kappa_{\mathrm{s}}) \sinh(2nR) + g[1 + \kappa_{\mathrm{s}} \cosh(2nR) + 2 \sinh^2(nR)]\}^{-1} \tag{5.6}$$

5.3 Electric fileds

Using the fact that $\boldsymbol{\mathcal{E}} = -\nabla \phi$ the electric fields are obtained for each region. For region 1, taking the Eq. (5.3)

$$\begin{aligned}
\mathcal{E}_x^{(1)} = -\frac{\partial \phi_1}{\partial x} &= \alpha \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} [2g\sinh^2(nR) + \kappa_\text{s}\sinh(2nR)] nk \sin(nkx) e^{-nkz} \\
&= \alpha k \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} [2g\sinh^2(nR) + \kappa_\text{s}\sinh(2nR)] \sin(nkx) e^{-nkz}, \qquad (5.7)\\
\mathcal{E}_z^{(1)} = -\frac{\partial \phi_1}{\partial z} &= -\alpha \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} [2g\sinh^2(nR) + \kappa_\text{s}\sinh(2nR)] \cos(nkx)(-nk) e^{-nkz} \\
&= \alpha k \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} [2g\sinh^2(nR) + \kappa_\text{s}\sinh(2nR)] \cos(nkx) e^{-nkz}. \qquad (5.8)
\end{aligned}$$

For region 2, taking the Eq. (5.4)

$$\begin{aligned}
\mathcal{E}_x^{(2)} = -\frac{\partial \phi_2}{\partial x} &= \alpha \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} nk \sin(nkx) [2g\sinh(nR)\sinh(nR+nkcz) + \kappa_\text{s}\sinh(2nR+nkcz) + \\
&\qquad + \sinh(nkcz)] \\
&= \alpha k \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} \sin(nkx) [2g\sinh(nR)\sinh(nR+nkcz) + \kappa_\text{s}\sinh(2nR+nkcz) + \\
&\qquad + \sinh(nkcz)], \qquad (5.9)\\
\mathcal{E}_z^{(2)} = -\frac{\partial \phi_2}{\partial z} &= -\frac{P_S A}{\varepsilon_0 \kappa_c} - \alpha \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} \cos(nkx) [2g\sinh(nR) nkc\cosh(nR+nkcz) + \\
&\qquad + \kappa_\text{s} nkc\cosh(2nR+nkcz) + nkc\cosh(nkcz)] \\
&= -\frac{P_S A}{\varepsilon_0 \kappa_c} - \alpha kc \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} \cos(nkx) [2g\sinh(nR)\cosh(nR+nkcz) + \\
&\qquad + \kappa_\text{s}\cosh(2nR+nkcz) + \cosh(nkcz)]. \qquad (5.10)
\end{aligned}$$

Finally, for region 3 it is taken the Eq. (5.5) in order to calculate the electric filed in this region using the gradient of this potential

$$\begin{aligned}
\mathcal{E}_x^{(3)} = -\frac{\partial \phi_1}{\partial x} &= -\alpha \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} [2g\sinh^2(nR) + \sinh(2nR)] nk \sin(nkx) e^{nk(z+d)} \\
&= -\alpha k \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} [2g\sinh^2(nR) + \sinh(2nR)] \sin(nkx) e^{nk(z+d)}, \qquad (5.11)\\
\mathcal{E}_z^{(3)} = -\frac{\partial \phi_1}{\partial z} &= \alpha \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n^2} [2g\sinh^2(nR) + \sinh(2nR)] \cos(nkx) nk e^{nk(z+d)} \\
&= \alpha k \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} [2g\sinh^2(nR) + \sinh(2nR)] \cos(nkx) e^{nk(z+d)}. \qquad (5.12)
\end{aligned}$$

5.4 Electrostatic energy

In order to obtain the depolarization energy per unit volume of this system, we have followed the same procedure as in Sec. 3.2.5. This development is detailed in Appendix F, where, using the same approximations as for the isolated thin film, we have found that

$$\frac{U_{\text{elec}}}{V} = \frac{4gP_{\text{S}}^2}{2\pi^3 c\kappa_c\varepsilon_0}\frac{1}{x}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\left\{(g^2+\kappa_{\text{s}})\sinh\left(n\pi cx\right)+g\left[1+\kappa_{\text{s}}\cosh\left(n\pi cx\right)+2\sinh^2\left(\frac{n\pi}{2}cx\right)\right]\right\}^{-2}\cdot$$
$$\cdot\left\{\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right)+\kappa_s\sinh\left(n\pi cx\right)\right]^2+\kappa_s\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right)+\sinh\left(n\pi cx\right)\right]^2+\right.$$
$$+4g^3\sinh^2\left(\frac{n\pi}{2}cx\right)\sinh\left(n\pi cx\right)+\frac{\kappa_s^2 g}{2}\sinh\left(2n\pi cx\right)+$$
$$+2g^2\kappa_s\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{3n\pi}{2}cx\right)+\sinh\left(\frac{n\pi}{2}cx\right)\right]+\frac{g}{2}\sinh\left(2n\pi cx\right)+$$
$$\left.+2g^2\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{n\pi}{2}cx\right)+\sinh\left(\frac{3n\pi}{2}cx\right)\right]+2g\kappa_s\sinh\left(n\pi cx\right)\right\} \tag{5.13}$$

Taking into account the Eq. (5.13), the depolarization energy per unit volume in the monodomain limit and a Kittel-like expression are obtained in Appendix F following the same procedure as in Sec. 3.2.5. In this way, this energy in the monodomain limit is

$$\frac{U_{\text{elec}}^{\text{mono}}}{V} = \frac{P_{\text{S}}^2}{2\kappa_c\varepsilon_0} \tag{5.14}$$

and the Kittel-like expression

$$\frac{U_{\text{elec}}^{\text{Kittel}}}{V} \approx \frac{P_{\text{S}}^2}{2\varepsilon_0}\beta(\kappa_s)\frac{1}{x} \tag{5.15}$$

where

$$\beta(\kappa_s) \approx \frac{8.414}{\pi^3}\frac{(g+\kappa_s)^2+\kappa_s(g+1)^2+2g^3+g\kappa_s^2+2g^2\kappa_s+g+2g^2}{\left[g^2+\kappa_s+g(\kappa_s+1)\right]^2} \tag{5.16}$$

5.5 Kittel law

Following the same procedure as in Sec. 3.2.6, the Kittel law for a ferroelectric on top of a substrate is calculated in Appendix G, assuming the electrostatic energy per unit volume in the Kittel limit as given in Eq. (5.15), minimizing the total energy per unit volume of the system with respect ω when $d >> \omega$. The Kittel law found is

$$\omega = \sqrt{l_k(\kappa_s)d} \tag{5.17}$$

where

$$l_k(\kappa_s) = \frac{2\varepsilon_0\Sigma}{P_{\text{S}}^2\beta(\kappa_s)} \tag{5.18}$$

is the Kittel length of this system.

Setting realistic values for the parameters, we can plot ω against d in physical units (Fig. 16). We can see in the red curve of Fig. 16 the results, numerically achieved, of the minimization of the total energy per unit volume, in which we have used the Eq. (5.13). From this Figure, the same conclusions as in the two previous systems can be drawn.

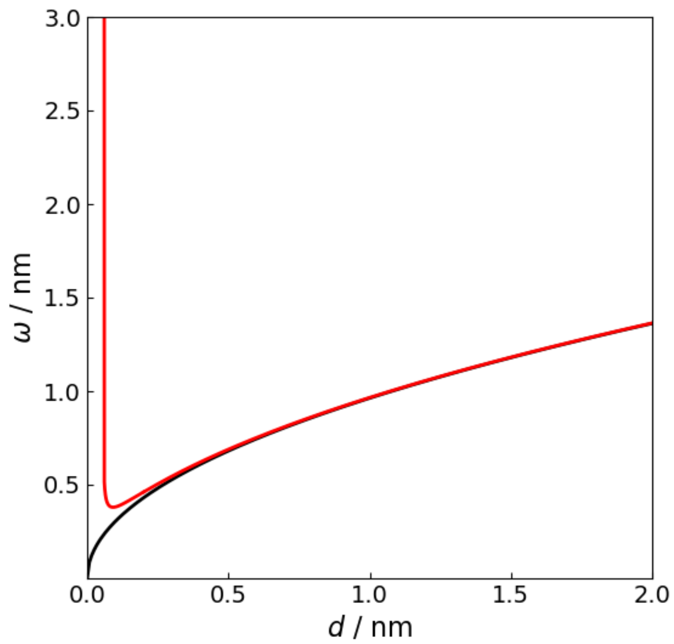


Figure 16: Domain width that minimizes the total energy per unit volume of the system formed by a ferroelectric and a substrate for different thicknesses of the ferroelectric thin film that are at the Kittel limit. The solid black line is the Kittel law and for the solid red line Eq. (5.13) has been used, taking into account the first 6 terms of the series.

6 Conclusions

We have study the domain formation in ferroelectric nanostructures taking into account three different cases: an isolated ferroelectric thin film, a ferroelectric layer on top of a substrate and a ferroelectric/paraelectric superlattice. In order to analyze this domain formation in each system, we have created a model in which we have done several assumptions and approximations:

- The domain wall is neglected.
- Surface or interface effects are neglected.
- The total polarization field $\mathbf{P}(\mathbf{r})$ is assumed to be fixed at the spontaneous polarization and it can only be varied from this value by a linear response to the electric depolarization field.
- The behaviour of the system along the y-direction is considered homogeneous.
- The origin of the coordinate system is chosen in such a way that the polarization profile is even.
- The free charge in the structures is zero.
- The geometry of the ferroelectric is tetragonal.
- The substrate is an isotropic material.
- The development of an in-plane polarization is no considered.
- The domain width is considered the same for both positive and negative polarization.
- In the superlattice case, the thickness of the ferroelectric and paraelectric layer are considered proportional.

In the three cases studied, the Kittel law is verified for large thicknesses of the ferroelectric film. As we reduce the thickness, the minimization of the total energy per unit volume leads to the appearance of a critical thickness where the domain size becomes minimal. If we continue reducing d, the domain width starts to increase until monodomain phases can be obtained.

Estimations of these critical thicknesses with realistic parameters can result in values that are not physical, below a unit cell.

The application of more realistic calculations from second-principles in well-studied systems leads us to the conclusion that the Kittel law is valid for ferroelectric film thicknesses greater than 3 nm, whereas using the model studied in this work, this law is valid for thicknesses larger than 6 nm.

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Appendix

A Fourier transform of the spontaneous polarization in the domain structure

In this appendix we shall compute the coefficients of the Fourier expansion of the spontaneous polarization [Eq. (3.1)] according to the Eq. (3.2).

For the coefficient a_0

$$
\begin{aligned}
a_0 &= \frac{2}{W}\int_{\frac{-W_+-W_-}{2}}^{\frac{W_++W_-}{2}} P_\mathrm{S}(t)dt \\
&= \frac{2}{W}\left(\int_{\frac{-W_+-W_-}{2}}^{\frac{-W_+}{2}} -P_\mathrm{S}dt + \int_{\frac{-W_+}{2}}^{\frac{W_+}{2}} P_\mathrm{S}dt + \int_{\frac{W_+}{2}}^{\frac{W_++W_-}{2}} -P_\mathrm{S}dt\right) \\
&= \frac{2}{W}\left[-P_\mathrm{S}\left(-\frac{W_+}{2}+\frac{W_++W_-}{2}\right)+P_\mathrm{S}\left(\frac{W_+}{2}+\frac{W_+}{2}\right)-P_\mathrm{S}\left(\frac{W_++W_-}{2}-\frac{W_-}{2}\right)\right] \\
&= \frac{2}{W}\left(-P_S\frac{W_-}{2}+P_\mathrm{S}W_+-P_\mathrm{S}\frac{W_-}{2}\right) \\
&= \frac{2}{W}(P_\mathrm{S}W_+-P_\mathrm{S}W_-) \\
&= 2P_\mathrm{S}\left(\frac{W_+-W_-}{W}\right) \\
&= 2P_\mathrm{S}A \quad \text{with} \quad A=\frac{W_+-W_-}{W_++W_-}.
\end{aligned} \tag{A.1}
$$

The coefficient a_n is obtained from

$$
\begin{aligned}
a_n &= \frac{2}{W}\int_{\frac{-W_+-W_-}{2}}^{\frac{W_++W_-}{2}} P_\mathrm{S}(t)\cos\left(\frac{2\pi n}{W}t\right)dt \\
&= \frac{2}{W}\left[\int_{\frac{-W_+-W_-}{2}}^{\frac{-W_+}{2}} -P_\mathrm{S}\cos\left(\frac{2\pi n}{W}t\right)dt + \int_{\frac{-W_+}{2}}^{\frac{W_+}{2}} P_\mathrm{S}\cos\left(\frac{2\pi n}{W}t\right)dt + \int_{\frac{W_+}{2}}^{\frac{W_++W_-}{2}} -P_\mathrm{S}\cos\left(\frac{2\pi n}{W}t\right)dt\right]
\end{aligned} \tag{A.2}
$$

The result of the first integral of Eq. (A.2) is

$$
\begin{aligned}
-P_\mathrm{S}\int_{\frac{-W_+-W_-}{2}}^{\frac{-W_+}{2}} \cos\left(\frac{2\pi n}{W}t\right)dt &= -\frac{P_\mathrm{S}W}{2\pi n}\sin\left(\frac{2\pi \mathrm{n}}{\mathrm{W}}\mathrm{t}\right)\Big|_{\frac{-W_+-W_-}{2}}^{\frac{-W_+}{2}} \\
&= \frac{P_\mathrm{S}W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right) - \frac{P_\mathrm{S}W}{2\pi n}\sin(\pi n) \\
&= \frac{P_\mathrm{S}W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right).
\end{aligned} \tag{A.3}
$$

The second integral is

$$
\begin{aligned}
P_\mathrm{S}\int_{\frac{-W_+}{2}}^{\frac{W_+}{2}} \cos\left(\frac{2\pi n}{W}t\right)dt &= \frac{P_\mathrm{S}W}{2\pi n}\sin\left(\frac{2\pi \mathrm{n}}{\mathrm{W}}\mathrm{t}\right)\Big|_{\frac{-W_+}{2}}^{\frac{W_+}{2}} \\
&= \frac{P_\mathrm{S}W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right) + \frac{P_\mathrm{S}W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right) \\
&= \frac{P_\mathrm{S}W}{\pi n}\sin\left(\frac{\pi n W_+}{W}\right).
\end{aligned} \tag{A.4}
$$

And the result of the third integral is

$$-P_S \int_{\frac{W_+}{2}}^{\frac{W_++W_-}{2}} \cos\left(\frac{2\pi n}{W}t\right) dt = -\frac{P_S W}{2\pi n}\sin\left(\frac{2\pi \mathrm{n}}{\mathrm{W}}\mathrm{t}\right)\Big|_{\frac{W_+}{2}}^{\frac{W_++W_-}{2}}$$
$$= -\frac{P_S W}{2\pi n}\sin(\pi n) + \frac{P_S W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right)$$
$$= \frac{P_S W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right). \tag{A.5}$$

Substituting the results of these integrals into Eq. (A.2) gives the expression for a_n

$$a_n = \frac{2}{W}\left[\frac{P_S W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right) + \frac{P_S W}{\pi n}\sin\left(\frac{\pi n W_+}{W}\right) + \frac{P_S W}{2\pi n}\sin\left(\frac{\pi n W_+}{W}\right)\right]$$
$$= \frac{4P_S}{\pi n}\sin\left(\frac{\pi n W_+}{W}\right)$$
$$= \frac{4P_S}{\pi n}\sin\left(\frac{\pi n}{2}(A+1)\right). \tag{A.6}$$

The coefficients b_n are zero since the function to be expanded in Fourier series is an even function.

B Electrostatic potential of the superlattice system

We will focus our attention on the area specified in Fig. 12. The Laplace equations in the three regions, taking into account the same **assumptions** as in Sec. 3.2.3, are

$$\kappa_s \nabla^2 \phi_1 = \kappa_s \nabla^2 \phi_3 = 0 \tag{B.1}$$
$$\kappa_a \frac{\partial^2 \phi_2}{\partial x^2} + \kappa_c \frac{\partial^2 \phi_2}{\partial z^2} = 0 \tag{B.2}$$

following the same procedure as in that section. These equations have the same solutions as Eq. (3.25) and Eq. (3.26). For this reason, the potentials that satisfy these Laplace equations are those given in the Eq.(3.46)

$$\phi_1(x,z) = a_0^{(1)}(z) + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(1)} e^{nkz} + d_n'^{(1)} e^{-nkz})$$
$$\phi_2(x,z) = a_0^{(2)}(z) + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(2)} e^{nkcz} + d_n'^{(2)} e^{-nkcz})$$
$$\phi_3(x,z) = a_0^{(3)}(z) + \sum_{n=1}^{\infty} \cos(nkx)(c_n'^{(3)} e^{nkz} + d_n'^{(3)} e^{-nkz}) \tag{B.3}$$

where the even parity in the x-direction has already been taken into account.

The next step is to find the expression for the coefficients $a_0^{(i)}(z)$. In order to do this, **we assume there is a constant field inside both of the layers**, in this way.

$$\frac{\mathrm{d}a_0^{(1)}}{\mathrm{d}z} = a \tag{B.4}$$
$$\frac{\mathrm{d}a_0^{(2)}}{\mathrm{d}z} = c \tag{B.5}$$
$$\frac{\mathrm{d}a_0^{(3)}}{\mathrm{d}z} = a \tag{B.6}$$

where regions 1 and 3 have the same electric field due to the periodicity of the system. Integrating the three differential equations, the zero term of the potential of each region is obtained

$$a_0^{(1)}(z) = az + b \tag{B.7}$$
$$a_0^{(2)}(z) = cz \tag{B.8}$$
$$a_0^{(3)}(z) = az + d \tag{B.9}$$

With the aim of knowing the value of the different constants of these potentials, we are going to use our **boundary conditions** defined in Sec. 4.2. Applying the condition that the potentials must be equal at the interfaces

$$a_0^{(1)}(z = d_\mathrm{P}/2) = a_0^{(2)}(z = d_\mathrm{P}/2) \quad \Rightarrow \quad a\frac{d_\mathrm{P}}{2} + b = c\frac{d_\mathrm{P}}{2} \quad \Rightarrow \quad (a-c)\frac{d_\mathrm{P}}{2} = -b \tag{B.10}$$

$$a_0^{(2)}(z = -d_\mathrm{P}/2) = a_0^{(3)}(z = -d_\mathrm{P}/2) \quad \Rightarrow \quad -c\frac{d_\mathrm{P}}{2} = -a\frac{d_\mathrm{P}}{2} + d \quad \Rightarrow \quad (a-c)\frac{d_\mathrm{P}}{2} = d \tag{B.11}$$

we obtain

$$d = -b \tag{B.12}$$

From the condition that the potentials must be equal at the limits in z of the study area

$$a_0^{(1)}(z = D/2) = a_0^{(3)}(z = -D/2) \quad \Rightarrow \quad a\frac{D}{2} - d = -a\frac{D}{2} + d \quad \Rightarrow \quad aD = 2d \quad \Rightarrow \quad d = a\frac{D}{2} \tag{B.13}$$

Knowing the Eq. (B.12) and the Eq. (B.13), the Eq.(B.10) and the Eq.(B.11) can be expressed as

$$(a-c)\frac{d_\mathrm{P}}{2} = a\frac{D}{2} \tag{B.14}$$

and, therefore, the zero term potential in each region is

$$a_0^{(1)}(z) = a\left(z - \frac{D}{2}\right) \tag{B.15}$$

$$a_0^{(2)}(z) = cz \tag{B.16}$$

$$a_0^{(3)}(z) = a\left(z + \frac{D}{2}\right) \tag{B.17}$$

Now, we apply the condition of the continuity of the normal component of the displacement fields at the interface to these last expressions of the potentials. Starting with the upper interface

$$\kappa_c \frac{\partial a_0^{(2)}}{\partial z}\bigg|_{z=\frac{d_\mathrm{P}}{2}} - \kappa_s \frac{\partial a_0^{(1)}}{\partial z}\bigg|_{z=\frac{d_\mathrm{P}}{2}} = \frac{P_\mathrm{S}^{n=0}(x)}{\varepsilon_0} \quad \Rightarrow \quad \kappa_c c - \kappa_s a = \frac{AP_\mathrm{S}}{\varepsilon_0} \tag{B.18}$$

The same result is obtained in the lower interface. Combining the Eq.(B.14) and Eq.(B.18) we will be able to know the expression of the constants a and c of the term zero of the potential. From the Eq.(B.14), it is found that

$$c = \frac{a(d_\mathrm{P} - D)}{d_\mathrm{P}} \tag{B.19}$$

which can be substituted in the Eq.(B.18)

$$\begin{aligned}
\frac{AP_\mathrm{S}}{\varepsilon_0} &= \kappa_c c - \kappa_s a \\
&= \kappa_c \frac{a(d_\mathrm{P} - D)}{d_\mathrm{P}} - \kappa_s a \\
&= \left[\kappa_c \frac{(d_\mathrm{P} - D)}{d_\mathrm{P}} - \kappa_s\right] a \\
&= \left[\kappa_c \frac{(d_\mathrm{P} - d_\mathrm{P} - d_\mathrm{S})}{d_\mathrm{P}} - \kappa_s\right] a \\
&= -\left(\kappa_c \frac{d_\mathrm{S}}{d_\mathrm{P}} + \kappa_s\right) a \\
&= -\left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) a d_\mathrm{S}
\end{aligned} \tag{B.20}$$

and obtain the expression for the constant a

$$a = -\frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{S}} \tag{B.21}$$

This expression can be substituted in the Eq.(B.19) to get the constant c

$$
\begin{aligned}
c &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}d_{\mathrm{P}}}(d_{\mathrm{P}}-D)\\
&= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}d_{\mathrm{P}}}(d_{\mathrm{P}}-d_{\mathrm{P}}-d_{\mathrm{S}})\\
&= \frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{P}}} \qquad \text{(B.22)}
\end{aligned}
$$

Knowing these constants, the final expression for the monodomain term of the potential can be achieved

$$
a_0^{(1)}(z) = -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right) \qquad \text{(B.23)}
$$

$$
a_0^{(2)}(z) = \frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{P}}}z \qquad \text{(B.24)}
$$

$$
a_0^{(3)}(z) = -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z+\frac{D}{2}\right) \qquad \text{(B.25)}
$$

With this terms, the full potential is therefore

$$
\begin{aligned}
\phi_1(x,z) &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right)+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(1)}e^{nkz}+d_n'^{(1)}e^{-nkz})\\
\phi_2(x,z) &= \frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{P}}}z+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(2)}e^{nkcz}+d_n'^{(2)}e^{-nkcz})\\
\phi_3(x,z) &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z+\frac{D}{2}\right)+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(3)}e^{nkz}+d_n'^{(3)}e^{-nkz}) \qquad \text{(B.26)}
\end{aligned}
$$

Hereafter, we are going to obtain the different coefficients of the series using the full potential. Applying the symmetry of the system under $z \to -z$

$$
\begin{aligned}
\phi_1(x,z) = -\phi_3(x,-z) \quad \Rightarrow \quad & -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right)+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(1)}e^{nkz}+d_n'^{(1)}e^{-nkz}) =\\
&= \frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(-z+\frac{D}{2}\right)-\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(3)}e^{-nkz}+d_n'^{(3)}e^{nkz}) \qquad \text{(B.27)}
\end{aligned}
$$

we have a relation between different coefficients

$$
\begin{aligned}
c_n'^{(1)} &= -d_n'^{(3)}\\
d_n'^{(1)} &= -c_n'^{(3)} \qquad \text{(B.28)}
\end{aligned}
$$

Now, the potentials can be written as

$$
\begin{aligned}
\phi_1(x,z) &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right)+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(1)}e^{nkz}+d_n'^{(1)}e^{-nkz}),\\
\phi_2(x,z) &= \frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{P}}}z+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(2)}e^{nkcz}+d_n'^{(2)}e^{-nkcz}),\\
\phi_3(x,z) &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z+\frac{D}{2}\right)-\sum_{n=1}^{\infty}\cos(nkx)(d_n'^{(1)}e^{nkz}+c_n'^{(1)}e^{-nkz}). \qquad \text{(B.29)}
\end{aligned}
$$

If we use Eq. (4.2) for the last full potential

$$\phi_1(x,z=D/2)=\phi_3(x,z=-D/2) \quad\Rightarrow\quad -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(\frac{D}{2}-\frac{D}{2}\right)+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(1)}e^{nk\frac{D}{2}}+d_n'^{(1)}e^{-nk\frac{D}{2}})=$$
$$=-\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(-\frac{D}{2}+\frac{D}{2}\right)-\sum_{n=1}^{\infty}\cos(nkx)(d_n'^{(1)}e^{-nk\frac{D}{2}}+c_n'^{(1)}e^{nk\frac{D}{2}}) \tag{B.30}$$

so

$$\begin{aligned} c_n'^{(1)}e^{nk\frac{D}{2}}+d_n'^{(1)}e^{-nk\frac{D}{2}} &= -d_n'^{(1)}e^{-nk\frac{D}{2}}-c_n'^{(1)}e^{nk\frac{D}{2}} \\ 2c_n'^{(1)}e^{nk\frac{D}{2}} &= -2d_n'^{(1)}e^{-nk\frac{D}{2}} \end{aligned} \tag{B.31}$$

Thus, the relation between $d_n'^{(1)}$ y $c_n'^{(1)}$ is

$$d_n'^{(1)}=-c_n'^{(1)}e^{nkD} \tag{B.32}$$

Taking into account this last relation, the potentials are

$$\begin{aligned}
\phi_1(x,z) &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right)+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(1)}e^{nkz}-c_n'^{(1)}e^{nkD}e^{-nkz}) \\
&= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right)+\sum_{n=1}^{\infty}c_n'^{(1)}\cos(nkx)e^{nk\frac{D}{2}}(e^{nkz-nk\frac{D}{2}}-e^{-nkz+nk\frac{D}{2}}) \\
&= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z-\frac{D}{2}\right)+\sum_{n=1}^{\infty}2c_n'^{(1)}\cos(nkx)e^{nk\frac{D}{2}}\sinh\left[nk\left(z-\frac{D}{2}\right)\right], \\
\phi_2(x,z) &= \frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{P}}}z+\sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(2)}e^{nkcz}+d_n'^{(2)}e^{-nkcz}), \\
\phi_3(x,z) &= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z+\frac{D}{2}\right)-\sum_{n=1}^{\infty}\cos(nkx)(-c_n'^{(1)}e^{nkD}e^{nkz}+c_n'^{(1)}e^{-nkz}) \\
&= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z+\frac{D}{2}\right)+\sum_{n=1}^{\infty}c_n'^{(1)}\cos(nkx)e^{nk\frac{D}{2}}(e^{nkz+nk\frac{D}{2}}-e^{-nkz-nk\frac{D}{2}}) \\
&= -\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(z+\frac{D}{2}\right)+\sum_{n=1}^{\infty}2c_n'^{(1)}\cos(nkx)e^{nk\frac{D}{2}}\sinh\left[nk\left(z+\frac{D}{2}\right)\right]
\end{aligned} \tag{B.33}$$

A relation between $c_n'^{(2)}$ and $d_n'^{(2)}$ can be obtained using the condition that the potentials must be equal at the interfaces. In the upper interface

$$\phi_1(x,z=d_{\mathrm{P}}/2)=\phi_2(x,z=d_{\mathrm{P}}/2)\Rightarrow-\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\left(\frac{d_{\mathrm{P}}}{2}-\frac{D}{2}\right)+$$
$$+\sum_{n=1}^{\infty}2c_n'^{(1)}\cos(nkx)e^{nk\frac{D}{2}}\sinh\left[nk\left(\frac{d_{\mathrm{P}}}{2}-\frac{D}{2}\right)\right]=$$
$$=\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{P}}}\frac{d_{\mathrm{P}}}{2}+\sum_{n=1}^{\infty}\cos(nkx)\left(c_n'^{(2)}e^{nkc\frac{d_{\mathrm{P}}}{2}}+d_n'^{(2)}e^{-nkc\frac{d_{\mathrm{P}}}{2}}\right) \tag{B.34}$$

Using the fact that $D=d_{\mathrm{P}}+d_{\mathrm{S}}$

$$-\sum_{n=1}^{\infty}2c_n'^{(1)}\cos(nkx)e^{nk\frac{D}{2}}\sinh\left(nk\frac{d_{\mathrm{S}}}{2}\right)=\sum_{n=1}^{\infty}\cos(nkx)\left(c_n'^{(2)}e^{nkc\frac{d_{\mathrm{P}}}{2}}+d_n'^{(2)}e^{-nkc\frac{d_{\mathrm{P}}}{2}}\right) \tag{B.35}$$

Studying now the continuity of the potential in the lower interface

$$\begin{aligned}
\phi_2(x, z = -d_\mathrm{P}/2) = \phi_3(x, z = -d_\mathrm{P}/2) \Rightarrow -\frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{P}} \frac{d_\mathrm{P}}{2} + \sum_{n=1}^{\infty} \cos(nkx) \left(c_n'^{(2)} e^{-nkc\frac{d_\mathrm{P}}{2}} + d_n'^{(2)} e^{nkc\frac{d_\mathrm{P}}{2}}\right) &= \\
= -\frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{S}} \left(-\frac{d_\mathrm{P}}{2} + \frac{D}{2}\right) &+ \\
+ \sum_{n=1}^{\infty} 2c_n'^{(1)} \cos(nkx) e^{nk\frac{D}{2}} \sinh\left[nk\left(-\frac{d_\mathrm{P}}{2} + \frac{D}{2}\right)\right] &
\end{aligned} \tag{B.36}$$

and applying the same expression for D as before

$$\sum_{n=1}^{\infty} \cos(nkx) \left(c_n'^{(2)} e^{-nkc\frac{d_\mathrm{P}}{2}} + d_n'^{(2)} e^{nkc\frac{d_\mathrm{P}}{2}}\right) = \sum_{n=1}^{\infty} 2c_n'^{(1)} \cos(nkx) e^{nk\frac{D}{2}} \sinh\left(nk\frac{d_\mathrm{S}}{2}\right) \tag{B.37}$$

If we compare the Eq. (B.35) and the Eq. (B.37), we can see

$$-\sum_{n=1}^{\infty} \cos(nkx) \left(c_n'^{(2)} e^{-nkc\frac{d_\mathrm{P}}{2}} + d_n'^{(2)} e^{nkc\frac{d_\mathrm{P}}{2}}\right) = \sum_{n=1}^{\infty} \cos(nkx) \left(c_n'^{(2)} e^{nkc\frac{d_\mathrm{P}}{2}} + d_n'^{(2)} e^{-nkc\frac{d_\mathrm{P}}{2}}\right) \tag{B.38}$$

Developing the previous equality

$$\begin{aligned}
-c_n'^{(2)} e^{-nkc\frac{d_\mathrm{P}}{2}} - d_n'^{(2)} e^{nkc\frac{d_\mathrm{P}}{2}} &= c_n'^{(2)} e^{nkc\frac{d_\mathrm{P}}{2}} + d_n'^{(2)} e^{-nkc\frac{d_\mathrm{P}}{2}} \\
c_n'^{(2)} \left(e^{nkc\frac{d_\mathrm{P}}{2}} + e^{-nkc\frac{d_\mathrm{P}}{2}}\right) &= -d_n'^{(2)} \left(e^{nkc\frac{d_\mathrm{P}}{2}} + e^{-nkc\frac{d_\mathrm{P}}{2}}\right)
\end{aligned} \tag{B.39}$$

we obtain the desired relation

$$c_n'^{(2)} = -d_n'^{(2)} \tag{B.40}$$

If we take into account this last relation, the expression for the full potential is now

$$\begin{aligned}
\phi_1(x, z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{S}} \left(z - \frac{D}{2}\right) + \sum_{n=1}^{\infty} 2c_n'^{(1)} \cos(nkx) e^{nk\frac{D}{2}} \sinh\left[nk\left(z - \frac{D}{2}\right)\right] \\
\phi_2(x, z) &= \frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{P}} z + \sum_{n=1}^{\infty} 2c_n'^{(2)} \cos(nkx) \sinh(nkcz) \\
\phi_3(x, z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0 \left(\frac{\kappa_c}{d_\mathrm{P}} + \frac{\kappa_s}{d_\mathrm{S}}\right) d_\mathrm{S}} \left(z + \frac{D}{2}\right) + \sum_{n=1}^{\infty} 2c_n'^{(1)} \cos(nkx) e^{nk\frac{D}{2}} \sinh\left[nk\left(z + \frac{D}{2}\right)\right]
\end{aligned} \tag{B.41}$$

The last relation between coefficients that remains to be found is the relation between $c_n'^{(1)}$ and $c_n'^{(2)}$. For this purpose, the relation between $c_n'^{(2)}$ and $d_n'^{(2)}$ will be applied in Eq. (B.35)

$$\begin{aligned}
-\sum_{n=1}^{\infty} 2c_n'^{(1)} \cos(nkx) e^{nk\frac{D}{2}} \sinh\left(nk\frac{d_\mathrm{S}}{2}\right) &= \sum_{n=1}^{\infty} \cos(nkx) c_n'^{(2)} \left(e^{nkc\frac{d_\mathrm{P}}{2}} - e^{-nkc\frac{d_\mathrm{P}}{2}}\right) \\
&= \sum_{n=1}^{\infty} 2\cos(nkx) c_n'^{(2)} \sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)
\end{aligned} \tag{B.42}$$

With this last expression, we obtain

$$-c_n'^{(1)} e^{nk\frac{D}{2}} \sinh\left(nk\frac{d_\mathrm{S}}{2}\right) = c_n'^{(2)} \sinh\left(nkc\frac{d_\mathrm{P}}{2}\right) \quad \Rightarrow \quad c_n'^{(1)} = -\frac{\sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)}{\sinh\left(nk\frac{d_\mathrm{S}}{2}\right)} e^{-nk\frac{D}{2}} c_n'^{(2)} = -\delta_n e^{-nk\frac{D}{2}} c_n'^{(2)} \tag{B.43}$$

where

$$\delta_n = \frac{\sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)}{\sinh\left(nk\frac{d_\mathrm{S}}{2}\right)} \tag{B.44}$$

Taking into account this last relation, the full expression of the potentials becomes

$$\begin{aligned}
\phi_1(x,z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\left(z-\frac{D}{2}\right)-\sum_{n=1}^{\infty}2\delta_n c_n^{\prime(2)}\cos(nkx)\sinh\left[nk\left(z-\frac{D}{2}\right)\right]\\
\phi_2(x,z) &= \frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{P}}z+\sum_{n=1}^{\infty}2c_n^{\prime(2)}\cos(nkx)\sinh(nkcz)\\
\phi_3(x,z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\left(z+\frac{D}{2}\right)-\sum_{n=1}^{\infty}2\delta_n c_n^{\prime(2)}\cos(nkx)\sinh\left[nk\left(z+\frac{D}{2}\right)\right]
\end{aligned}\tag{B.45}$$

In order to find the expression of the single coefficient on which the potentials depend, i.e. $c_n^{\prime(2)}$, we will use the continuity of the normal component of the displacement vector at the interface between the regions 1 and 2, located at $z=\frac{d_\mathrm{P}}{2}$. We will use the displacement vectors defined in the boundary conditions in Sec. 4.2

$$\kappa_c\left.\frac{\partial\phi_2}{\partial z}\right|_{z=\frac{d_\mathrm{P}}{2}}-\kappa_s\left.\frac{\partial\phi_1}{\partial z}\right|_{z=\frac{d_\mathrm{P}}{2}}=\frac{P_\mathrm{S}(x)}{\varepsilon_0}\tag{B.46}$$

Since the potentials and the spontaneous polarization are expressed as a linear combination of periodic functions with different harmonics, we can apply Eq. (B.46) to each of them. Doing so for the zero-th order term ($n=0$),

$$\frac{\kappa_c AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{P}}+\frac{\kappa_s AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}=\frac{AP_\mathrm{S}}{\varepsilon_0}\tag{B.47}$$

Developing the equality

$$\begin{aligned}
\frac{AP_\mathrm{S}}{\varepsilon_0}\left[\frac{\kappa_c}{\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{P}}+\frac{\kappa_s}{\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\right] &= \frac{AP_\mathrm{S}}{\varepsilon_0}\\
\frac{AP_\mathrm{S}}{\varepsilon_0}\left[\frac{1}{\left(\frac{1}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}\kappa_c}\right)d_\mathrm{P}}+\frac{1}{\left(\frac{\kappa_c}{d_\mathrm{P}\kappa_s}+\frac{1}{d_\mathrm{S}}\right)d_\mathrm{S}}\right] &= \frac{AP_\mathrm{S}}{\varepsilon_0}\\
\frac{AP_\mathrm{S}}{\varepsilon_0}\left(\frac{1}{1+\frac{\kappa_s d_\mathrm{P}}{d_\mathrm{S}\kappa_c}}+\frac{1}{\frac{\kappa_c d_\mathrm{S}}{d_\mathrm{P}\kappa_s}+1}\right) &= \frac{AP_\mathrm{S}}{\varepsilon_0}\\
\frac{AP_\mathrm{S}}{\varepsilon_0}\left(\frac{d_\mathrm{S}\kappa_c}{d_\mathrm{S}\kappa_c+\kappa_s d_\mathrm{P}}+\frac{d_\mathrm{P}\kappa_s}{d_\mathrm{S}\kappa_c+\kappa_s d_\mathrm{P}}\right) &= \frac{AP_\mathrm{S}}{\varepsilon_0}\\
\frac{AP_\mathrm{S}}{\varepsilon_0} &= \frac{AP_\mathrm{S}}{\varepsilon_0}
\end{aligned}\tag{B.48}$$

If the same is done for the higher-order terms

$$\begin{aligned}
\frac{1}{\varepsilon_0}\sum_{n=1}^{\infty}\frac{4P_\mathrm{S}}{n\pi}\sin\left(\frac{n\pi}{2}(A+1)\right)\cos(nkx) &= \sum_{n=1}^{\infty}2c_n^{\prime(2)}\cos(nkx)\kappa_c cnk\cosh\left(nkc\frac{d_\mathrm{P}}{2}\right)+\\
&+\sum_{n=1}^{\infty}2\delta_n c_n^{\prime(2)}\cos(nkx)\kappa_s nk\cosh\left[nk\left(\frac{d_\mathrm{P}}{2}-\frac{D}{2}\right)\right]
\end{aligned}\tag{B.49}$$

Taking into account Eq. (B.48) and Eq. (B.49), the continuity of the normal component of the displacement vector at the upper surface of the ferroelectric [Eq. (B.46)] becomes

$$\sum_{n=1}^{\infty}2c_n^{\prime(2)}nk\left\{c\kappa_c\cosh\left(nkc\frac{d_\mathrm{P}}{2}\right)+\delta_n\kappa_s\cosh\left[nk\left(\frac{d_\mathrm{P}}{2}-\frac{D}{2}\right)\right]\right\}=\sum_{n=1}^{\infty}\frac{4P_\mathrm{S}}{n\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right)\tag{B.50}$$

from which the expression for the coefficient $c_n'^{(2)}$ is directly obtained

$$\begin{aligned} c_n'^{(2)} &= \frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\left[g\cosh\left(nkc\frac{d_\mathrm{P}}{2}\right)+\delta_n\kappa_s\cosh\left(nk\frac{d_\mathrm{S}}{2}\right)\right]^{-1} \\ &= \frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\left[g\cosh\left(nkc\frac{d_\mathrm{P}}{2}\right)+\frac{\sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)}{\sinh\left(nk\frac{d_\mathrm{S}}{2}\right)}\kappa_s\cosh\left(nk\frac{d_\mathrm{S}}{2}\right)\right]^{-1} \\ &= \frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\left[g\cosh\left(nkc\frac{d_\mathrm{P}}{2}\right)+\kappa_s\sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)\coth\left(nk\frac{d_\mathrm{S}}{2}\right)\right]^{-1} \\ &= \frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\theta_n \end{aligned} \tag{B.51}$$

where

$$\theta_n = \left[g\cosh\left(nkc\frac{d_\mathrm{P}}{2}\right)+\kappa_s\sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)\coth\left(nk\frac{d_\mathrm{S}}{2}\right)\right]^{-1} \tag{B.52}$$

and the previously defined expressions for $g = c\kappa_c$, $D = d_\mathrm{P} + d_\mathrm{S}$ and $\delta_n = \frac{\sinh\left(nkc\frac{d_\mathrm{P}}{2}\right)}{\sinh\left(nk\frac{d_\mathrm{S}}{2}\right)}$ have been used.

Finally, introducing the expression of this coefficient in the Eq. (B.45), the potential for region 1 is

$$\begin{aligned} \phi_1(x,z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\left(z-\frac{D}{2}\right)-\sum_{n=1}^{\infty}2\delta_n\frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\theta_n\cos(nkx)\sinh\left[nk\left(z-\frac{D}{2}\right)\right], \\ &= -\frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\left(z-\frac{D}{2}\right)-\sum_{n=1}^{\infty}\delta_n\nu_n\theta_n\cos(nkx)\sinh\left[nk\left(z-\frac{D}{2}\right)\right] \end{aligned} \tag{B.53}$$

For the potential in region 2, we have

$$\begin{aligned} \phi_2(x,z) &= \frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{P}}z+\sum_{n=1}^{\infty}2\frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\theta_n\cos(nkx)\sinh(nkcz), \\ &= \frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{P}}z+\sum_{n=1}^{\infty}\nu_n\theta_n\cos(nkx)\sinh(nkcz) \end{aligned} \tag{B.54}$$

and for the potential in the third region,

$$\begin{aligned} \phi_3(x,z) &= -\frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\left(z+\frac{D}{2}\right)-\sum_{n=1}^{\infty}2\delta_n\frac{1}{2}\frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)\theta_n\cos(nkx)\sinh\left[nk\left(z+\frac{D}{2}\right)\right] \\ &= -\frac{AP_\mathrm{S}}{\varepsilon_0\left(\frac{\kappa_c}{d_\mathrm{P}}+\frac{\kappa_s}{d_\mathrm{S}}\right)d_\mathrm{S}}\left(z+\frac{D}{2}\right)-\sum_{n=1}^{\infty}\delta_n\nu_n\theta_n\cos(nkx)\sinh\left[nk\left(z+\frac{D}{2}\right)\right] \end{aligned} \tag{B.55}$$

In the potential of the three regions, we have used

$$\nu_n = \frac{4P_\mathrm{S}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right) \tag{B.56}$$

C Electrostatic energy of the superlattice system

Within the paraelectric layer, the total electrostatic energy is given by

$$U_\mathrm{para}^\mathrm{elec} = \frac{\varepsilon_0}{2}\int \boldsymbol{\mathcal{E}}\cdot\mathbf{D}\ dV \tag{C.1}$$

where the integral is taken over the volume of the paraelectric layer.

Let us compute the electrostatic energy stored in the paraelectric region 1. The square of the electric fields given by Eq. (4.14) and Eq. (4.15) is

$$\mathcal{E}_x^{(1)2} = k^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \sin(nkx) n \sinh\left[nk\left(z-\frac{D}{2}\right)\right] \delta_m \nu_m \theta_m \sin(mkx) m \sinh\left[mk\left(z-\frac{D}{2}\right)\right]$$

$$\begin{aligned}\mathcal{E}_z^{(1)2} = & \left[\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\right]^2 + 2\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\sum_{n=1}^{\infty}\delta_n\nu_n\theta_n\cos(nkx)nk\cosh\left[nk\left(z-\frac{D}{2}\right)\right] + \\ & + k^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) n \cosh\left[nk\left(z-\frac{D}{2}\right)\right] \delta_m \nu_m \theta_m \cos(mkx) m \cosh\left[mk\left(z-\frac{D}{2}\right)\right] \end{aligned} \quad (C.2)$$

Considering these expressions, $U^{\mathrm{elec}}_{\mathrm{para}(1)}$ can be calculated from Eq. (C.1). Since we have assumed that all the physical magnitudes are periodic along the y-direction, we can integrate only in the $(x,\ z)$ plane to obtain the energy per unit length along y.

$$\begin{aligned}\frac{U^{\mathrm{elec}}_{\mathrm{para}(1)}}{L_y} = & \int \frac{\varepsilon_0}{2}\kappa_s\left[\mathcal{E}_x^{(1)2}+\mathcal{E}_z^{(1)2}\right]dxdz \\ = & \frac{\varepsilon_0}{2}\kappa_s \int \left\{ k^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \sin(nkx) n \sinh\left[nk\left(z-\frac{D}{2}\right)\right] \delta_m \nu_m \theta_m \sin(mkx) m \sinh\left[mk\left(z-\frac{D}{2}\right)\right] + \right. \\ & + \left[\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\right]^2 + 2\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\sum_{n=1}^{\infty}\delta_n\nu_n\theta_n\cos(nkx)nk\cosh\left[nk\left(z-\frac{D}{2}\right)\right] + \\ & \left. + k^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) n \cosh\left[nk\left(z-\frac{D}{2}\right)\right] \delta_m \nu_m \theta_m \cos(mkx) m \cosh\left[mk\left(z-\frac{D}{2}\right)\right]\right\} dxdz \end{aligned} \quad (C.3)$$

Let us integrate this electrostatic energy over one period of length W along the x direction and over the extension of the paraelectric region 1 (with z ranging between $d_{\mathrm{P}}/2$ and $D/2$). If the result is divided by the domain width, the electrostatic energy will be given in units of energy/domain area.

$$\begin{aligned}\frac{U^{\mathrm{elec}}_{\mathrm{para}(1)}}{L_y W} = & \frac{\varepsilon_0}{2W}\kappa_s k^2 \sum_{n=1}^{\infty} \delta_n^2\nu_n^2\theta_n^2 n^2 \int_{-\frac{W}{2}}^{\frac{W}{2}} \sin^2(nkx)dx \int_{\frac{d_{\mathrm{P}}}{2}}^{\frac{D}{2}} \sinh^2\left[nk\left(z-\frac{D}{2}\right)\right]dz + \\ & + \frac{\varepsilon_0}{2W}\kappa_s \int_{-\frac{W}{2}}^{\frac{W}{2}} \left[\frac{AP_{\mathrm{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\mathrm{P}}}+\frac{\kappa_s}{d_{\mathrm{S}}}\right)d_{\mathrm{S}}}\right]^2 dx \int_{\frac{d_{\mathrm{P}}}{2}}^{\frac{D}{2}} dz + \\ & + \frac{\varepsilon_0}{2W}\kappa_s k^2 \sum_{n=1}^{\infty} \delta_n^2\nu_n^2\theta_n^2 n^2 \int_{-\frac{W}{2}}^{\frac{W}{2}} \cos^2(nkx)dx \int_{\frac{d_{\mathrm{P}}}{2}}^{\frac{D}{2}} \cosh^2\left[nk\left(z-\frac{D}{2}\right)\right]dz \end{aligned} \quad (C.4)$$

where we have applied the orthogonality relations of sines and cosines defined in Eq. (3.103). Now, using Eq. (3.104) and Eq. (3.105)

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{para}(1)}}{L_y W} &= \frac{\varepsilon_0}{2W}\kappa_s \left\{ \left[\frac{AP_{\text{S}}}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right) d_{\text{S}}} \right]^2 W \left(\frac{D}{2} - \frac{d_{\text{P}}}{2} \right) + \right. \\
&\quad \left. + k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \frac{W}{2} \left\{ \int_{\frac{d_{\text{P}}}{2}}^{\frac{D}{2}} \sinh^2 \left[nk \left(z - \frac{D}{2} \right) \right] dz + \int_{\frac{d_{\text{P}}}{2}}^{\frac{D}{2}} \cosh^2 \left[nk \left(z - \frac{D}{2} \right) \right] dz \right\} \right\} \\
&= \frac{\varepsilon_0}{2}\kappa_s \left\{ \left[\frac{AP_{\text{S}}}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right) d_{\text{S}}} \right]^2 \frac{d_{\text{S}}}{2} + k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \frac{1}{2} \int_{\frac{d_{\text{P}}}{2}}^{\frac{D}{2}} \cosh \left[2nk \left(z - \frac{D}{2} \right) \right] dz \right\} \\
&= \frac{\varepsilon_0}{4}\kappa_s \left\{ \frac{A^2 P_{\text{S}}^2}{\varepsilon_0^2 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right)^2 d_{\text{S}}} + k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \frac{1}{2nk} \sinh \left[2nk \left(z - \frac{D}{2} \right) \right] \Bigg|_{\frac{d_{\text{P}}}{2}}^{\frac{D}{2}} \right\} \\
&= \frac{\varepsilon_0}{4}\kappa_s \left\{ \frac{A^2 P_{\text{S}}^2}{\varepsilon_0^2 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right)^2 d_{\text{S}}} - k \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n \frac{1}{2} \sinh \left[2nk \left(\frac{d_{\text{P}}}{2} - \frac{D}{2} \right) \right] \right\} \\
&= \frac{\kappa_s}{4} \frac{A^2 P_{\text{S}}^2}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right)^2 d_{\text{S}}} + \frac{\varepsilon_0 \kappa_s}{8} k \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n \sinh(nkd_{\text{S}})
\end{aligned} \tag{C.5}
$$

where we have used again the fact that $D = d_{\text{P}} + d_{\text{S}}$ and we have applied $\cosh(2x) = \cosh^2(x) + \sinh^2(x)$.

Following the same procedure, we can compute the electrostatic energy stored in the paraelectric region 3. The square of the electric fields given by Eq. (4.18) and Eq. (4.19) are

$$
\begin{aligned}
\mathcal{E}_x^{(3)2} &= k^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \sin(nkx) n \sinh \left[nk \left(z + \frac{D}{2} \right) \right] \delta_m \nu_m \theta_m \sin(mkx) m \sinh \left[mk \left(z + \frac{D}{2} \right) \right] \\
\mathcal{E}_z^{(1)2} &= \left[\frac{AP_{\text{S}}}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right) d_{\text{S}}} \right]^2 + 2 \frac{AP_{\text{S}}}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right) d_{\text{S}}} \sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) nk \cosh \left[nk \left(z + \frac{D}{2} \right) \right] + \\
&\quad + k^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) n \cosh \left[nk \left(z + \frac{D}{2} \right) \right] \delta_m \nu_m \theta_m \cos(mkx) m \cosh \left[mk \left(z + \frac{D}{2} \right) \right]
\end{aligned} \tag{C.6}
$$

Then, $U^{\text{elec}}_{\text{para}(3)}$ can be calculated again from Eq. (C.1). Due to the same reasoning, we can do the same as before to obtain the energy per unit length along y in this region

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{para}(3)}}{L_y} &= \int \frac{\varepsilon_0}{2}\kappa_s \left[\mathcal{E}_x^{(3)2} + \mathcal{E}_z^{(3)2} \right] dxdz \\
&= \frac{\varepsilon_0}{2}\kappa_s \int \left\{ k^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \sin(nkx) n \sinh \left[nk \left(z + \frac{D}{2} \right) \right] \delta_m \nu_m \theta_m \sin(mkx) m \sinh \left[mk \left(z + \frac{D}{2} \right) \right] + \right. \\
&\quad + \left[\frac{AP_{\text{S}}}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right) d_{\text{S}}} \right]^2 + 2 \frac{AP_{\text{S}}}{\varepsilon_0 \left(\frac{\kappa_c}{d_{\text{P}}} + \frac{\kappa_s}{d_{\text{S}}} \right) d_{\text{S}}} \sum_{n=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) nk \cosh \left[nk \left(z + \frac{D}{2} \right) \right] + \\
&\quad \left. + k^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \delta_n \nu_n \theta_n \cos(nkx) n \cosh \left[nk \left(z + \frac{D}{2} \right) \right] \delta_m \nu_m \theta_m \cos(mkx) m \cosh \left[mk \left(z + \frac{D}{2} \right) \right] \right\} dxdz
\end{aligned} \tag{C.7}
$$

Doing the same as in the previous region but, in this case, integrating in z from $-D/2$ to $-d_{\text{P}}/2$, the electrostatic energy of the region 3 will be given in units of energy/domain area as well

$$\frac{U^{\text{elec}}_{\text{para}(3)}}{L_y W} = \frac{\varepsilon_0}{2W}\kappa_s k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \int_{-\frac{W}{2}}^{\frac{W}{2}} \sin^2(nkx)dx \int_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} \sinh^2\left[nk\left(z+\frac{D}{2}\right)\right] dz+$$
$$+\frac{\varepsilon_0}{2W}\kappa_s \int_{-\frac{W}{2}}^{\frac{W}{2}} \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{S}}}\right]^2 dx \int_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} dz+$$
$$+\frac{\varepsilon_0}{2W}\kappa_s k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \int_{-\frac{W}{2}}^{\frac{W}{2}} \cos^2(nkx)dx \int_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} \cosh^2\left[nk\left(z+\frac{D}{2}\right)\right] dz \tag{C.8}$$

also due to the orthogonality relations of sines and cosines. Using again the Eq. (3.104) and the Eq. (3.105)

$$\frac{U^{\text{elec}}_{\text{para}(3)}}{L_y W} = \frac{\varepsilon_0}{2W}\kappa_s \left\{ \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{S}}}\right]^2 W\left(-\frac{d_{\text{P}}}{2}+\frac{D}{2}\right)+\right.$$
$$\left. + k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \frac{W}{2} \left\{ \int_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} \sinh^2\left[nk\left(z+\frac{D}{2}\right)\right] dz + \int_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} \cosh^2\left[nk\left(z+\frac{D}{2}\right)\right] dz \right\}\right\}$$
$$= \frac{\varepsilon_0}{2}\kappa_s \left\{ \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{S}}}\right]^2 \frac{d_{\text{S}}}{2} + k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \frac{1}{2} \int_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} \cosh\left[2nk\left(z+\frac{D}{2}\right)\right] dz \right\}$$
$$= \frac{\varepsilon_0}{4}\kappa_s \left\{ \frac{A^2 P_{\text{S}}^2}{\varepsilon_0^2\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{S}}} + k^2 \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n^2 \frac{1}{2nk} \sinh\left[2nk\left(z+\frac{D}{2}\right)\right]\Bigg|_{-\frac{D}{2}}^{-\frac{d_{\text{P}}}{2}} \right\}$$
$$= \frac{\varepsilon_0}{4}\kappa_s \left\{ \frac{A^2 P_{\text{S}}^2}{\varepsilon_0^2\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{S}}} + k \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n \frac{1}{2} \sinh\left[2nk\left(-\frac{d_{\text{P}}}{2}+\frac{D}{2}\right)\right] \right\}$$
$$= \frac{\kappa_s}{4} \frac{A^2 P_{\text{S}}^2}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{S}}} + \frac{\varepsilon_0 \kappa_s}{8} k \sum_{n=1}^{\infty} \delta_n^2 \nu_n^2 \theta_n^2 n \sinh(nkd_{\text{S}}) \tag{C.9}$$

where we have used again the definition of D and the property of the $\cosh(2x)$ applied in the previous paraelectric region.

Within the ferroelectric region 2, taking the square of the electric field in Eq. (4.16) and Eq. (4.17)

$$\mathcal{E}_x^{(2)2} = k^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \nu_n\theta_n \sin(nkx) n \sinh(nkcz) \nu_m\theta_m \sin(mkx) m \sinh(mkcz)$$
$$\mathcal{E}_z^{(2)2} = \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}}\right]^2 + 2\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}} \sum_{n=1}^{\infty} \nu_n\theta_n \cos(nkx) nkc \cosh(nkcz)+$$
$$+(kc)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \nu_n\theta_n \cos(nkx) n \cosh(nkcz) \nu_m\theta_m \cos(mkx) m \cosh(mkcz) \tag{C.10}$$

$U^{\text{elec}}_{\text{ferro}(2)}$ can be calculated from the following expression using Eq. (3.99). Doing the same as before to obtain this electrostatic energy per unit length along y

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y} &= \int \frac{\varepsilon_0}{2}\left[\kappa_a \mathcal{E}_x^{(3)2} + \kappa_c \mathcal{E}_z^{(3)2}\right] dxdz \\
&= \frac{\varepsilon_0}{2}\int \left\{\kappa_a k^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \nu_n\theta_n \sin(nkx) n \sinh(nkcz)\nu_m\theta_m \sin(mkx) m \sinh(mkcz) + \right. \\
&\quad + \kappa_c \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}}\right]^2 + 2\kappa_c \frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}}\sum_{n=1}^{\infty}\nu_n\theta_n\cos(nkx)nkc\cosh(nkcz) + \\
&\quad \left. + \kappa_c (kc)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\nu_n\theta_n\cos(nkx)n\cosh(nkcz)\nu_m\theta_m\cos(mkx)m\cosh(mkcz)\right\} dxdz \qquad \text{(C.11)}
\end{aligned}$$

Doing the same as before, but integrating over the entire thickness of the ferroelectric layer along z, we obtain the electrostatic energy in this region in units of energy/domain area

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} &= \frac{\varepsilon_0}{2W}\kappa_a k^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \int_{-\frac{W}{2}}^{\frac{W}{2}} \sin^2(nkx)dx \int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \sinh^2(nkcz)dz + \\
&\quad + \frac{\varepsilon_0}{2W}\kappa_c \int_{-\frac{W}{2}}^{\frac{W}{2}} \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}}\right]^2 dx \int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} dz + \\
&\quad + \frac{\varepsilon_0}{2W}\kappa_c (kc)^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \int_{-\frac{W}{2}}^{\frac{W}{2}} \cos^2(nkx)dx \int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \cosh^2(nkcz)dz \qquad \text{(C.12)}
\end{aligned}$$

where we have applied again the orthogonality relations of sines and cosines. Now, using another time the result of the integral of $\sin^2(x)$ and $\cos^2(x)$ over one period in x and calculating trivially the integral of the constants, we have

$$\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} = \frac{\varepsilon_0}{2}\kappa_c \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}}\right]^2 d_{\text{P}} + \frac{\varepsilon_0}{4}\kappa_a k^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \left[\int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \sinh^2(nkcz)dz + \int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \cosh^2(nkcz)dz\right] \qquad \text{(C.13)}$$

remembering that $c = \sqrt{\frac{\kappa_a}{\kappa_c}}$. Applying the hyperbolic property of $\cosh(2x) = \cosh^2(x) + \sinh^2(x)$

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} &= \frac{\varepsilon_0}{2}\kappa_c \left[\frac{AP_{\text{S}}}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)d_{\text{P}}}\right]^2 d_{\text{P}} + \frac{\varepsilon_0}{4}\kappa_a k^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \cosh(2nkcz)dz \\
&= \frac{A^2 P_{\text{S}}^2 \kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0}{4}\kappa_a k^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \int_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \cosh(2nkcz)dz \\
&= \frac{A^2 P_{\text{S}}^2 \kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0}{4}\kappa_a k^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \frac{1}{2nkc}\sinh(2nkcz)\Big|_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \\
&= \frac{A^2 P_{\text{S}}^2 \kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0}{4}\kappa_a k^2 \sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n^2 \frac{1}{2nkc}\sinh(2nkcz)\Big|_{-\frac{d_{\text{P}}}{2}}^{\frac{d_{\text{P}}}{2}} \\
&= \frac{A^2 P_{\text{S}}^2 \kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0\kappa_a k}{8c}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n \left[\sinh\left(2nkc\frac{d_{\text{P}}}{2}\right) - \sinh\left(-2nkc\frac{d_{\text{P}}}{2}\right)\right] \\
&= \frac{A^2 P_{\text{S}}^2 \kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0\kappa_a k}{8c}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n 2\sinh(nkcd_{\text{P}}) \qquad \text{(C.14)}
\end{aligned}$$

Now, using again the definition of the constant c

$$\begin{aligned}\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_yW} &= \frac{A^2P_{\text{S}}^2\kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0 c^2\kappa_c k}{4c}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\sinh(nkcd_{\text{P}})\\ &= \frac{A^2P_{\text{S}}^2\kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0 c\kappa_c k}{4}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\sinh(nkcd_{\text{P}})\end{aligned} \tag{C.15}$$

and applying the fact that $g = c\kappa_c$

$$\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_yW} = \frac{A^2P_{\text{S}}^2\kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0 gk}{4}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\sinh(nkcd_{\text{P}}) \tag{C.16}$$

Adding the Eq. (C.5), Eq. (C.9) and Eq. (C.16) together, it is obtained the total depolarization energy per unit area

$$\begin{aligned}\frac{U_{\text{elec}}}{L_yW} = &\frac{\kappa_s}{4}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{S}}} + \frac{\varepsilon_0\kappa_s}{8}k\sum_{n=1}^{\infty}\delta_n^2\nu_n^2\theta_n^2 n\sinh(nkd_{\text{S}}) + \frac{\kappa_s}{4}\frac{A^2P_{\text{S}}^2}{\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{S}}}+\\ &+\frac{\varepsilon_0\kappa_s}{8}k\sum_{n=1}^{\infty}\delta_n^2\nu_n^2\theta_n^2 n\sinh(nkd_{\text{S}}) + \frac{A^2P_{\text{S}}^2\kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0 gk}{4}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\sinh(nkcd_{\text{P}})\end{aligned} \tag{C.17}$$

which, when it is simplified, becomes

$$\begin{aligned}\frac{U_{\text{elec}}}{L_yW} &= \frac{A^2P_{\text{S}}^2\kappa_s}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{S}}} + \frac{A^2P_{\text{S}}^2\kappa_c}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2 d_{\text{P}}} + \frac{\varepsilon_0\kappa_s}{4}k\sum_{n=1}^{\infty}\delta_n^2\nu_n^2\theta_n^2 n\sinh(nkd_{\text{S}}) + \frac{\varepsilon_0 gk}{4}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\sinh(nkcd_{\text{P}})\\ &= \frac{A^2P_{\text{S}}^2}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)^2}\left(\frac{\kappa_s}{d_{\text{S}}}+\frac{\kappa_c}{d_{\text{P}}}\right) + \frac{\varepsilon_0 k}{4}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\left[\delta_n^2\kappa_s\sinh(nkd_{\text{S}})+g\sinh(nkcd_{\text{P}})\right]\\ &= \frac{A^2P_{\text{S}}^2}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)} + \frac{\varepsilon_0 k}{4}\sum_{n=1}^{\infty}\nu_n^2\theta_n^2 n\left[\delta_n^2\kappa_s\sinh(nkd_{\text{S}})+g\sinh(nkcd_{\text{P}})\right]\end{aligned} \tag{C.18}$$

Making use of $\nu_n = \frac{4P_{\text{S}}}{n^2\pi\varepsilon_0 k}\sin\left(\frac{n\pi}{2}(A+1)\right)$

$$\begin{aligned}\frac{U_{\text{elec}}}{L_yW} &= \frac{A^2P_{\text{S}}^2}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)} + \frac{\varepsilon_0 k}{4}\sum_{n=1}^{\infty}\frac{16P_{\text{S}}^2}{n^4\pi^2\varepsilon_0^2k^2}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\theta_n^2 n\left[\delta_n^2\kappa_s\sinh(nkd_{\text{S}})+g\sinh(nkcd_{\text{P}})\right]\\ &= \frac{A^2P_{\text{S}}^2}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)} + \frac{4P_{\text{S}}^2}{\pi^2\varepsilon_0 k}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\theta_n^2\left[\delta_n^2\kappa_s\sinh(nkd_{\text{S}})+g\sinh(nkcd_{\text{P}})\right]\end{aligned} \tag{C.19}$$

Next, we are going to apply the hyperbolic property of $\sinh(2x) = 2\sinh(x)\cosh(x)$ and the definition of $\delta_n = \frac{\sinh\left(nkc\frac{d_{\text{P}}}{2}\right)}{\sinh\left(nk\frac{d_{\text{S}}}{2}\right)}$

$$\begin{aligned}\frac{U_{\text{elec}}}{L_yW} = &\frac{A^2P_{\text{S}}^2}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)} + \frac{4P_{\text{S}}^2}{\pi^2\varepsilon_0 k}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\theta_n^2\left[\frac{\sinh^2\left(nkc\frac{d_{\text{P}}}{2}\right)}{\sinh^2\left(nk\frac{d_{\text{S}}}{2}\right)}\kappa_s 2\sinh\left(\frac{nkd_{\text{S}}}{2}\right)\cosh\left(\frac{nkd_{\text{S}}}{2}\right)+\right.\\ &\left.+g2\sinh\left(\frac{nkcd_{\text{P}}}{2}\right)\cosh\left(\frac{nkcd_{\text{P}}}{2}\right)\right]\end{aligned} \tag{C.20}$$

Using now the expression for $k = \frac{2\pi}{W}$

$$\begin{aligned}\frac{U_{\text{elec}}}{L_yW} = &\frac{A^2P_{\text{S}}^2}{2\varepsilon_0\left(\frac{\kappa_c}{d_{\text{P}}}+\frac{\kappa_s}{d_{\text{S}}}\right)} + \frac{4P_{\text{S}}^2}{\pi^2\varepsilon_0\frac{2\pi}{W}}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}(A+1)\right)}{n^3}\theta_n^2\left[\frac{\sinh^2\left(n\frac{2\pi}{W}c\frac{d_{\text{P}}}{2}\right)}{\sinh^2\left(n\frac{2\pi}{W}\frac{d_{\text{S}}}{2}\right)}\kappa_s 2\sinh\left(n\frac{2\pi}{W}\frac{d_{\text{S}}}{2}\right)\cosh\left(n\frac{2\pi}{W}\frac{d_{\text{S}}}{2}\right)+\right.\\ &\left.+g2\sinh\left(n\frac{2\pi}{W}\frac{cd_{\text{P}}}{2}\right)\cosh\left(n\frac{2\pi}{W}\frac{cd_{\text{P}}}{2}\right)\right]\end{aligned} \tag{C.21}$$

In the following, **we shall consider $W_+ = W_- = \omega$, which leads to $W = 2\omega$, and $A = \frac{W_+ - W_-}{W_+ + W_-} = 0$**

$$\begin{aligned}
\frac{U_{\text{elec}}}{L_y W} &= \frac{4P_{\text{S}}^2}{\pi^2\varepsilon_0 \frac{2\pi}{2\omega}} \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\theta_n^2 \left[\frac{\sinh^2\left(n\frac{2\pi}{2\omega}c\frac{d_{\text{P}}}{2}\right)}{\sinh^2\left(n\frac{2\pi}{2\omega}\frac{d_{\text{S}}}{2}\right)}\kappa_s 2\sinh\left(n\frac{2\pi}{2\omega}\frac{d_{\text{S}}}{2}\right)\cosh\left(n\frac{2\pi}{2\omega}\frac{d_{\text{S}}}{2}\right) + \right. \\
&\qquad \left. + g 2\sinh\left(n\frac{2\pi}{2\omega}\frac{cd_{\text{P}}}{2}\right)\cosh\left(n\frac{2\pi}{2\omega}\frac{cd_{\text{P}}}{2}\right)\right] \\
&= \frac{4P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\theta_n^2 \left[\frac{\sinh^2\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)}{\sinh^2\left(\frac{n\pi d_{\text{S}}}{2\omega}\right)}\kappa_s 2\sinh\left(\frac{n\pi d_{\text{S}}}{2\omega}\right)\cosh\left(\frac{n\pi d_{\text{S}}}{2\omega}\right) + \right. \\
&\qquad \left. + g 2\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\cosh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\right] \\
&= \frac{4P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\theta_n^2 \left[2\kappa_s \sinh^2\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\coth\left(\frac{n\pi d_{\text{S}}}{2\omega}\right) + 2g\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\cosh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\right] \\
&= \frac{4P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\theta_n^2 2\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\left[\kappa_s\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\coth\left(\frac{n\pi d_{\text{S}}}{2\omega}\right) + g\cosh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\right]
\end{aligned} \tag{C.22}$$

Remembering the definition of $\theta_n = \left[g\cosh\left(nkc\frac{d_{\text{P}}}{2}\right) + \kappa_s\sinh\left(nkc\frac{d_{\text{P}}}{2}\right)\coth\left(nk\frac{d_{\text{S}}}{2}\right)\right]^{-1}$, we can see that the term in brackets has the same expression, in this way

$$\begin{aligned}
\frac{U_{\text{elec}}}{L_y W} &= \frac{4P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\theta_n^2 2\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\theta_n^{-1} \\
&= \frac{4P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} 2\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\theta_n
\end{aligned} \tag{C.23}$$

Now, using the expression of θ_n we obtain the final expression of the electrostatic energy per unit area

$$\begin{aligned}
\frac{U_{\text{elec}}}{L_y W} &= \frac{4P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{2\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)}{\kappa_s\sinh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)\coth\left(\frac{n\pi d_{\text{S}}}{2\omega}\right) + g\cosh\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)} \\
&= \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{1}{\kappa_s\coth\left(\frac{n\pi d_{\text{S}}}{2\omega}\right) + g\coth\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)}
\end{aligned} \tag{C.24}$$

This electrostatic energy is divided by the length $D = d_{\text{P}} + d_{\text{S}}$ to obtain the depolarization energy per unit volume

$$\frac{U_{\text{elec}}}{L_y W D} = \frac{U_{\text{elec}}}{V} = \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0(d_{\text{P}} + d_{\text{S}})}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{1}{\kappa_s\coth\left(\frac{n\pi d_{\text{S}}}{2\omega}\right) + g\coth\left(\frac{n\pi cd_{\text{P}}}{2\omega}\right)} \tag{C.25}$$

It is wanted to write the energy of the Eq. (C.25) in terms of the ratio x of the thickness of the ferroelectric to width

$$x = \frac{d_{\text{P}}}{\omega} \tag{C.26}$$

For this, **an approximation will be made, where $d_{\text{P}} = d$ and $d_{\text{S}} = \frac{d_{\text{S}}}{d}d = \alpha d$.** Taking into account this approximation, the energy per unit volume can be expressed as

$$\begin{aligned}
\frac{U_{\text{elec}}}{V} &= \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0(d + \alpha d)}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{1}{\kappa_s\coth\left(\frac{n\pi\alpha d}{2\omega}\right) + g\coth\left(\frac{n\pi cd}{2\omega}\right)} \\
&= \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0(1 + \alpha)d}\omega \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{1}{\kappa_s\coth\left(\frac{n\pi\alpha d}{2\omega}\right) + g\coth\left(\frac{n\pi cd}{2\omega}\right)} \\
&= \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0(1 + \alpha)}\frac{1}{x} \sum_{n=1}^{\infty} \frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \frac{1}{\kappa_s\coth\left(\frac{n\pi\alpha}{2}x\right) + g\coth\left(\frac{n\pi c}{2}x\right)}
\end{aligned} \tag{C.27}$$

and we can examine the behaviour in terms in the different limits. The monodomain energy $\frac{U_{\text{elec}}^{\text{mono}}}{V}$ is obtained when $x \to 0$

$$\lim_{x\to 0} \frac{1}{x\left[\kappa_s\coth\left(\frac{n\pi\alpha}{2}x\right) + g\coth\left(\frac{n\pi c}{2}x\right)\right]} \tag{C.28}$$

Expanding the function of the denominator to first order and solving the limit

$$
\begin{aligned}
\lim_{x\to 0}\frac{1}{x\left[\kappa_s\coth\left(\frac{n\pi\alpha}{2}x\right)+g\coth\left(\frac{n\pi c}{2}x\right)\right]} &= \lim_{x\to 0}\frac{1}{x\left[\frac{2\kappa_s}{n\pi\alpha x}+\frac{\kappa_s n\pi\alpha x}{6}+\frac{2g}{n\pi c x}+\frac{gn\pi c x}{6}\right]}\\
&= \lim_{x\to 0}\frac{1}{\frac{2\kappa_s}{n\pi\alpha}+\frac{\kappa_s n\pi\alpha x^2}{6}+\frac{2g}{n\pi c}+\frac{gn\pi c x^2}{6}}\\
&= \frac{1}{\frac{2\kappa_s}{n\pi\alpha}+\frac{2g}{n\pi c}}\\
&= \frac{n\pi c\alpha}{2g\alpha+2\kappa_s c}
\end{aligned} \tag{C.29}
$$

that yields to

$$
\begin{aligned}
\lim_{x\to 0}\frac{U_{\text{elec}}}{V} &= \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0(1+\alpha)}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\frac{n\pi c\alpha}{2g\alpha+2\kappa_s c}\\
&= \frac{8P_{\text{S}}^2 c\alpha}{2\pi^2\varepsilon_0(1+\alpha)(g\alpha+\kappa_s c)}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^2}\\
&= \frac{8P_{\text{S}}^2 c}{2\pi^2\varepsilon_0(1+\alpha)(g+\alpha^{-1}\kappa_s c)}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^2}
\end{aligned} \tag{C.30}
$$

Using the result of the infinite sum obtained in Eq. (3.130)

$$
\begin{aligned}
\frac{U_{\text{elec}}^{\text{mono}}}{V} &= \frac{8P_{\text{S}}^2 c}{2\pi^2\varepsilon_0(1+\alpha)(g+\alpha^{-1}\kappa_s c)}\frac{\pi^2}{8}\\
&= \frac{P_{\text{S}}^2 c}{2\varepsilon_0(1+\alpha)(g+\alpha^{-1}\kappa_s c)}
\end{aligned} \tag{C.31}
$$

and the definition of $g = c\kappa_c$

$$
\frac{U_{\text{elec}}^{\text{mono}}}{V} = \frac{P_{\text{S}}^2}{2\varepsilon_0(1+\alpha)(\kappa_c+\alpha^{-1}\kappa_s)} \tag{C.32}
$$

On the other hand, the electrostatic in the Kittel limit $\frac{U_{\text{elec}}^{\text{Kittel}}}{V}$ can be also approximated using

$$
\lim_{x\to\infty}\coth\left(\frac{n\pi c}{2}x\right) = \lim_{x\to\infty}\coth\left(\frac{n\pi\alpha}{2}x\right) = 1 \tag{C.33}
$$

so we can obtain

$$
\begin{aligned}
\lim_{x\to\infty}\frac{U_{\text{elec}}}{V} &= \frac{8P_{\text{S}}^2}{\pi^3\varepsilon_0(1+\alpha)(g+\kappa_s)}\frac{1}{x}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\\
&= \frac{16P_{\text{S}}^2}{2\pi^3\varepsilon_0(1+\alpha)(g+\kappa_s)}\frac{1}{x}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}
\end{aligned} \tag{C.34}
$$

The result of the infinite series is achieved in Eq. (3.134), so it is obtained a Kittel-like expression in the limit $x\to\infty$

$$
\frac{U_{\text{elec}}^{\text{Kittel}}}{V} \approx \frac{P_{\text{S}}^2}{2\varepsilon_0}\beta(\kappa_s.\alpha)\frac{1}{x} \tag{C.35}
$$

where

$$
\beta(\kappa_s,\alpha) = \frac{16}{\pi^3(1+\alpha)(g+\kappa_s)}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \approx \frac{16.829}{\pi^3(1+\alpha)(g+\kappa_s)} \tag{C.36}
$$

D Kittel law of the superlattice system

As described at the beginning of Sec. 3.2, the total energy per unit volume U of the system when $d >> \omega$ is

$$
U = \frac{(P-P_{\text{S}})^2}{2\varepsilon_0\chi_c} + \frac{P_{\text{S}}^2}{2\varepsilon_0}\beta(\kappa_s,\alpha)\frac{\omega}{d} + \frac{\Sigma}{\omega} \tag{D.1}
$$

Minimizing this total energy per unit volume with respect ω

$$\frac{\partial U}{\partial \omega} = \frac{P_S^2}{2\varepsilon_0}\beta(\kappa_s,\alpha)\frac{1}{d} - \frac{\Sigma}{\omega^2} = 0 \tag{D.2}$$

Kittel Law is obtained

$$\omega = \sqrt{l_k(\kappa_s,\alpha)d} \tag{D.3}$$

where

$$l_k(\kappa_s,\alpha) = \frac{2\varepsilon_0\Sigma}{P_S^2\beta(\kappa_s,\alpha)} \tag{D.4}$$

is the Kittel length, which defines a characteristic length scale of the system.

E Electrostatic potential of the system formed by a ferroelectric thin film and a substrate

The Laplace equation for the potential in the three regions of space, taking into account the same **assumptions** as in Sec. 3.2.3, are

$$\nabla^2\phi_1 = \kappa_s\nabla^2\phi_3 = 0 \tag{E.1}$$

$$\kappa_a\frac{\partial^2\phi_2}{\partial x^2} + \kappa_c\frac{\partial^2\phi_2}{\partial z^2} = 0 \tag{E.2}$$

where κ_s is the electronic dielectric constant of the substrate. These equations have the same solutions as Eq. (3.25) and Eq. (3.26). For this reason, the potentials that satisfy these Laplace equations are those given in Eq. (3.46)

$$\begin{aligned}
\phi_1(x,z) &= a_0^{(1)}(z) + \sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(1)}e^{nkz} + d_n'^{(1)}e^{-nkz}) \\
\phi_2(x,z) &= a_0^{(2)}(z) + \sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(2)}e^{nkcz} + d_n'^{(2)}e^{-nkcz}) \\
\phi_3(x,z) &= a_0^{(3)}(z) + \sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(3)}e^{nkz} + d_n'^{(3)}e^{-nkz})
\end{aligned} \tag{E.3}$$

where the even parity in the x-direction has already been taken into account.

The next step is to find the expression for the coefficients $a_0^{(i)}(z)$. We have used the same procedure as in Sec. 3.2.3 from Eq. (3.53) until Eq. (3.57). Knowing these coefficients and applying the fact that the electric filed vanishes when $z \to +\infty$ and $z \to -\infty$, we can write the potentials as

$$\begin{aligned}
\phi_1(x,z) &= \sum_{n=1}^{\infty} d_n'^{(1)}\cos(nkx)e^{-nkz} \\
\phi_2(x,z) &= \frac{P_S A}{\varepsilon_0\kappa_c}z + \sum_{n=1}^{\infty}\cos(nkx)(c_n'^{(2)}e^{nkcz} + d_n'^{(2)}e^{-nkcz}) \\
\phi_3(x,z) &= -\frac{P_S A}{\varepsilon_0\kappa_c}d + \sum_{n=1}^{\infty} c_n'^{(3)}\cos(nkx)e^{nkz}
\end{aligned} \tag{E.4}$$

In order to obtain the expression for the remaining unknown coefficients in Eq. (E.4), the fact that the potential and the normal component of the displacement vectors must be equal on the surfaces of the thin film can be used. In this way, since the expressions of the potentials are the same as in the case of the isolated film before applying the previous boundary conditions, and the normal component of the displacement vectors only differs from that of region 3 by a factor of κ_s, the relations between the different coefficients will remain the same except for Eq. (3.70), which will be modified in the second term of the left part due to the definition of the displacement vector in region 3 [Eq. (5.2)].

$$d_n'^{(1)} = c_n'^{(2)} + d_n'^{(2)} \tag{E.5}$$

$$c_n'^{(3)}e^{-nkd} = c_n'^{(2)}e^{-2nR} + d_n'^{(2)}e^{2nR} \tag{E.6}$$

$$nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + d_n'^{(1)}nk = \frac{4P_S}{n\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right) \tag{E.7}$$

$$nkc\kappa_c(c_n'^{(2)}e^{-nkcd} - d_n'^{(2)}e^{nkcd}) - nk\kappa_s c_n'^{(3)}e^{-nkd} = \frac{4P_S}{n\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right) \tag{E.8}$$

Since the right-hand side of Eq. (E.7) and the right-hand side of Eq (E.8) are equal

$$c\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + d_n'^{(1)} = c\kappa_c(c_n'^{(2)}e^{-nkcd} - d_n'^{(2)}e^{nkcd}) - \kappa_s c_n'^{(3)}e^{-nkd} \tag{E.9}$$

Now, replacing Eq. (E.5) and Eq. (E.6) into Eq. (E.9)

$$c\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + c_n'^{(2)} + d_n'^{(2)} = c\kappa_c(c_n'^{(2)}e^{-2nR} - d_n'^{(2)}e^{2nR}) - \kappa_s(c_n'^{(2)}e^{-2nR} + d_n'^{(2)}e^{2nR}) \tag{E.10}$$

where we have used $R = \frac{\pi cd}{W}$. Within Eq. (E.10), the terms in which $d_n'^{(2)}$ will be joined on one side of the equality and on the other side those with $c_n'^{(2)}$, obtaining a relation between these two coefficients

$$d_n'^{(2)} = \frac{(c\kappa_c - \kappa_s)e^{-2nR} - (c\kappa_c + 1)}{(c\kappa_c + \kappa_s)e^{2nR} - (c\kappa_c - 1)}c_n'^{(2)} \tag{E.11}$$

Carrying out various operations

$$\begin{aligned}
d_n'^{(2)} &= \frac{g - \kappa_s - (g+1)e^{2nR}}{(g+\kappa_s)e^{2nR} - (g-1)}e^{-2nR}c_n'^{(2)} \\
&= -\frac{g(e^{2nR}-1) + \kappa_s + e^{2nR}}{g(e^{2nR}-1) + \kappa_s e^{2nR} + 1}e^{-2nR}c_n'^{(2)} \\
&= -\frac{ge^{nR}(e^{nR} - e^{-nR}) + \kappa_s + e^{2nR}}{ge^{nR}(e^{nR} - e^{-nR}) + \kappa_s e^{2nR} + 1}e^{-2nR}c_n'^{(2)} \\
&= -\frac{2ge^{nR}\sinh(nR) + \kappa_s + e^{2nR}}{2ge^{nR}\sinh(nR) + \kappa_s e^{2nR} + 1}e^{-2nR}c_n'^{(2)} \\
&= -\frac{2g\sinh(nR) + \kappa_s e^{-nR} + e^{nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}e^{-2nR}c_n'^{(2)}
\end{aligned} \tag{E.12}$$

where we have used the fact that $g = c\kappa_c$. Since the relation between $d_n'^{(2)}$ and $c_n'^{(2)}$ has already been obtained, the ratio of all other coefficients with $c_n'^{(2)}$ can be found. For example, from Eq. (E.5)

$$\begin{aligned}
d_n'^{(1)} &= c_n'^{(2)} + d_n'^{(2)} \\
&= c_n'^{(2)} - \frac{2g\sinh(nR) + \kappa_s e^{-nR} + e^{nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}e^{-2nR}c_n'^{(2)} \\
&= \frac{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR} - 2g\sinh(nR)e^{-2nR} - \kappa_s e^{-nR}e^{-2nR} - e^{nR}e^{-2nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)} \\
&= \frac{2g\sinh(nR)e^{-nR}(e^{nR} - e^{-nR}) + \kappa_s e^{-nR}(e^{2nR} - e^{-2nR})}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)} \\
&= \frac{4g\sinh^2(nR)e^{-nR} + 2\kappa_s\sinh(2nR)e^{-nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)}
\end{aligned} \tag{E.13}$$

and from Eq. (E.6)

$$\begin{aligned}
c_n'^{(3)}e^{-nkd} &= c_n'^{(2)}e^{-2nR} + d_n'^{(2)}e^{2nR} \\
&= e^{-2nR}c_n'^{(2)} - \frac{2g\sinh(nR) + \kappa_s e^{-nR} + e^{nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)} \\
&= \frac{2g\sinh(nR)e^{-2nR} + \kappa_s e^{nR}e^{-2nR} + e^{-nR}e^{-2nR} - 2g\sinh(nR) - \kappa_s e^{-nR} - e^{nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)} \\
&= \frac{2g\sinh(nR)e^{-nR}(e^{-nR} - e^{nR}) + e^{-nR}(e^{-2nR} - e^{2nR})}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)} \\
&= -\frac{4g\sinh^2(nR)e^{-nR} + 2\sinh(2nR)e^{-nR}}{2g\sinh(nR) + \kappa_s e^{nR} + e^{-nR}}c_n'^{(2)}
\end{aligned} \tag{E.14}$$

From Eq. (E.7), Eq. (E.12) and Eq. (E.13)

$$\frac{4P_S}{n\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right) = nkc\kappa_c(c_n'^{(2)} - d_n'^{(2)}) + d_n'^{(1)}nk$$

$$\frac{4P_S}{n\pi\varepsilon_0}\sin\left(\frac{n\pi}{2}(A+1)\right) = nkc\kappa_c\left[c_n'^{(2)} + \frac{2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}e^{-2nR}c_n'^{(2)}\right] + $$
$$+\frac{4g\sinh^2(nR)e^{-nR}+2\kappa_s\sinh(2nR)e^{-nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}nkc_n'^{(2)}$$

Therefore, the expression for $c_n'^{(2)}$ can be written as

$$c_n'^{(2)} = \frac{4P_S W}{n^2\pi\varepsilon_0 2\pi}\sin\left(\frac{n\pi}{2}(A+1)\right)\left\{c\kappa_c\left[1+\frac{2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}e^{-2nR}\right]+\right.$$
$$\left.+\frac{4g\sinh^2(nR)e^{-nR}+2\kappa_s\sinh(2nR)e^{-nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}\right\}^{-1} \tag{E.15}$$

where we have used $k=\frac{2\pi}{W}$. The term between braces will now be developed

$$\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{[2g^2\sinh(nR)+g\kappa_s e^{nR}+ge^{-nR}+2g^2\sinh(nR)e^{-2nR}+g\kappa_s e^{-3nR}+ge^{-nR}+4g\sinh^2(nR)e^{-nR}+2\kappa_s\sinh(2nR)e^{-nR}]}$$
$$\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{4g^2\sinh(nR)e^{-nR}\cosh(nR)+2\kappa_s e^{-nR}\sinh(2nR)+ge^{-nR}[2+2\kappa_s\cosh(2nR)+4\sinh^2(nR)]}$$
$$\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2g^2\sinh(2nR)e^{-nR}+2\kappa_s e^{-nR}\sinh(2nR)+ge^{-nR}[2+2\kappa_s\cosh(2nR)+4\sinh^2(nR)]}$$
$$\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}} \tag{E.16}$$

If this expression is introduced into Eq. (E.15), the final expression for the coefficient $c_n'^{(2)}$ is

$$c_n'^{(2)} = \frac{4P_S W}{n^2\pi\varepsilon_0 2\pi}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}}$$
$$= \frac{1}{4\pi\varepsilon_0}\left(\frac{8P_S cd}{R}\right)\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}}$$
$$= \alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}} \tag{E.17}$$

using $\alpha=\frac{1}{4\pi\varepsilon_0}\left(\frac{8P_S cd}{R}\right)$. Then, from Eq. (E.12)

$$d_n'^{(2)} = -\frac{2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}e^{-2nR}c_n^2$$
$$= -\frac{2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}e^{-2nR}\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\cdot$$
$$\cdot\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}}$$
$$= \alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}}{2e^{nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}} \tag{E.18}$$

and from Eq. (E.13)

$$d_n'^{(1)} = \frac{4g\sinh^2(nR)e^{-nR}+2\kappa_s\sinh(2nR)e^{-nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}c_n^2$$
$$= \frac{4g\sinh^2(nR)e^{-nR}+2\kappa_s\sinh(2nR)e^{-nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\cdot$$
$$\cdot\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}}$$
$$= \alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{2g\sinh^2(nR)+\kappa_s\sinh(2nR)}{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]} \tag{E.19}$$

Finally, from Eq. (E.14)

$$\begin{aligned}
c_n'^{(3)} &= -e^{nkd}\frac{4g\sinh^2(nR)e^{-nR}+2\sinh(2nR)e^{-nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}c_n^2 \\
&= -e^{nkd}\frac{4g\sinh^2(nR)e^{-nR}+2\sinh(2nR)e^{-nR}}{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\cdot \\
&\quad\cdot\frac{2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}}{2e^{-nR}\{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}} \\
&= -\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{2g\sinh^2(nR)+\sinh(2nR)}{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]}e^{nkd}
\end{aligned}\tag{E.20}$$

To simplify the notation, we are going to rename

$$\mu_n = \{(g^2+\kappa_s)\sinh(2nR)+g[1+\kappa_s\cosh(2nR)+2\sinh^2(nR)]\}^{-1}\tag{E.21}$$

Thus, the final expression of the coefficients is

$$\begin{aligned}
c_n'^{(2)} &= \alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{[2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}]\mu_n}{2e^{-nR}} \\
d_n'^{(2)} &= \alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{[2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}]\mu_n}{2e^{nR}} \\
d_n'^{(1)} &= \alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]\mu_n \\
c_n'^{(3)} &= -\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}[2g\sinh^2(nR)+\sinh(2nR)]\mu_n e^{nkd}
\end{aligned}\tag{E.22}$$

Every coefficient that appear in Eq. (E.4) is known. Replacing them, we get the final expression for the potential in the three regions.

$$\phi_1(x,z) = \sum_{n=1}^{\infty}\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]\mu_n\cos(nkx)e^{-nkz}\tag{E.23}$$

For the potential in region 2, we have

$$\begin{aligned}
\phi_2(x,z) &= \frac{P_S A}{\varepsilon_0\kappa_c}z+\sum_{n=1}^{\infty}\cos(nkx)\left\{\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{[2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}]\mu_n e^{nkcz}}{2e^{-nR}}-\right. \\
&\qquad\left.-\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}\frac{[2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}]\mu_n e^{-nkcz}}{2e^{nR}}\right\} \\
&= \frac{P_S A}{\varepsilon_0\kappa_c}z+\sum_{n=1}^{\infty}\cos(nkx)\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n^2}\left\{\frac{[2g\sinh(nR)+\kappa_s e^{nR}+e^{-nR}]e^{nkcz}}{2e^{-nR}}-\right. \\
&\qquad\left.-\frac{[2g\sinh(nR)+\kappa_s e^{-nR}+e^{nR}]e^{-nkcz}}{2e^{nR}}\right\} \\
&= \frac{P_S A}{\varepsilon_0\kappa_c}z+\sum_{n=1}^{\infty}\cos(nkx)\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n^2}\left\{\frac{2g\sinh(nR)e^{nR+nkcz}+\kappa_s e^{2nR+nkcz}+e^{nkcz}}{2}-\right. \\
&\qquad\left.-\frac{2g\sinh(nR)e^{-nR-nkcz}+\kappa_s e^{-2nR-nkcz}+e^{-nkcz}}{2}\right\} \\
&= \frac{P_S A}{\varepsilon_0\kappa_c}z+\sum_{n=1}^{\infty}\cos(nkx)\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n^2}[2g\sinh(nR)\sinh(nR+nkcz)+\kappa_s\sinh(2nR+nkcz)+ \\
&\qquad+\sinh(nkcz)]
\end{aligned}\tag{E.24}$$

Finally, for the potential in the third region,

$$\begin{aligned}
\phi_3(x,z) &= -\frac{P_S A}{\varepsilon_0\kappa_c}d-\sum_{n=1}^{\infty}\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}[2g\sinh^2(nR)+\sinh(2nR)]\mu_n e^{nkd}\cos(nkx)e^{nkz} \\
&= -\frac{P_S A}{\varepsilon_0\kappa_c}d-\sum_{n=1}^{\infty}\alpha\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{1}{n^2}[2g\sinh^2(nR)+\sinh(2nR)]\mu_n\cos(nkx)e^{nk(z+d)}
\end{aligned}\tag{E.25}$$

F Electrostatic energy of the system formed by a ferroelectric thin film and a substrate

Let us compute the electrostatic energy stored in the vacuum region 1. The square of the electric fields given by Eq.(5.7) and Eq.(5.8) is

$$\begin{aligned}
\mathcal{E}_x^{(1)2} = (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\left[2g\sinh^2(nR)+\kappa_s\sinh(2nR)\right]\sin(nkx)e^{-nkz}\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\cdot \\
\cdot\left[2g\sinh^2(mR)+\kappa_s\sinh(2mR)\right]\sin(mkx)e^{-mkz}, \\
\mathcal{E}_z^{(1)2} = (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\left[2g\sinh^2(nR)+\kappa_s\sinh(2nR)\right]\cos(nkx)e^{-nkz}\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\cdot \\
\cdot\left[2g\sinh^2(mR)+\kappa_s\sinh(2mR)\right]\cos(mkx)e^{-mkz}
\end{aligned} \tag{F.1}$$

Considering these expressions, $U^{\mathrm{elec}}_{\mathrm{vacuum}(1)}$ can be calculated from Eq. (3.98). Since we have also assumed that all the physical magnitudes are periodic along y-direction, we can integrate only in the $(x,\ z)$ plane to obtain the energy per unit length along y.

$$\begin{aligned}
\frac{U^{\mathrm{elec}}_{\mathrm{vacuum}(1)}}{L_y} = \frac{\varepsilon_0}{2}(\alpha k)^2 \int \Bigg\{ \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\left[2g\sinh^2(nR)+\kappa_s\sinh(2nR)\right]\sin(nkx)e^{-nkz}\cdot \\
\cdot\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\left[2g\sinh^2(mR)+\kappa_s\sinh(2mR)\right]\sin(mkx)e^{-mkz}+ \\
+\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\left[2g\sinh^2(nR)+\kappa_s\sinh(2nR)\right]\cos(nkx)e^{-nkz}\cdot \\
\cdot\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\left[2g\sinh^2(mR)+\kappa_s\sinh(2mR)\right]\cos(mkx)e^{-mkz}\Bigg\}\,dxdz
\end{aligned} \tag{F.2}$$

Next, we will integrate this electrostatic energy over one period of length W along the x direction, and over the extension of the vacuum region 1 (with z ranging between 0 and ∞). If the result is divided by the domain width, the electrostatic energy will be given in units of energy/domain area

$$\begin{aligned}
\frac{U^{\mathrm{elec}}_{\mathrm{vacuum}(1)}}{L_y W} = \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\left[2g\sinh^2(nR)+\kappa_s\sinh(2nR)\right]^2\frac{1}{W}\cdot \\
\cdot\left[\int_{-W/2}^{W/2}\sin^2(nkx)dx\int_0^{\infty}e^{-2nkz}dz+\int_{-W/2}^{W/2}\cos^2(nkx)dx\int_0^{\infty}e^{-2nkz}dz\right]
\end{aligned} \tag{F.3}$$

where we have applied the orthogonality relations of sines and cosines expressed in Eq.(3.103). Using Eq.(3.104) and Eq.(3.105)

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{vacuum}(1)}}{L_y W} &= \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2 \cdot \\
&\quad \cdot \left[\frac{1}{2}\left(-\frac{1}{2nk}e^{-2nkz}\Big|_0^{\infty}\right)+\frac{1}{2}\left(-\frac{1}{2nk}e^{-2nkz}\Big|_0^{\infty}\right)\right] \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2\left(\frac{1}{2}\frac{1}{2nk}+\frac{1}{2}\frac{1}{2nk}\right) \\
&= \frac{\varepsilon_0}{2}(\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2\frac{1}{2nk} \\
&= \frac{\varepsilon_0}{4}\alpha^2 k \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2 \\
&= \frac{\varepsilon_0}{4}\frac{1}{16\varepsilon_0^2\pi^2}\left(\frac{64P_{\text{S}}^2c^2d^2}{R^2}\right)\frac{2\pi}{W}\sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2 \\
&= \frac{1}{4}\frac{4P_{\text{S}}^2c^2d^2}{\varepsilon_0\pi^2 R\frac{\pi cd}{W}}\frac{2\pi}{W}\sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2 \\
&= \frac{1}{2}\frac{4P_{\text{S}}^2gd}{\pi^2\varepsilon_0\kappa_c R}\sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2
\end{aligned} \tag{F.4}$$

Following the same procedure, we can obtain the electrostatic energy in the substrate region 3. The square of the electric fields expressed in Eq.(5.11) and Eq.(5.12) is

$$\begin{aligned}
\mathcal{E}_x^{(3)2} &= (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}[2g\sinh^2(nR)+\sinh(2nR)]\sin(nkx)e^{nk(z+d)}\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\cdot \\
&\quad \cdot [2g\sinh^2(mR)+\sinh(2mR)]\sin(mkx)e^{mk(z+d)} \\
\mathcal{E}_z^{(3)2} &= (\alpha k)^2 \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}[2g\sinh^2(nR)+\sinh(2nR)]\cos(nkx)e^{nk(z+d)}\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\cdot \\
&\quad \cdot [2g\sinh^2(mR)+\sinh(2mR)]\cos(mkx)e^{mk(z+d)}
\end{aligned} \tag{F.5}$$

Then, $U^{\text{elec}}_{\text{subs}(3)}$ can be calculated from Eq. (C.1). Integrating only in the (x, z) plane, we obtain $U^{\text{elec}}_{\text{subs}(3)}$ per unit length along y

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{subs}(3)}}{L_y} &= \frac{\varepsilon_0}{2}\kappa_s(\alpha k)^2 \int \Bigg\{\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}[2g\sinh^2(nR)+\sinh(2nR)]\sin(nkx)e^{nk(z+d)}\cdot \\
&\quad \cdot \sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}[2g\sinh^2(mR)+\sinh(2mR)]\sin(mkx)e^{mk(z+d)}+ \\
&\quad + \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}[2g\sinh^2(nR)+\sinh(2nR)]\cos(nkx)e^{nk(z+d)}\cdot \\
&\quad \cdot \sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}[2g\sinh^2(mR)+\sinh(2mR)]\cos(mkx)e^{mk(z+d)}\Bigg\}\,dxdz
\end{aligned} \tag{F.6}$$

Doing the same as in the previous region but, in this case, integrating in z over all the extension of the substrate (between $-\infty$ and $-d$), the electrostatic energy in this region will be given in units of energy/domain area

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{subs}(3)}}{L_y W} &= \frac{\varepsilon_0}{2}\kappa_s(\alpha k)^2 \sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}[2g\sinh^2(nR)+\sinh(2nR)]^2\frac{1}{W}\cdot \\
&\quad \cdot \left[\int_{-W/2}^{W/2}\sin^2(nkx)dx\int_{-\infty}^{-d}e^{2nk(z+d)}dz+\int_{-W/2}^{W/2}\cos^2(nkx)dx\int_{-\infty}^{-d}e^{2nk(z+d)}dz\right]
\end{aligned} \tag{F.7}$$

also due to the orthogonality relations of sines and cosines expressed in Eq.(3.103). Using again Eq.(3.104) and Eq.(3.105)

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{subs}(3)}}{L_y W} &= \frac{\varepsilon_0}{2}\kappa_s(\alpha k)^2\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}[2g\sinh^2(nR)+\sinh(2nR)]^2\frac{1}{W}2\frac{W}{2}\int_{-\infty}^{-d}e^{2nk(z+d)}dz\\
&= \frac{\varepsilon_0}{2}\kappa_s(\alpha k)^2\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}[2g\sinh^2(nR)+\sinh(2nR)]^2\frac{1}{2nk}e^{2nk(z+d)}\Big|_{-\infty}^{-d}\\
&= \frac{\varepsilon_0}{4}\kappa_s\alpha^2 k\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\sinh(2nR)]^2\\
&= \frac{\varepsilon_0}{4}\kappa_s\frac{1}{16\pi^2\varepsilon_0^2}\left(\frac{64P_S^2c^2d^2}{R^2}\right)k\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\sinh(2nR)]^2\\
&= \frac{1}{4}\kappa_s\frac{4P_S^2c^2d^2}{\pi^2\varepsilon_0 R\frac{\pi cd}{W}}\frac{2\pi}{W}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\sinh(2nR)]^2\\
&= \frac{1}{2}\kappa_s\frac{4P_S^2cd}{\pi^2\varepsilon_0 R}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\sinh(2nR)]^2\\
&= \frac{1}{2}\frac{4P_S^2gd}{\pi^2\varepsilon_0\kappa_c R}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\kappa_s[2g\sinh^2(nR)+\sinh(2nR)]^2
\end{aligned}
\tag{F.8}
$$

Finally, within the ferroelectric region 2, taking the square of the electric fields in Eq. (5.9) and Eq. (5.10),

$$
\begin{aligned}
\mathcal{E}_x^{(2)2} &= (\alpha k)^2\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\sin(nkx)[2g\sinh(nR)\sinh(nR+nkcz)+\kappa_s\sinh(2nR+nkcz)+\\
&\qquad +\sinh(nkcz)]\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\sin(mkx)\cdot\\
&\qquad \cdot[2g\sinh(mR)\sinh(mR+mkcz)+\kappa_s\sinh(2mR+mkcz)+\sinh(mkcz)],\\
\mathcal{E}_z^{(2)2} &= \left(\frac{P_SA}{\varepsilon_0\kappa_c}\right)^2+(\alpha kc)^2\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\cos(nkx)[2g\sinh(nR)\cosh(nR+nkcz)+\\
&\qquad +\kappa_s\cosh(2nR+nkcz)+\cosh(nkcz)]\cdot\\
&\qquad \cdot\sin\left(\frac{m\pi}{2}(A+1)\right)\frac{\mu_m}{m}\cos(mkx)[2g\sinh(mR)\cosh(mR+mkcz)+\\
&\qquad +\kappa_s\cosh(2mR+mkcz)+\cosh(mkcz)]+\\
&\quad +2\frac{P_SA}{\varepsilon_0\kappa_c}\alpha kc\sum_{n=1}^{\infty}\sin\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n}{n}\cos(nkx)[2g\sinh(nR)\cosh(nR+nkcz)+\kappa_s\cosh(2nR+nkcz)+\\
&\qquad +\cosh(nkcz)].
\end{aligned}
\tag{F.9}
$$

Then, $U^{\text{elec}}_{\text{ferro}(2)}$ can be calculated from Eq.(3.99). Doing the same as before, we can obtain this electrostatic energy per unit length along y

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro(2)}}}{L_y} = \frac{\varepsilon_0}{2} \int \Bigg\{ & \kappa_a (\alpha k)^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} \sin(nkx) \cdot \\
& \cdot [2g \sinh(nR) \sinh(nR + nkcz) + \kappa_s \sinh(2nR + nkcz) + \sinh(nkcz)] \cdot \\
& \cdot \sin\left(\frac{m\pi}{2}(A+1)\right) \frac{\mu_m}{m} \sin(mkx) [2g \sinh(mR) \sinh(mR + mkcz) + \\
& + \kappa_s \sinh(2mR + mkcz) + \sinh(mkcz)] + \\
& + \kappa_c \Bigg\{ \left(\frac{P_S A}{\varepsilon_0 \kappa_c}\right)^2 + (\alpha kc)^2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} \cos(nkx) \cdot \\
& \cdot [2g \sinh(nR) \cosh(nR + nkcz) + \kappa_s \cosh(2nR + nkcz) + \\
& + \cosh(nkcz)] \sin\left(\frac{m\pi}{2}(A+1)\right) \frac{\mu_m}{m} \cdot \cos(mkx) \cdot \\
& \cdot [2g \sinh(mR) \cosh(mR + mkcz) + \kappa_s \cosh(2mR + mkcz) + \\
& + \cosh(mkcz)] + \\
& + 2 \frac{P_S A}{\varepsilon_0 \kappa_c} \alpha kc \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} \cos(nkx) \cdot \\
& \cdot [2g \sinh(nR) \cosh(nR + nkcz) + \kappa_s \cosh(2nR + nkcz) \\
& + \cosh(nkcz)] \Bigg\} \Bigg\} dx dz
\end{aligned} \tag{F.10}
$$

Next, we will obtain the electrostatic energy in units of energy/domain area, as we did with the two previous regions, but now integrating in z over the ferroelectric region

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro(2)}}}{L_y W} = \frac{\varepsilon_0}{2} \Bigg\{ & \frac{1}{\kappa_c} \left(\frac{P_S A}{\varepsilon_0}\right)^2 \frac{1}{W} \int_{-W/2}^{W/2} dx \int_{-d}^{0} dz + \\
& + \kappa_a (\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n^2}{n^2} \frac{1}{W} \int_{-W/2}^{W/2} \sin^2(nkx) dx \cdot \\
& \cdot \int_{-d}^{0} [2g \sinh(nR) \sinh(nR + nkcz) + \kappa_s \sinh(2nR + nkcz) + \sinh(nkcz)]^2 dz + \\
& + \kappa_c (\alpha kc)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n^2}{n^2} \frac{1}{W} \int_{-W/2}^{W/2} \cos^2(nkx) dx \cdot \\
& \cdot \int_{-d}^{0} [2g \sinh(nR) \cosh(nR + nkcz) + \kappa_s \cosh(2nR + nkcz) + \cosh(nkcz)]^2 dz + \\
& + 2 \frac{P_S A}{\varepsilon_0} \alpha kc \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{2}(A+1)\right) \frac{\mu_n}{n} \frac{1}{W} \int_{-W/2}^{W/2} \cos(nkx) dx \cdot \\
& \cdot \int_{-d}^{0} [2g \sinh(nR) \cosh(nR + nkcz) + \kappa_s \cosh(2nR + nkcz) + \cosh(nkcz)] dz \Bigg\}
\end{aligned} \tag{F.11}
$$

also using the orthogonality relations of sines and cosines expressed in Eq. (3.103). Making use of Eq. (3.104), Eq. (3.105) and Eq. (3.115)

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro(2)}}}{L_y W} =& \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0 \kappa_c} d + \\
&+ \frac{\varepsilon_0}{4}\kappa_a (\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\cdot \\
&\qquad \cdot \int_{-d}^{0} [2g\sinh(nR)\sinh(nR+nkcz) + \kappa_s \sinh(2nR+nkcz) + \sinh(nkcz)]^2 dz + \\
&+ \frac{\varepsilon_0}{4}\kappa_c (\alpha kc)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\cdot \\
&\qquad \cdot \int_{-d}^{0} [2g\sinh(nR)\cosh(nR+nkcz) + \kappa_s \cosh(2nR+nkcz) + \cosh(nkcz)]^2 dz
\end{aligned} \tag{F.12}
$$

Developing the square in the integrant of the two integrals in this equation, the electrostatic energy per domain area is

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro(2)}}}{L_y W} =& \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0 \kappa_c} d + \\
&+ \frac{\varepsilon_0}{4}\kappa_a (\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\cdot \\
&\qquad \cdot \int_{-d}^{0} [4g^2\sinh^2(nR)\sinh^2(nR+nkcz) + \kappa_s^2 \sinh^2(2nR+nkcz) + \\
&\qquad + 4g\sinh(nR)\sinh(nR+nkcz)\kappa_s\sinh(2nR+nkcz) + \sinh^2(nkcz) + \\
&\qquad + 4g\sinh(nR)\sinh(nR+nkcz)\sin(nkcz) + \\
&\qquad + 2\kappa_s \sinh(2nR+nkcz)\sinh(nkcz)]dz + \\
&+ \frac{\varepsilon_0}{4}\kappa_c (\alpha kc)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\cdot \\
&\qquad \cdot \int_{-d}^{0} [4g^2\sinh^2(nR)\cosh^2(nR+nkcz) + \kappa_s^2 \cosh^2(2nR+nkcz) + \\
&\qquad + 4g\sinh(nR)\cosh(nR+nkcz)\kappa_s\cosh(2nR+nkcz) + \cosh^2(nkcz) + \\
&\qquad + 4g\sinh(nR)\cosh(nR+nkcz)\cosh(nkcz) + \\
&\qquad + 2\kappa_s \cosh(2nR+nkcz)\cosh(nkcz)]dz
\end{aligned} \tag{F.13}
$$

Now, we use the fact that $\kappa_a = \kappa_c c^2$ and we put together inside the same integral the hiperbolic functions with the same argument

$$\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} =& \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0 \kappa_c} d + \\
&+ \frac{\varepsilon_0}{4}\kappa_a(\alpha k)^2 \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\cdot \\
&\qquad \cdot \Bigg\{ 4g^2\sinh^2(nR)\int_{-d}^{0}[\sinh^2(nR+nkcz)+\cosh^2(nR+nkcz)]dz + \\
&\qquad + \kappa_s^2\int_{-d}^{0}[\sinh^2(2nR+nkcz)+\cosh^2(2nR+nkcz)]dz + \\
&\qquad + 4g\kappa_s\sinh(nR)\int_{-d}^{0}[\sinh(nR+nkcz)\sinh(2nR+nkcz) + \\
&\qquad\qquad + \cosh(nR+nkcz)\cosh(2nR+nkcz)]dz + \\
&\qquad + \int_{-d}^{0}[\sinh^2(nkcz)+\cosh^2(nkcz)]dz + \\
&\qquad + 4g\sinh(nR)\int_{-d}^{0}[\sinh(nR+nkcz)\sin(nkcz)+\cosh(nR+nkcz)\cosh(nkcz)]dz + \\
&\qquad + 2\kappa_s\int_{-d}^{0}[\sinh(2nR+nkcz)\sinh(nkcz)+\cosh(2nR+nkcz)\cosh(nkcz)]dz \Bigg\}
\end{aligned} \tag{F.14}$$

Next, we are going to solve each of the integrals shown in Eq. (F.14). The first one

$$\begin{aligned}
\int_{-d}^{0}[\sinh^2(nR+nkcz)+\cosh^2(nR+nkcz)]dz &= \int_{-d}^{0}\cosh(2nR+2nkcz)dz \\
&= \frac{1}{2nkc}\sinh(2nR+2nkcz)\Big|_{-d}^{0} \\
&= \frac{1}{2nkc}[\sinh(2nR)-\sinh(2nR-2nkcd)] \\
&= \frac{1}{2nkc}\left[\sinh(2nR)-\sinh\left(2nR-2n\frac{2\pi}{W}cd\right)\right] \\
&= \frac{1}{2nkc}[\sinh(2nR)-\sinh(2nR-4nR)] \\
&= \frac{1}{2nkc}[\sinh(2nR)-\sinh(-2nR)] \\
&= \frac{1}{2nkc}[\sinh(2nR)+\sinh(2nR)] \\
&= \frac{1}{nkc}\sinh(2nR)
\end{aligned} \tag{F.15}$$

where we have used the fact that $\cosh(2x) = \cosh^2(x) + \sinh^2(x)$, $k = \frac{2\pi}{W}$ and $R = \frac{\pi cd}{W}$. In order to solve the other integrals, k and R have been used. The second integral can be solved this way

$$\begin{aligned}\int_{-d}^{0}[\sinh^2(2nR+nkcz)+\cosh^2(2nR+nkcz)]dz &= \int_{-d}^{0}\cosh(4nR+2nkcz)dz \\ &= \frac{1}{2nkc}\sinh(4nR+2nkcz)\Big|_{-d}^{0} \\ &= \frac{1}{2nkc}[\sinh(4nR)-\sinh(4nR-2nkcd)] \\ &= \frac{1}{2nkc}\left[\sinh(4nR)-\sinh\left(4nR-2n\frac{2\pi}{W}cd\right)\right] \\ &= \frac{1}{2nkc}[\sinh(4nR)-\sinh\left(4nR-4nR\right)] \\ &= \frac{1}{2nkc}\sinh(4nR) \qquad \text{(F.16)}\end{aligned}$$

where we have used the same hyperbolic property as before. Continuing with the third integral

$$\begin{aligned}&\int_{-d}^{0}[\sinh(nR+nkcz)\sinh(2nR+nkcz)+ \\ &\quad +\cosh(nR+nkcz)\cosh(2nR+nkcz)]dz = \\ &= \int_{-d}^{0}\left[\frac{1}{2}\cosh(nR+nkcz+2nR+nkcz)-\right. \\ &\quad -\frac{1}{2}\cosh(nR+nkcz-2nR-nkcz)+ \\ &\quad +\frac{1}{2}\cosh(nR+nkcz+2nR+nkcz)+ \\ &\quad \left.+\frac{1}{2}\cosh(nR+nkcz-2nR-nkcz)\right]dz \\ &= \int_{-d}^{0}\left[\frac{1}{2}\cosh(nR+nkcz+2nR+nkcz)-\right. \\ &\quad \left.+\frac{1}{2}\cosh(nR+nkcz+2nR+nkcz)\right]dz \\ &= \int_{-d}^{0}\left[\frac{1}{2}\cosh(3nR+2nkcz)+\frac{1}{2}\cosh(3nR+2nkcz)\right]dz \\ &= \int_{-d}^{0}\cosh(3nR+2nkcz)dz \\ &= \frac{1}{2nkc}\sinh(3nR+2nkcz)\Big|_{-d}^{0} \\ &= \frac{1}{2nkc}[\sinh(3nR)-\sinh(3nR-2nkcd)] \\ &= \frac{1}{2nkc}\left[\sinh(3nR)-\sinh\left(3nR-2n\frac{2\pi}{W}cd\right)\right] \\ &= \frac{1}{2nkc}[\sinh(3nR)-\sinh\left(3nR-4nR\right)] \\ &= \frac{1}{2nkc}[\sinh(3nR)+\sinh(nR)] \qquad \text{(F.17)}\end{aligned}$$

where we have applied these hyperbolic properties: $\sinh(x)\sinh(y)=\frac{1}{2}[\cosh(x+y)-\cosh(x-y)]$ and $\cosh(x)\cosh(y)=\frac{1}{2}[\cosh(x+y)+\cosh(x-y)]$.

The fourth one

$$\begin{aligned}
\int_{-d}^{0} [\sinh^2(nkcz) + \cosh^2(nkcz)]dz &= \int_{-d}^{0} \cosh(2nkcz)dz \\
&= \frac{1}{2nkc} \sinh(2nkcz)\bigg|_{-d}^{0} \\
&= \frac{1}{2nkc}[-\sinh(-2nkcd)] \\
&= \frac{1}{2nkc}\left[-\sinh\left(-2n\frac{2\pi}{W}cd\right)\right] \\
&= \frac{1}{2nkc}[-\sinh(-4nR)] \\
&= \frac{1}{2nkc}\sinh(4nR) \qquad \text{(F.18)}
\end{aligned}$$

where we have used the same hyperbolic property as in Eq. (F.15).

Next, we will solved the fifth integral

$$\begin{aligned}
&\int_{-d}^{0} [\sinh(nR + nkcz)\sinh(nkcz)+ \\
&\quad + \cosh(nR + nkcz)\cosh(nkcz)]dz = \\
&= \int_{-d}^{0} \left[\frac{1}{2}\cosh(nR + nkcz + nkcz) - \right. \\
&\quad - \frac{1}{2}\cosh(nR + nkcz - nkcz) + \\
&\quad + \frac{1}{2}\cosh(nR + nkcz + nkcz) + \\
&\quad \left. + \frac{1}{2}\cosh(nR + nkcz - nkcz)\right] dz \\
&= \int_{-d}^{0} \left[\frac{1}{2}\cosh(nR + nkcz + nkcz) - \right. \\
&\quad \left. + \frac{1}{2}\cosh(nR + nkcz + nkcz)\right] dz \\
&= \int_{-d}^{0} \cosh(nR + 2nkcz)dz \\
&= \frac{1}{2nkc}\sinh(nR + 2nkcz)\bigg|_{-d}^{0} \\
&= \frac{1}{2nkc}[\sinh(nR) - \sinh(nR - 2nkcd)] \\
&= \frac{1}{2nkc}\left[\sinh(nR) - \sinh\left(nR - 2n\frac{2\pi}{W}cd\right)\right] \\
&= \frac{1}{2nkc}[\sinh(nR) - \sinh(nR - 4nR)] \\
&= \frac{1}{2nkc}[\sinh(nR) + \sinh(3nR)] \qquad \text{(F.19)}
\end{aligned}$$

and finally, the sixth integral is solved now

$$
\begin{aligned}
\int_{-d}^{0} & [\sinh(2nR+nkcz)\sinh(nkcz)+ \\
& + \cosh(2nR+nkcz)\cosh(nkcz)]dz = \\
&= \int_{-d}^{0}\left[\frac{1}{2}\cosh(2nR+nkcz+nkcz)- \right.\\
&\quad -\frac{1}{2}\cosh(2nR+nkcz-nkcz)+\\
&\quad +\frac{1}{2}\cosh(2nR+nkcz+nkcz)+\\
&\quad \left.+\frac{1}{2}\cosh(2nR+nkcz-nkcz)\right]dz\\
&= \int_{-d}^{0}\left[\frac{1}{2}\cosh(2nR+nkcz+nkcz)- \right.\\
&\quad \left.+\frac{1}{2}\cosh(2nR+nkcz+nkcz)\right]dz\\
&= \int_{-d}^{0}\cosh(2nR+2nkcz)dz\\
&= \frac{1}{2nkc}\sinh(2nR+2nkcz)\Big|_{-d}^{0}\\
&= \frac{1}{2nkc}[\sinh(2nR)-\sinh(2nR-2nkcd)]\\
&= \frac{1}{2nkc}\left[\sinh(2nR)-\sinh\left(2nR-2n\frac{2\pi}{W}cd\right)\right]\\
&= \frac{1}{2nkc}[\sinh(2nR)-\sinh(2nR-4nR)]\\
&= \frac{1}{2nkc}[\sinh(2nR)+\sinh(2nR)]\\
&= \frac{1}{nkc}\sinh(2nR) \qquad \text{(F.20)}
\end{aligned}
$$

In these two last integrals we have applied the same properties as in Eq. (F.17). We include now the result of these integrals in Eq. (F.14) to obtain the electrostatic energy per unit area of region 2

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro}(2)}}{L_y W} = & \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0\kappa_c}d+\frac{\varepsilon_0}{4}\kappa_a(\alpha k)^2\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^2}\left\{\frac{4g^2\sinh^2(nR)}{nkc}\sinh(2nR)+\frac{\kappa_s^2}{2nkc}\sinh(4nR)+\right.\\
&+\frac{4g\kappa_s\sinh(nR)}{2nkc}[\sinh(3nR)+\sinh(nR)]+\\
&+\frac{\sinh(4nR)}{2nkc}+\\
&+\frac{4g\sinh(nR)}{2nkc}[\sinh(nR)+\sinh(3nR)]+\\
&\left.+\frac{2\kappa_s}{nkc}\sinh(2nR)\right\} \qquad \text{(F.21)}
\end{aligned}
$$

Simplifying Eq. (F.21), we achieve the final expression of the electrostatic energy per unit area of this region

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro(2)}}}{L_y W} =& \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0 \kappa_c} d + \frac{\varepsilon_0}{4c}\kappa_a \alpha^2 k \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\Bigg\{ 4g^2 \sinh^2(nR)\sinh(2nR) + \frac{\kappa_s^2}{2}\sinh(4nR) + \\
& + 2g\kappa_s \sinh(nR)[\sinh(3nR)+\sinh(nR)] + \\
& + \frac{\sinh(4nR)}{2} + \\
& + 2g\sinh(nR)[\sinh(nR)+\sinh(3nR)] + \\
& + 2\kappa_s \sinh(2nR)\Bigg\} \\
=& \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0 \kappa_c} d + \frac{\varepsilon_0}{4c}\kappa_a \frac{1}{16\pi^2\varepsilon_0^2}\frac{64 P_{\text{S}}^2 c^2 d^2}{R^2} k \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\cdot \\
& \cdot \Bigg\{ 4g^2 \sinh^2(nR)\sinh(2nR) + \frac{\kappa_s^2}{2}\sinh(4nR) + \\
& + 2g\kappa_s \sinh(nR)[\sinh(3nR)+\sinh(nR)] + \\
& + \frac{\sinh(4nR)}{2} + \\
& + 2g\sinh(nR)[\sinh(nR)+\sinh(3nR)] + \\
& + 2\kappa_s \sinh(2nR)\Bigg\}
\end{aligned} \tag{F.22}
$$

where we have introduced the value of $\alpha = \frac{1}{4\pi\varepsilon_0}\left(\frac{8P_{\text{S}}cd}{R}\right)$. Using now the fact that $g = c\kappa_c$, $k = \frac{2\pi}{W}$ and $R = \frac{\pi cd}{W}$

$$
\begin{aligned}
\frac{U^{\text{elec}}_{\text{ferro(2)}}}{L_y W} =& \frac{1}{2}\frac{(P_S A)^2}{\varepsilon_0 \kappa_c} d + \frac{1}{4}\kappa_a \frac{1}{\pi^2\varepsilon_0}\frac{4 P_{\text{S}}^2 c d^2}{R\frac{\pi cd}{W}}\frac{2\pi}{W} \sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\cdot \\
& \cdot \Bigg\{ 4g^2 \sinh^2(nR)\sinh(2nR) + \frac{\kappa_s^2}{2}\sinh(4nR) + \\
& + 2g\kappa_s \sinh(nR)[\sinh(3nR)+\sinh(nR)] + \\
& + \frac{\sinh(4nR)}{2} + \\
& + 2g\sinh(nR)[\sinh(nR)+\sinh(3nR)] + \\
& + 2\kappa_s \sinh(2nR)\Bigg\} \\
=& \frac{1}{2}\frac{P_{\text{S}}^2 d}{\kappa_c \varepsilon_0}\Bigg\{ A^2 + \frac{4g^2}{\pi^2 R}\sum_{n=1}^{\infty} \sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\Bigg\{ 4g^2 \sinh^2(nR)\sinh(2nR) + \frac{\kappa_s^2}{2}\sinh(4nR) + \\
& + 2g\kappa_s \sinh(nR)[\sinh(3nR)+\sinh(nR)] + \\
& + \frac{\sinh(4nR)}{2} + \\
& + 2g\sinh(nR)[\sinh(nR)+\sinh(3nR)] + \\
& + 2\kappa_s \sinh(2nR)\Bigg\}\Bigg\}
\end{aligned} \tag{F.23}
$$

Adding the Eq. (F.4), Eq. (F.8) and Eq. (F.23) together, it is obtained the total depolarization energy per unit are

$$
\begin{aligned}
\frac{U_{\text{elec}}}{L_y W} &= \frac{1}{2}\frac{4P_{\text{S}}^2 gd}{\pi^2\varepsilon_0\kappa_c R}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2+\\
&+\frac{1}{2}\frac{4P_{\text{S}}^2 gd}{\pi^2\varepsilon_0\kappa_c R}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\kappa_s[2g\sinh^2(nR)+\sinh(2nR)]^2+\\
&+\frac{1}{2}\frac{P_{\text{S}}^2 d}{\kappa_c\varepsilon_0}\left\{A^2+\frac{4g^2}{\pi^2 R}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\left\{4g^2\sinh^2(nR)\sinh(2nR)+\frac{\kappa_s^2}{2}\sinh(4nR)+\right.\right.\\
&\qquad+2g\kappa_s\sinh(nR)[\sinh(3nR)+\sinh(nR)]+\\
&\qquad+\frac{\sinh(4nR)}{2}+\\
&\qquad+2g\sinh(nR)[\sinh(nR)+\sinh(3nR)]+\\
&\qquad\left.\left.+2\kappa_s\sinh(2nR)\right\}\right\}\\
&=\frac{1}{2}\frac{P_{\text{S}}^2 d}{\kappa_c\varepsilon_0}\left\{A^2+\frac{4g}{\pi^2 R}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}(A+1)\right)\frac{\mu_n^2}{n^3}\left\{[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2+\right.\right.\\
&\qquad+\kappa_s[2g\sinh^2(nR)+\sinh(2nR)]^2+\\
&\qquad+4g^3\sinh^2(nR)\sinh(2nR)+\frac{\kappa_s^2 g}{2}\sinh(4nR)+\\
&\qquad+2g^2\kappa_s\sinh(nR)[\sinh(3nR)+\sinh(nR)]+\\
&\qquad+\frac{g}{2}\sinh(4nR)+\\
&\qquad+2g^2\sinh(nR)[\sinh(nR)+\sinh(3nR)]+\\
&\qquad\left.\left.+2g\kappa_s\sinh(2nR)\right\}\right\}
\end{aligned}
\tag{F.24}
$$

In the following, **we shall consider $W_+ = W_- = \omega$, which leads to $W = 2\omega$, and $A = \frac{W_+ - W_-}{W_+ + W_-} = 0$**. If this last expression is divided by the thickness of the ferroelectric thin film d, we obtain the depolarization energy per unit volume. Under these assumptions, this energy simplifies to

$$
\begin{aligned}
\frac{U_{\text{elec}}}{L_y W d} = \frac{U_{\text{elec}}}{V} &= \frac{4gP_{\text{S}}^2}{2\pi^2 R\kappa_c\varepsilon_0}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi}{2}\right)\frac{\mu_n^2}{n^3}\left\{[2g\sinh^2(nR)+\kappa_s\sinh(2nR)]^2+\right.\\
&\qquad+\kappa_s[2g\sinh^2(nR)+\sinh(2nR)]^2+\\
&\qquad+4g^3\sinh^2(nR)\sinh(2nR)+\frac{\kappa_s^2 g}{2}\sinh(4nR)+\\
&\qquad+2g^2\kappa_s\sinh(nR)[\sinh(3nR)+\sinh(nR)]+\\
&\qquad+\frac{g}{2}\sinh(4nR)+\\
&\qquad+2g^2\sinh(nR)[\sinh(nR)+\sinh(3nR)]+\\
&\qquad\left.+2g\kappa_s\sinh(2nR)\right\}
\end{aligned}
\tag{F.25}
$$

It is turned to write the energy of the Eq. (F.25) in terms of the ratio x of the thickness to width [Eq. (3.125)], so that, using the constant $R = \frac{\pi c d}{W}$ and the definition of $\mu_n = \{(g^2+\kappa_\mathrm{s})\sinh(2nR) + g[1+\kappa_\mathrm{s}\cosh(2nR) + 2\sinh^2(nR)]\}^{-1}$

$$\begin{aligned}
\frac{U_\mathrm{elec}}{V} &= \frac{4gP_\mathrm{S}^2}{2\pi^2\frac{\pi cd}{2\omega}\kappa_c\varepsilon_0}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\left\{(g^2+\kappa_\mathrm{s})\sinh\left(2n\frac{\pi cd}{2\omega}\right) + g\left[1+\kappa_\mathrm{s}\cosh\left(2n\frac{\pi cd}{2\omega}\right) + 2\sinh^2\left(n\frac{\pi cd}{2\omega}\right)\right]\right\}^{-2}\cdot \\
&\quad\cdot\left\{\left[2g\sinh^2\left(n\frac{\pi cd}{2\omega}\right) + \kappa_s\sinh\left(2n\frac{\pi cd}{2\omega}\right)\right]^2 + \kappa_s\left[2g\sinh^2\left(n\frac{\pi cd}{2\omega}\right) + \sinh\left(2n\frac{\pi cd}{2\omega}\right)\right]^2 + \right.\\
&\quad + 4g^3\sinh^2\left(n\frac{\pi cd}{2\omega}\right)\sinh\left(2n\frac{\pi cd}{2\omega}\right) + \frac{\kappa_s^2 g}{2}\sinh\left(4n\frac{\pi cd}{2\omega}\right) + \\
&\quad + 2g^2\kappa_s\sinh\left(n\frac{\pi cd}{2\omega}\right)\left[\sinh\left(3n\frac{\pi cd}{2\omega}\right) + \sinh\left(n\frac{\pi cd}{2\omega}\right)\right] + \frac{g}{2}\sinh\left(4n\frac{\pi cd}{2\omega}\right) + \\
&\quad \left. + 2g^2\sinh\left(n\frac{\pi cd}{2\omega}\right)\left[\sinh\left(n\frac{\pi cd}{2\omega}\right) + \sinh\left(3n\frac{\pi cd}{2\omega}\right)\right] + 2g\kappa_s\sinh\left(2n\frac{\pi cd}{2\omega}\right)\right\} \\
&= \frac{8gP_\mathrm{S}^2}{2\pi^3 c\kappa_c\varepsilon_0}\frac{1}{x}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\left\{(g^2+\kappa_\mathrm{s})\sinh(n\pi cx) + g\left[1+\kappa_\mathrm{s}\cosh(n\pi cx) + 2\sinh^2\left(\frac{n\pi}{2}cx\right)\right]\right\}^{-2}\cdot \\
&\quad\cdot\left\{\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right) + \kappa_s\sinh(n\pi cx)\right]^2 + \kappa_s\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right) + \sinh(n\pi cx)\right]^2 + \right.\\
&\quad + 4g^3\sinh^2\left(\frac{n\pi}{2}cx\right)\sinh(n\pi cx) + \frac{\kappa_s^2 g}{2}\sinh(2n\pi cx) + \\
&\quad + 2g^2\kappa_s\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{3n\pi}{2}cx\right) + \sinh\left(\frac{n\pi}{2}cx\right)\right] + \frac{g}{2}\sinh(2n\pi cx) + \\
&\quad \left. + 2g^2\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{n\pi}{2}cx\right) + \sinh\left(\frac{3n\pi}{2}cx\right)\right] + 2g\kappa_s\sinh(n\pi cx)\right\}
\end{aligned} \tag{F.26}$$

and we can examine the behaviour in terms in the different limits. The monodomain energy $\frac{U_\mathrm{elec}^\mathrm{mono}}{V}$ is obtained when $x \to 0$ in Eq. (F.26)

$$\begin{aligned}
&\lim_{x\to 0}\frac{1}{x}\left\{(g^2+\kappa_\mathrm{s})\sinh(n\pi cx) + g\left[1+\kappa_\mathrm{s}\cosh(n\pi cx) + 2\sinh^2\left(\frac{n\pi}{2}cx\right)\right]\right\}^{-2}\cdot \\
&\quad\cdot\left\{\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right) + \kappa_s\sinh(n\pi cx)\right]^2 + \kappa_s\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right) + \sinh(n\pi cx)\right]^2 + \right.\\
&\quad + 4g^3\sinh^2\left(\frac{n\pi}{2}cx\right)\sinh(n\pi cx) + \frac{\kappa_s^2 g}{2}\sinh(2n\pi cx) + \\
&\quad + 2g^2\kappa_s\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{3n\pi}{2}cx\right) + \sinh\left(\frac{n\pi}{2}cx\right)\right] + \frac{g}{2}\sinh(2n\pi cx) + \\
&\quad \left. + 2g^2\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{n\pi}{2}cx\right) + \sinh\left(\frac{3n\pi}{2}cx\right)\right] + 2g\kappa_s\sinh(n\pi cx)\right\}
\end{aligned} \tag{F.27}$$

For this purpose, we will expand every hyperbolic function to first order

$$\sinh(n\pi cx) = n\pi cx \tag{F.28}$$

$$\sinh\left(\frac{n\pi}{2}cx\right) = \frac{n\pi}{2}cx \tag{F.29}$$

$$\sinh^2\left(\frac{n\pi}{2}cx\right) = \frac{n^2\pi^2}{4}c^2x^2 \tag{F.30}$$

$$\sinh(2n\pi cx) = 2n\pi cx \tag{F.31}$$

$$\sinh\left(\frac{3n\pi}{2}cx\right) = \frac{3n\pi}{2}cx \tag{F.32}$$

$$\cosh(n\pi cx) = 1 \tag{F.33}$$

and we solve the limit. First, we will solve the limit of $\mu_n^2 = \Big\{(g^2+\kappa_{\mathrm{s}})\sinh(n\pi cx) + g\left[1+\kappa_{\mathrm{s}}\cosh(n\pi cx) + \right.$ $\left. +2\sinh^2\left(\frac{n\pi}{2}cx\right)\right]\Big\}^{-2}$ so that the subsequent expressions are simple

$$\begin{aligned}
\lim_{x\to 0}\Big\{&(g^2+\kappa_{\mathrm{s}})\sinh(n\pi cx) + \\
&+ g\left[1+\kappa_{\mathrm{s}}\cosh(n\pi cx) + 2\sinh^2\left(\frac{n\pi}{2}cx\right)\right]\Big\}^{-2} = \lim_{x\to 0}\left\{(g^2+\kappa_{\mathrm{s}})n\pi cx + g\left[1+\kappa_{\mathrm{s}}+2\frac{n^2\pi^2}{4}c^2x^2\right]\right\}^{-2} \\
&= \frac{1}{g^2(1+\kappa_s)^2}
\end{aligned} \tag{F.34}$$

where we have used the Eq. (F.28), Eq. (F.30) and Eq. (F.33). For the first term of the limit we will apply also Eq. (F.28) and Eq. (F.30),

$$\begin{aligned}
\lim_{x\to 0}\frac{\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right)+\kappa_s\sinh(n\pi cx)\right]^2}{x} &= \lim_{x\to 0}\frac{\left[2g\frac{n^2\pi^2}{4}c^2x^2+\kappa_s n\pi cx\right]^2}{x} \\
&= \lim_{x\to 0}\left[2g\frac{n^2\pi^2}{4}c^2x+\kappa_s n\pi c\right]^2 x \\
&= 0
\end{aligned} \tag{F.35}$$

and for the second one the same equations will be used, too

$$\begin{aligned}
\lim_{x\to 0}\frac{\kappa_s\left[2g\sinh^2\left(\frac{n\pi}{2}cx\right)+\sinh(n\pi cx)\right]^2}{x} &= \lim_{x\to 0}\frac{\kappa_s\left[2g\frac{n^2\pi^2}{4}c^2x^2+n\pi cx\right]^2}{x} \\
&= \lim_{x\to 0}\kappa_s\left[2g\frac{n^2\pi^2}{4}c^2x+n\pi c\right]^2 x \\
&= 0
\end{aligned} \tag{F.36}$$

The limit of the third and fourth terms is

$$\begin{aligned}
\lim_{x\to 0}\frac{4g^3\sinh^2\left(\frac{n\pi}{2}cx\right)\sinh(n\pi cx)+\frac{\kappa_s^2 g}{2}\sinh(2n\pi cx)}{x} &= \lim_{x\to 0}\frac{4g^3\frac{n^2\pi^2}{4}c^2x^2n\pi cx+\frac{\kappa_s^2 g}{2}2n\pi cx}{x} \\
&= \lim_{x\to 0}4g^3\frac{n^2\pi^2}{4}c^2x^2n\pi c+\frac{\kappa_s^2 g}{2}2n\pi c \\
&= \kappa_s^2 gn\pi c
\end{aligned} \tag{F.37}$$

and of the fifth and sixth terms

$$\begin{aligned}
\lim_{x\to 0}\frac{2g^2\kappa_{\mathrm{s}}\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{3n\pi}{2}cx\right)+\sinh\left(\frac{n\pi}{2}cx\right)\right]+\frac{g}{2}\sinh(2n\pi cx)}{x} &= \lim_{x\to 0}\frac{\frac{2g^2\kappa_s n\pi cx}{2}\left[\frac{3n\pi}{2}cx+\frac{n\pi}{2}cx\right]+\frac{g}{2}2n\pi cx}{x} \\
&= \lim_{x\to 0}\frac{2g^2\kappa_s n\pi c}{2}\left[\frac{3n\pi}{2}cx+\frac{n\pi}{2}cx\right]+\frac{g}{2}2n\pi c \\
&= gn\pi c
\end{aligned} \tag{F.38}$$

Finally, the limit of the two last terms is

$$\begin{aligned}
\lim_{x\to 0}\frac{2g^2\sinh\left(\frac{n\pi}{2}cx\right)\left[\sinh\left(\frac{n\pi}{2}cx\right)+\sinh\left(\frac{3n\pi}{2}cx\right)\right]+2g\kappa_s\sinh(n\pi cx)}{x} &= \lim_{x\to 0}\frac{2g^2\frac{n\pi}{2}cx\left[\frac{n\pi}{2}cx+\frac{3n\pi}{2}cx\right]+2g\kappa_s n\pi cx}{x} \\
&= \lim_{x\to 0}2g^2\frac{n\pi}{2}c\left[\frac{n\pi}{2}cx+\frac{3n\pi}{2}cx\right]+2g\kappa_s n\pi c \\
&= 2g\kappa_s n\pi c
\end{aligned} \tag{F.39}$$

Taking into account the Eq. (F.34), Eq. (F.35), Eq. (F.36), Eq. (F.37), Eq. (F.38) and Eq. (F.39), the depolarization energy per unit volume in the monodomain limit can be expressed as

$$\begin{aligned}
\lim_{x\to 0}\frac{U_{\mathrm{elec}}}{V} &= \frac{8gP_{\mathrm{S}}^2}{2\pi^3 c\kappa_c\varepsilon_0}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3}\frac{\kappa_s^2 gn\pi c+gn\pi c+2g\kappa_s n\pi c}{g^2(1+\kappa_s)^2} \\
&= \frac{8P_{\mathrm{S}}^2}{2\pi^2\kappa_c\varepsilon_0}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^2}\frac{\kappa_s^2+1+2\kappa_s}{(1+\kappa_s)^2} \\
&= \frac{8P_{\mathrm{S}}^2}{2\pi^2\kappa_c\varepsilon_0}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^2} \\
&= \frac{8P_{\mathrm{S}}^2}{2\pi^2\kappa_c\varepsilon_0}\frac{\pi^2}{8} \\
&= \frac{P_{\mathrm{S}}^2}{2\kappa_c\varepsilon_0}
\end{aligned} \tag{F.40}$$

where we have used the Eq. (3.130).

In the limit, $x\to\infty$, we will use the following equalities (valid in this limit) of the involved hyperbolic functions to obtain the electrostatic energy per unit volume in the Kittel limit $\frac{U_{\mathrm{elec}}^{\mathrm{Kittel}}}{V}$

$$\sinh(n\pi cx) = \frac{e^{n\pi cx}}{2} \tag{F.41}$$

$$\sinh\left(\frac{n\pi}{2}cx\right) = \frac{e^{\frac{n\pi}{2}cx}}{2} \tag{F.42}$$

$$\sinh^2\left(\frac{n\pi}{2}cx\right) = \frac{e^{n\pi cx}}{4} \tag{F.43}$$

$$\sinh(2n\pi cx) = \frac{e^{2n\pi cx}}{2} \tag{F.44}$$

$$\sinh\left(\frac{3n\pi}{2}cx\right) = \frac{e^{\frac{3n\pi}{2}cx}}{2} \tag{F.45}$$

$$\cosh(n\pi cx) = \frac{e^{n\pi cx}}{2} \tag{F.46}$$

thus leaving the limit that needs to be solved

$$\begin{aligned}
&\lim_{x\to\infty}\left\{(g^2+\kappa_{\mathrm{s}})\frac{e^{n\pi cx}}{2}+g\left[1+\kappa_{\mathrm{s}}\frac{e^{n\pi cx}}{2}+2\frac{e^{n\pi cx}}{4}\right]\right\}^{-2}\cdot \\
&\cdot\left\{\left[2g\frac{e^{n\pi cx}}{4}+\kappa_s\frac{e^{n\pi cx}}{2}\right]^2+\kappa_s\left[2g\frac{e^{n\pi cx}}{4}+\frac{e^{n\pi cx}}{2}\right]^2+4g^3\frac{e^{n\pi cx}}{4}\frac{e^{n\pi cx}}{2}+\frac{\kappa_s^2 g}{2}\frac{e^{2n\pi cx}}{2}+\right. \\
&\left.+2g^2\kappa_s\frac{e^{\frac{n\pi}{2}cx}}{2}\left[\frac{e^{\frac{3n\pi}{2}cx}}{2}+\frac{e^{\frac{n\pi}{2}cx}}{2}\right]+\frac{g}{2}\frac{e^{2n\pi cx}}{2}+2g^2\frac{e^{\frac{n\pi}{2}cx}}{2}\left[\frac{e^{\frac{n\pi}{2}cx}}{2}+\frac{e^{\frac{3n\pi}{2}cx}}{2}\right]+2g\kappa_s\frac{e^{n\pi cx}}{2}\right\}
\end{aligned} \tag{F.47}$$

When x tends to infinity the number one of the second term of the first factor of the limit is negligible compared to the exponentials, so

$$\begin{aligned}
&\lim_{x\to\infty}\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^{-2}e^{-2n\pi cx}\cdot \\
&\cdot\left\{\left[2g\frac{e^{n\pi cx}}{4}+\kappa_s\frac{e^{n\pi cx}}{2}\right]^2+\kappa_s\left[2g\frac{e^{n\pi cx}}{4}+\frac{e^{n\pi cx}}{2}\right]^2+4g^3\frac{e^{n\pi cx}}{4}\frac{e^{n\pi cx}}{2}+\frac{\kappa_s^2 g}{2}\frac{e^{2n\pi cx}}{2}+\right. \\
&\left.+2g^2\kappa_s\frac{e^{\frac{n\pi}{2}cx}}{2}\left[\frac{e^{\frac{3n\pi}{2}cx}}{2}+\frac{e^{\frac{n\pi}{2}cx}}{2}\right]+\frac{g}{2}\frac{e^{2n\pi cx}}{2}+2g^2\frac{e^{\frac{n\pi}{2}cx}}{2}\left[\frac{e^{\frac{n\pi}{2}cx}}{2}+\frac{e^{\frac{3n\pi}{2}cx}}{2}\right]+2g\kappa_s\frac{e^{n\pi cx}}{2}\right\}
\end{aligned} \tag{F.48}$$

Now, we will solve Eq. (F.48) for each term. The limit of the first and the second one

$$\lim_{x\to\infty}\frac{\left[2g\frac{e^{n\pi cx}}{4}+\kappa_s\frac{e^{n\pi cx}}{2}\right]^2+\kappa_s\left[2g\frac{e^{n\pi cx}}{4}+\frac{e^{n\pi cx}}{2}\right]^2}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{2n\pi cx}}=\lim_{x\to\infty}\frac{\left[\frac{g}{2}+\frac{\kappa_s}{2}\right]^2+\kappa_s\left[\frac{g}{2}+\frac{1}{2}\right]^2}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2}$$
$$=\frac{\frac{(g+\kappa_s)^2+\kappa_s(g+1)^2}{4}}{\frac{[g^2+\kappa_s+g(\kappa_s+1)]^2}{4}}$$
$$=\frac{(g+\kappa_s)^2+\kappa_s(g+1)^2}{[g^2+\kappa_s+g(\kappa_s+1)]^2} \tag{F.49}$$

Continuing with the limit of the third and the fourth term

$$\lim_{x\to\infty}\frac{4g^3\frac{e^{n\pi cx}}{4}\frac{e^{n\pi cx}}{2}+\frac{\kappa_s^2 g}{2}\frac{e^{2n\pi cx}}{2}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{2n\pi cx}}=\lim_{x\to\infty}\frac{\frac{g^3}{2}+\frac{\kappa_s^2 g}{4}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2}$$
$$=\frac{\frac{2g^3+\kappa_s^2 g}{4}}{\frac{[g^2+\kappa_s+g(\kappa_s+1)]^2}{4}}$$
$$=\frac{2g^3+\kappa_s^2 g}{[g^2+\kappa_s+g(\kappa_s+1)]^2} \tag{F.50}$$

Next, we will solve the limit of the fifth and the sixth term

$$\lim_{x\to\infty}\frac{2g^2\kappa_s\frac{e^{\frac{n\pi}{2}cx}}{2}\left[\frac{e^{\frac{3n\pi}{2}cx}}{2}+\frac{e^{\frac{n\pi}{2}cx}}{2}\right]+\frac{g}{2}\frac{e^{2n\pi cx}}{2}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{2n\pi cx}}=\lim_{x\to\infty}\frac{\frac{g^2\kappa_s}{2}+\frac{g}{4}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2}+\lim_{x\to\infty}\frac{\frac{g^2\kappa_s e^{n\pi cx}}{2}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{2n\pi cx}}$$
$$=\frac{\frac{2g^2\kappa_s+g}{4}}{\frac{[g^2+\kappa_s+g(\kappa_s+1)]^2}{4}}+\lim_{x\to\infty}\frac{\frac{g^2\kappa_s}{2}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{n\pi cx}}$$
$$=\frac{2g^2\kappa_s+g}{[g^2+\kappa_s+g(\kappa_s+1)]^2} \tag{F.51}$$

Finally, the limit of the two las terms is

$$\lim_{x\to\infty}\frac{2g^2\frac{e^{\frac{n\pi}{2}cx}}{2}\left[\frac{e^{\frac{n\pi}{2}cx}}{2}+\frac{e^{\frac{3n\pi}{2}cx}}{2}\right]+2g\kappa_s\frac{e^{n\pi cx}}{2}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{2n\pi cx}}=\lim_{x\to\infty}\frac{\frac{g^2}{2}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2}+\lim_{x\to\infty}\frac{\left(\frac{g^2}{2}+g^2\kappa_s\right)e^{n\pi cx}}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{2n\pi cx}}$$
$$=\frac{\frac{g^2}{2}}{\frac{[g^2+\kappa_s+g(\kappa_s+1)]^2}{4}}+\lim_{x\to\infty}\frac{\left(\frac{g^2}{2}+g^2\kappa_s\right)}{\left[\frac{g^2+\kappa_s}{2}+g\left(\frac{\kappa_s}{2}+\frac{1}{2}\right)\right]^2 e^{n\pi cx}}$$
$$=\frac{2g^2}{[g^2+\kappa_s+g(\kappa_s+1)]^2} \tag{F.52}$$

Taking into account Eq. (F.49), Eq. (F.50), Eq. (F.51), Eq. (F.52), we can obtain

$$\lim_{x\to\infty}\frac{U_{\text{elec}}}{V}=\frac{8P_{\text{S}}^2}{2\pi^3\varepsilon_0}\frac{1}{x}\frac{(g+\kappa_s)^2+\kappa_s(g+1)^2+2g^3+\kappa_s^2 g+2g^2\kappa_s+g+2g^2}{[g^2+\kappa_s+g(\kappa_s+1)]^2}\sum_{n=1}^{\infty}\frac{\sin^2\left(\frac{n\pi}{2}\right)}{n^3} \tag{F.53}$$

and making use of Eq. (3.134) a Kittel-like expression is obtained

$$\frac{U_{\text{elec}}^{\text{Kittel}}}{V}\approx\frac{P_{\text{S}}^2}{2\varepsilon_0}\beta(\kappa_s)\frac{1}{x} \tag{F.54}$$

where

$$\beta(\kappa_s)=\frac{8.414}{\pi^3}\frac{(g+\kappa_s)^2+\kappa_s(g+1)^2+2g^3+\kappa_s^2 g+2g^2\kappa_s+g+2g^2}{[g^2+\kappa_s+g(\kappa_s+1)]^2} \tag{F.55}$$

G Kittel law of the ferroelectric thin film and a substrate

The total energy per unit volume U of the system when $d >> \omega$, as describes at the beginning of Sec. 3.2, is

$$U = \frac{(P - P_{\mathrm{S}})^2}{2\varepsilon_0 \chi_c} + \frac{P_{\mathrm{S}}^2}{2\varepsilon_0} \beta(\kappa_s) \frac{\omega}{d} + \frac{\Sigma}{\omega} \tag{G.1}$$

Minimizing this total energy per unit volume with respect ω

$$\frac{\partial U}{\partial \omega} = \frac{P_{\mathrm{S}}^2}{2\varepsilon_0} \beta(\kappa_s) \frac{1}{d} - \frac{\Sigma}{\omega^2} = 0 \tag{G.2}$$

Kittel law is obtained

$$\omega = \sqrt{l_k(\kappa_s) d} \tag{G.3}$$

where

$$l_k(\kappa_s) = \frac{2\varepsilon_0 \Sigma}{P_{\mathrm{S}}^2 \beta(\kappa_s)} \tag{G.4}$$

is the Kittel length of this system.